Supplementary Information:

# Projectability disentanglement for accurate and automated electronic-structure Hamiltonians

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# S1 Comparison

## S1.1 Silicon

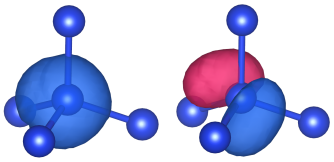
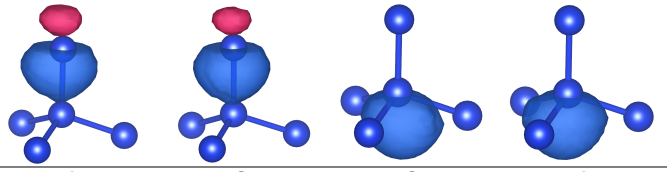
| | |  | | | |
|---|---|---|---|---|---|
| | multiplicity | 2 | 6 | | |
| **hydrogenic ED** | $d_{WFC}(Å)$ | 0.000 | 0.000 | | |
| | $\Omega_{WF}(Å^2)$ | 1.849 | 2.546 | | |
| **PAO ED** | $d_{WFC}(Å)$ | 0.000 | 0.000 | | |
| | $\Omega_{WF}(Å^2)$ | 1.849 | 2.546 | | |
| **PAO PD** | $d_{WFC}(Å)$ | 0.000 | 0.000 | | |
| | $\Omega_{WF}(Å^2)$ | 1.320 | 1.885 | | |
| **PAO PD+ED** | $d_{WFC}(Å)$ | 0.000 | 0.000 | | |
| | $\Omega_{WF}(Å^2)$ | 1.798 | 2.597 | | |
| | |  | | | |
| | multiplicity | 1 | 3 | 3 | 1 |
| **SCDM** | $d_{WFC}(Å)$ | 0.566 | 0.638 | 0.833 | 0.836 |
| | $\Omega_{WF}(Å^2)$ | 5.201 | 4.921 | 4.507 | 4.586 |

Figure S1: Silicon MLWF shapes, centers, and spreads for hydrogenic with ED, SCDM, PAO with ED, PAO with PD, and PAO with PD+ED. $d_{\mathrm{WF}}$ is the distance of WF centers from the nearest-neighbor atom, and $\Omega_{\mathrm{WF}}$ is the spread of each WF.

## S1.2 Copper

Here we test the five methods with a metal, copper. For PD and PD+ED, we choose $p_{\max} = 0.95$, $p_{\min} = 0.01$. As shown in Fig. S2, all the methods can accurately interpolate occupied bands. At first glance, the SCDM reproduces better the overall band structure. However, in the higher energy range for the bands at the X point at about 17 eV, the SCDM has an unphysical large discontinuity of bands along different directions, leading to its much larger spreads and irregular shapes in Fig. S3. For all other four methods, although the high-energy conduction bands do not overlap with DFT bands (as expected), they are still smoothly connected throughout the BZ. Thanks to the freezing of some high projectability states in the high-energy region, the PD and the PD+ED can reproduce better the high-energy unoccupied bands.

Apart from SCDM, MLWFs of all the other four methods are strictly atom-centered orbitals, and perfectly preserve the multiplicities of $s$, $p$, and $d$ orbitals. Note the PD and PD+ED reach the same set of MLWFs, since the PAOs are complete for all the bands inside the inner energy window. The high projectability ensures the freezing of all the bands in the inner energy window, thus in this case PD is enough.

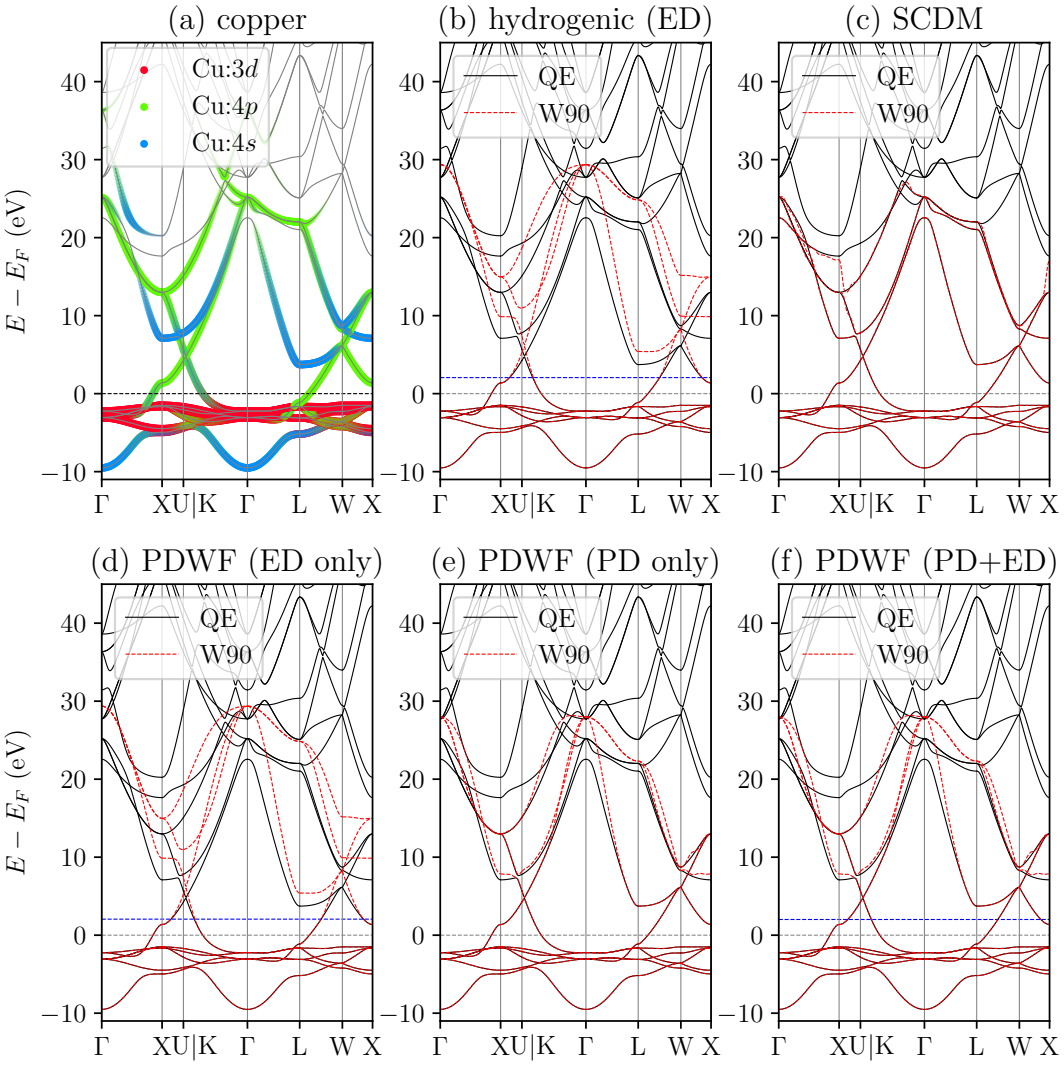



Figure S2: (a) Band structures of copper, shown as grey lines. The colored dots represent the projectability of copper $3d$ (red), $4p$ (green), and $4s$ (blue) orbitals. The size of the dot is proportional to the total projectability $p_{m\mathbf{k}}$ of the band $m$ at kpoint $\mathbf{k}$. Comparisons of QE and Wannier-interpolated bands for (b) hydrogenic with ED, (c) SCDM, (d) PAO with ED, (e) PAO with PD, and (f) PAO with PD+ED. The Fermi energy $E_F$ (horizontal black dashed line) is at zero. The horizontal blue dashed line denotes the top of inner energy window, which equals $E_F$+2 eV.

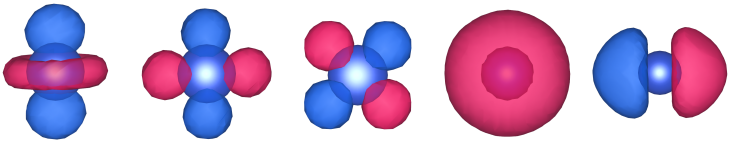
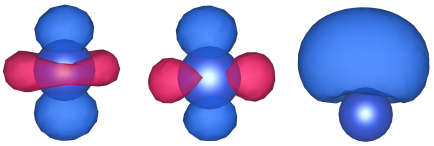
| | |  | | | | |
|---|---|---|---|---|---|---|
| | character | $d_{z^2}$ | $d_{x^2-y^2}$ | $d_{xy}, d_{xz}, d_{yz}$ | $s$ | $p_x, p_y, p_z$ |
| | multiplicity | 1 | 1 | 3 | 1 | 3 |
| **hydrogenic ED** | $d_{WFC}(Å)$ | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}(Å^2)$ | 0.370 | 0.370 | 0.364 | 1.227 | 1.271 |
| **PAO ED** | $d_{WFC}(Å)$ | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}(Å^2)$ | 0.370 | 0.370 | 0.364 | 1.227 | 1.271 |
| **PAO PD** | $d_{WFC}(Å)$ | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}(Å^2)$ | 0.340 | 0.340 | 0.336 | 1.531 | 2.000 |
| **PAO PD+ED** | $d_{WFC}(Å)$ | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}(Å^2)$ | 0.340 | 0.340 | 0.336 | 1.531 | 2.000 |
| | |  | | | | |
| **SCDM** | $d_{WFC}(Å)$ | 0.005 | 0.030 | 0.760 | | |
| | $\Omega_{WF}(Å^2)$ | 0.339 | 0.421 | 5.123 | | |
| | $d_{WFC}(Å)$ | 0.021 | | 0.997 | | |
| | $\Omega_{WF}(Å^2)$ | 0.402 | | 4.790 | | |
| | $d_{WFC}(Å)$ | 0.023 | | 1.063 | | |
| | $\Omega_{WF}(Å^2)$ | 0.409 | | 5.005 | | |
| | $d_{WFC}(Å)$ | 0.029 | | 1.296 | | |
| | $\Omega_{WF}(Å^2)$ | 0.453 | | 4.932 | | |

Figure S3: Copper MLWF shapes, centers, and spreads for hydrogenic with ED, SCDM, PAO with ED, PAO with PD, and PAO with PD+ED. For SCDM, all the 9 MLWFs are listed since their $d_{\mathrm{WF}}$, $\Omega_{\mathrm{WF}}$, and shapes are different. The 9 MLWFs are roughly categorized into 3 groups.

## S1.3 Strontium vanadate

Here we test a perovskite, $SrVO_3$. For PAO with PD and PAO with PD+ED, we choose $p_{\max} = 0.95$, $p_{\min} = 0.01$. Figure S4 shows the band structures. As shown in Fig. S4a, a large portion of conduction bands have high projectability; in such cases, it is relatively safe to increase the maximum inner energy window. However, in HT calculations, it is difficult to tune the inner energy window in an automated fashion. With the help of PD or PD+ED, the high-projectability states are automatically frozen, leading to overall much better interpolated bands when comparing Figs. S4e and S4f with Figs. S4b and S4d.

Figure S5 shows the MLWF shapes of the five methods. The MLWFs of both the hydrogenic with ED and PAO with ED are orbitals with the characteristic $s$, $p$, and $d$ shapes and are strictly atom-centered. For PAO with PD and PAO with PD+ED, although few MLWFs hybridize and slightly drift away from the atom centers, most of the MLWFs still resemble atomic orbitals. The SCDM MLWFs again have much larger spreads and irregular shapes.

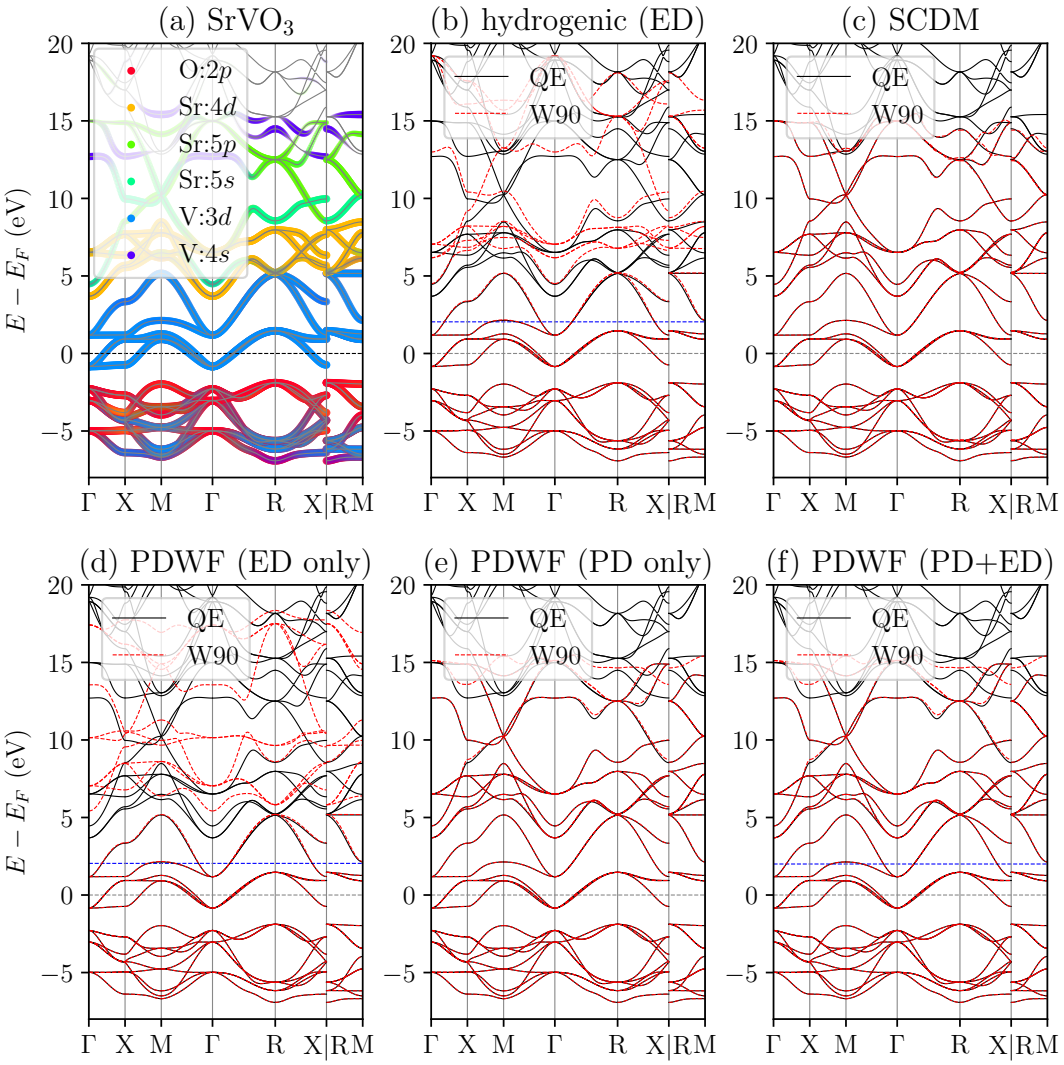
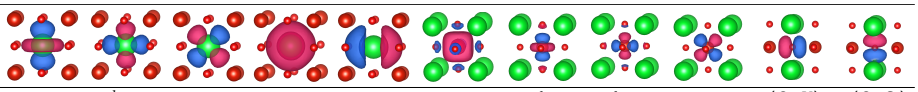
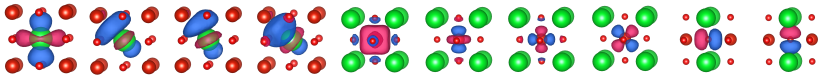



Figure S4: (a) Band structures of $SrVO_3$, shown as grey lines. The colored dots represent the projectability of oxygen $2p$ (red), strontium $4d$ (orange), strontium $5p$ (green), strontium $5s$ (cyan), vanadium $3d$ (blue), and vanadium $4s$ (purple) orbitals, respectively. The size of the dot is proportional to the total projectability $p_{m\mathbf{k}}$ of the band $m$ at kpoint $\mathbf{k}$. Comparisons of QE and Wannier-interpolated bands for (b) hydrogenic with ED, (c) SCDM, (d) PAO with ED, (e) PAO with PD, and (f) PAO with PD+ED. The Fermi energy $E_F$ (horizontal black dashed line) is at zero. The horizontal blue dashed line denotes the maximum inner energy window, which equals $E_F + 2\,\mathrm{eV}$.

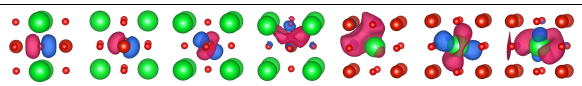


| | character | $d_{z^2}$ | $d_{x^2-y^2}$ | $d_{xy}, d_{xz}, d_{yz}$ | $s$ | $p_x, p_y, p_z$ | hybrid | $d_{z^2}$ | $d_{x^2-y^2}$ | $d_{xy}, d_{xz}, d_{yz}$ | $p(O-V)$ | $p(O-Sr)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | multiplicity | 1 | 1 | 3 | 1 | 3 | 1 | 1 | 1 | 3 | 3 | 6 |
| **hydrogenic ED** | $d_{WFC}$(Å) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}$(Å$^2$) | 1.287 | 1.287 | 1.395 | 2.648 | 2.717 | 1.758 | 0.527 | 0.527 | 0.660 | 0.626 | 0.646 |

| | character | $d_{z^2}$ | $d_{x^2-y^2}$ | $d_{xy}, d_{xz}, d_{yz}$ | hybrid | $p_x, p_y, p_z$ | hybrid | $d_{z^2}$ | $d_{x^2-y^2}$ | $d_{xy}, d_{xz}, d_{yz}$ | $p(O-V)$ | $p(O-Sr)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | multiplicity | 1 | 1 | 3 | 1 | 3 | 1 | 1 | 1 | 3 | 3 | 6 |
| **PAO ED** | $d_{WFC}$(Å) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}$(Å$^2$) | 1.022 | 1.022 | 2.178 | 2.850 | 2.792 | 1.778 | 0.528 | 0.528 | 0.643 | 0.618 | 0.642 |



| | character | $d_{z^2}$ | hybrid | hybrid | hybrid | hybrid | $d_{z^2}$ | $d_{x^2-y^2}$ | $d_{xy}, d_{xz}, d_{yz}$ | $p(O-V)$ | $p(O-Sr)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | multiplicity | 1 | 2 | 2 | 4 | 1 | 1 | 1 | 3 | 3 | 6 |
| **PAO PD** | $d_{WFC}$(Å) | 0.113 | 0.922 | 0.776 | 0.930 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}$(Å$^2$) | 2.042 | 2.266 | 2.249 | 2.215 | 3.095 | 0.558 | 0.558 | 0.648 | 0.628 | 0.587 |
| **PAO PD+ED** | $d_{WFC}$(Å) | 0.113 | 0.923 | 0.778 | 0.929 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}$(Å$^2$) | 2.043 | 2.267 | 2.250 | 2.215 | 3.097 | 0.559 | 0.558 | 0.648 | 0.632 | 0.587 |



| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **SCDM** | $d_{WFC}$(Å) | 0.020 | 0.012 | 0.005 | 0.681 | 1.382 | 0.325 | 0.225 | | | | |
| | $\Omega_{WF}$(Å$^2$) | 0.825 | 0.825 | 0.693 | 17.260 | 9.450 | 3.717 | 6.906 | | | | |
| | $d_{WFC}$(Å) | 0.024 | 0.006 | 0.012 | 0.807 | 1.370 | 0.406 | | | | | |
| | $\Omega_{WF}$(Å$^2$) | 0.849 | 0.793 | 0.776 | 16.208 | 8.097 | 4.249 | | | | | |
| | $d_{WFC}$(Å) | 0.037 | 0.013 | 0.012 | | | 0.106 | | | | | |
| | $\Omega_{WF}$(Å$^2$) | 0.888 | 0.789 | 0.682 | | | 3.285 | | | | | |
| | $d_{WFC}$(Å) | | 0.017 | 0.010 | | | 0.137 | | | | | |
| | $\Omega_{WF}$(Å$^2$) | | 0.691 | 0.718 | | | 3.369 | | | | | |
| | $d_{WFC}$(Å) | | 0.011 | 0.002 | | | 0.107 | | | | | |
| | $\Omega_{WF}$(Å$^2$) | | 0.788 | 0.604 | | | 4.414 | | | | | |
| | $d_{WFC}$(Å) | | 0.016 | | | | | | | | | |
| | $\Omega_{WF}$(Å$^2$) | | 0.693 | | | | | | | | | |

Figure S5: $SrVO_3$ MLWF shapes, centers, and spreads for hydrogenic with ED, SCDM, PAO with ED, PAO with PD, and PAO with PD+ED. For SCDM, all the 24 MLWFs are listed since their $d_{\mathrm{WF}}$, $\Omega_{\mathrm{WF}}$, and shapes are different. The 24 MLWFs are roughly categorized into 7 groups.

## S2 pw2wannier90.x parallelization

Since HT calculations are expensive, to improve their efficiency and fully utilize many-core CPUs we implement $k-$pool parallelization[1, 2] for `pw2wannier90.x`. Figure S6 shows the $k-$pool parallelization efficiency of our `pw2wannier90.x` implementation, tested on a $3 \times 3 \times 3$ silicon supercell. The speedup is defined as $T_{n_k}/T_1$ where $T_{n_k}$ is the wallclock time of a calculation with the number of $k-$pools equals $n_k$. Almost all the time is spent in computing `mmn` matrices, and the $k-$pool implementation performs well at reducing the wallclock time, e.g. comparing $n_k = 16$ with $n_k = 1$, the total wallclock time is reduced by 12 times.

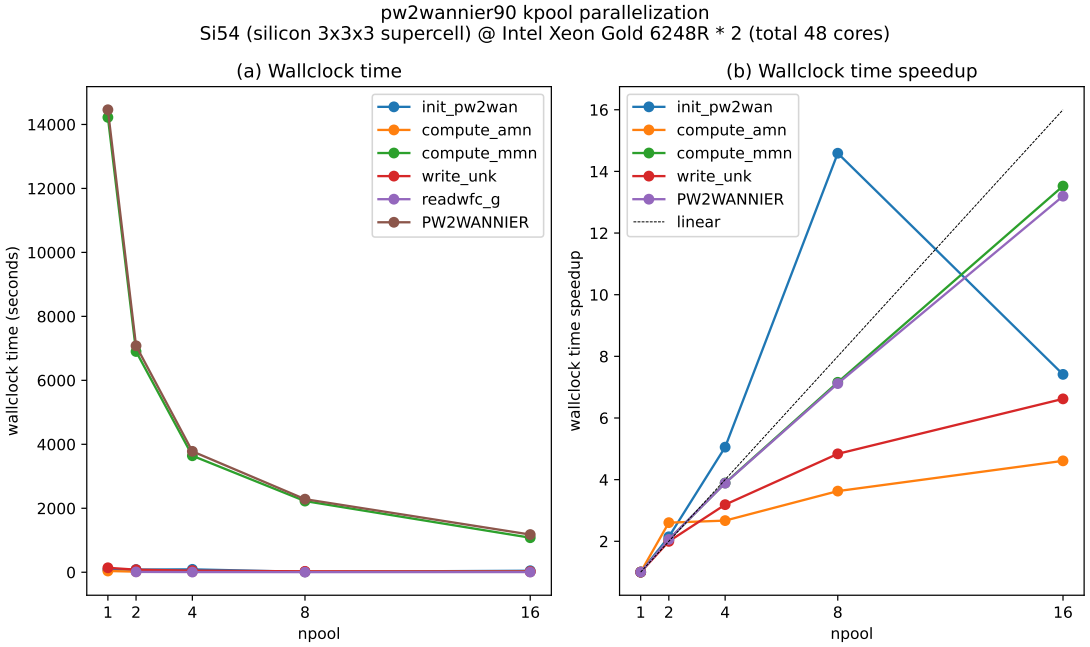



Figure S6: $k-$pool parallelization efficiency of `pw2wannier90.x` implementation. (a) Wallclock time and (b) wallclock time speedup for initialization (`init_pw2wan`), computation of `amn` matrices using PAO (`compute_amn`), computation of `mmn` matrices (`compute_mmn`), writing of `unk` matrices (`write_unk`), reading of wavefunctions (`readwfc_g`), and the total time of pw2wannier90 (`PW2WANNIER`).

# S3 Band distance

To allow a better overview of the band-distance histograms, Figs. S7 and S8 show the zoom out of the corresponding Fig. 5 in the main text. As discussed in the main text, the PDWF $\eta_0$ and $\eta_2$ are much more clustered towards $\eta = 0$. The conclusions are the same for $\eta_0^{\max}$ and $\eta_2^{\max}$, as shown in Fig. S8. Notice that in Figs. S7 and S8, for $\eta_0$, $\eta_2$, $\eta_0^{\max}$, and $\eta_2^{\max}$, the SCDM cumulative histograms do not reach 200 at the rightmost position of horizontal axes, i.e., there are some outliers with $\eta > 100\,\text{meV}$ or $\eta^{\max} > 500\,\text{meV}$. To allow comparison of successful calculations, i.e., excluding outlier calculations, we listed the $\eta^{\leq 20}$ (i.e., the average of all the calculations for which $\eta \leq 20\,\text{meV}$), $\eta^{\leq 100}$, $\eta^{\max,\leq 100}$ (the average of all the calculations for which $\eta^{\max} \leq 100\,\text{meV}$), and $\eta^{\max,\leq 500}$ in Table S1. $N$ in Table S1 denotes the number of successful calculations, which participate in the averagings of $\eta^{\leq 20}$, $\eta^{\leq 100}$, $\eta^{\max,\leq 100}$, or $\eta^{\max,\leq 500}$. As expected, SCDM is relatively better at interpolating high-energy conduction bands, while PDWF is more accurate at occupied and near-Fermi-energy bands.

For $\eta_4^{\leq 20}$, although PDWF (4.939 meV) is still more accurate than SCDM (around 5.892 meV), the SCDM outperforms PDWF with a higher success rate ($171/200 = 85.5\%$ compared with $108/200 = 54\%$). However, as we are not freezing all the states below $E_F + 4\,\text{eV}$, this is expected and in most practical cases it is not an issue since we usually focus on low-energy physics. In Table S1, we also compare $\eta_0^{\max,\leq 100}$, $\eta_2^{\max,\leq 100}$, $\eta_4^{\max,\leq 100}$, and extending the comparison range, i.e., $\eta_0^{\leq 100}$, $\eta_2^{\leq 100}$, $\eta_4^{\leq 100}$, $\eta_0^{\max,\leq 500}$, $\eta_2^{\max,\leq 500}$, $\eta_4^{\max,\leq 500}$, obtaining the same conclusions.

Table S1: Average of band distances for PDWF and SCDM projections. $\eta_\nu$ is the average of average band distance of the 200 structures below $E_F + \nu$, where $\nu =$ 0, 2, or 4 eV. $\eta_\nu^{\leq 20}$ is the average of structures with $\eta_\nu \leq 20$ meV. $\eta_\nu^{\max}$ is the average of max band distance of the 200 structures. $\eta_\nu^{\max,\leq 100}$ is the average of structures with $\eta_\nu^{\max} \leq 100$ meV. $N$ is the number of structures participating in the averagings.

| Type | PDWF | | SCDM | |
|---|---|---|---|---|
| | $\eta$ (meV) | $N$ | $\eta$ (meV) | $N$ |
| $\eta_0$ | 2.685 | 200 | 10.278 | 200 |
| $\eta_2$ | 4.231 | 200 | 11.201 | 200 |
| $\eta_4$ | 34.888 | 200 | 16.456 | 200 |
| $\eta_0^{\leq 20}$ | 1.902 | 196 | 5.094 | 185 |
| $\eta_2^{\leq 20}$ | 2.922 | 193 | 5.280 | 183 |
| $\eta_4^{\leq 20}$ | 4.939 | 108 | 5.892 | 171 |
| $\eta_0^{\leq 100}$ | 2.685 | 200 | 6.953 | 198 |
| $\eta_2^{\leq 100}$ | 4.231 | 200 | 7.714 | 198 |
| $\eta_4^{\leq 100}$ | 22.701 | 179 | 9.621 | 195 |
| $\eta_0^{\max}$ | 20.392 | 200 | 73.238 | 200 |
| $\eta_2^{\max}$ | 36.743 | 200 | 84.011 | 200 |
| $\eta_4^{\max}$ | 294.971 | 200 | 139.696 | 200 |
| $\eta_0^{\max,\leq 100}$ | 12.360 | 193 | 30.933 | 171 |
| $\eta_2^{\max,\leq 100}$ | 19.024 | 181 | 32.155 | 165 |
| $\eta_4^{\max,\leq 100}$ | 18.739 | 83 | 35.592 | 146 |
| $\eta_0^{\max,\leq 500}$ | 20.392 | 200 | 51.389 | 197 |
| $\eta_2^{\max,\leq 500}$ | 32.038 | 198 | 56.346 | 196 |
| $\eta_4^{\max,\leq 500}$ | 132.687 | 152 | 78.399 | 190 |

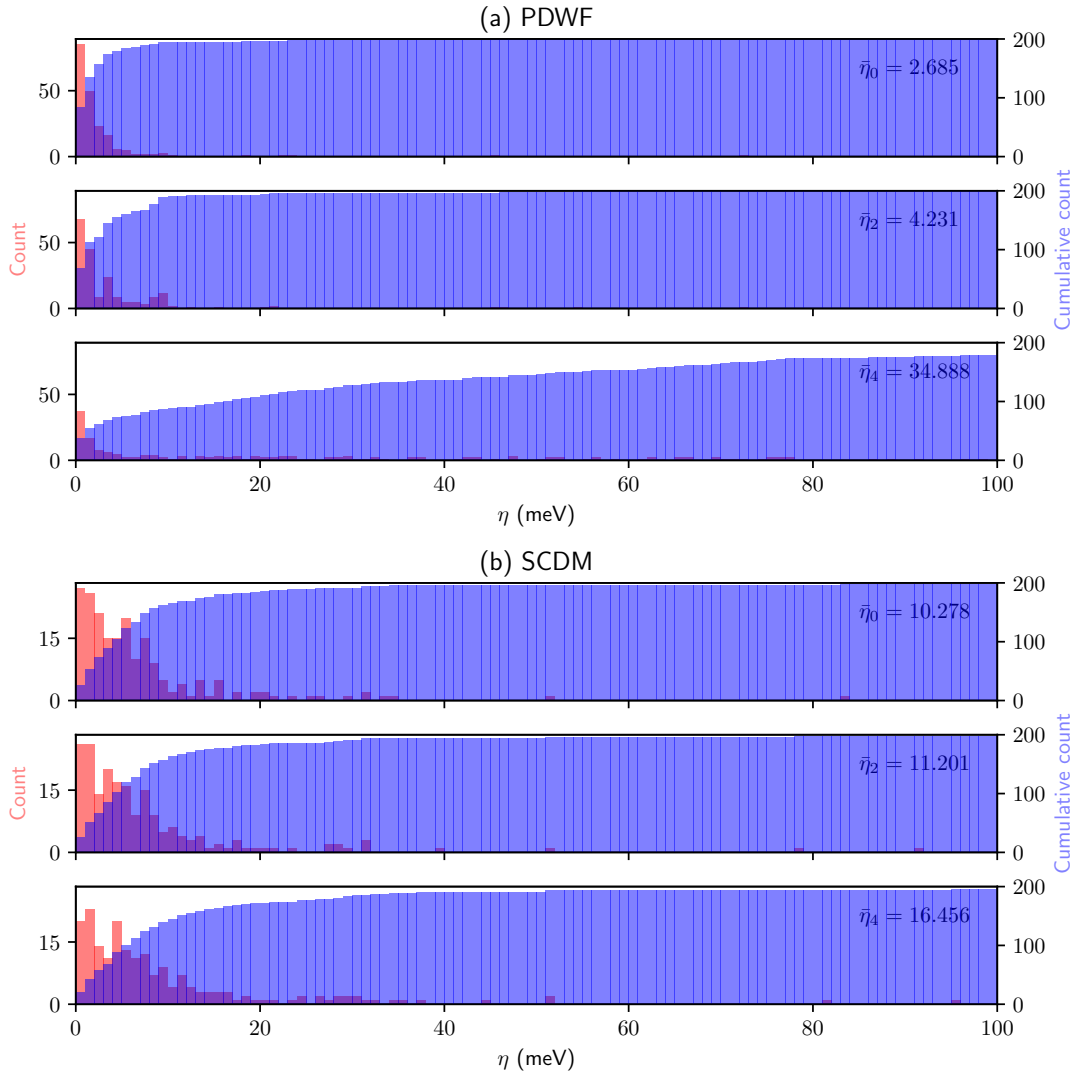



Figure S7: Histograms (red) and cumulative histograms (blue) of band distances $\eta_0$, $\eta_2$, and $\eta_4$ for 200 structures, using (a) PDWF and (b) SCDM. The top, center, and bottom plots in each panel are $\eta_0$, $\eta_2$, and $\eta_4$, respectively. The $\bar{\eta}$ at the top right of each panel is the mean value for the 200 structures.

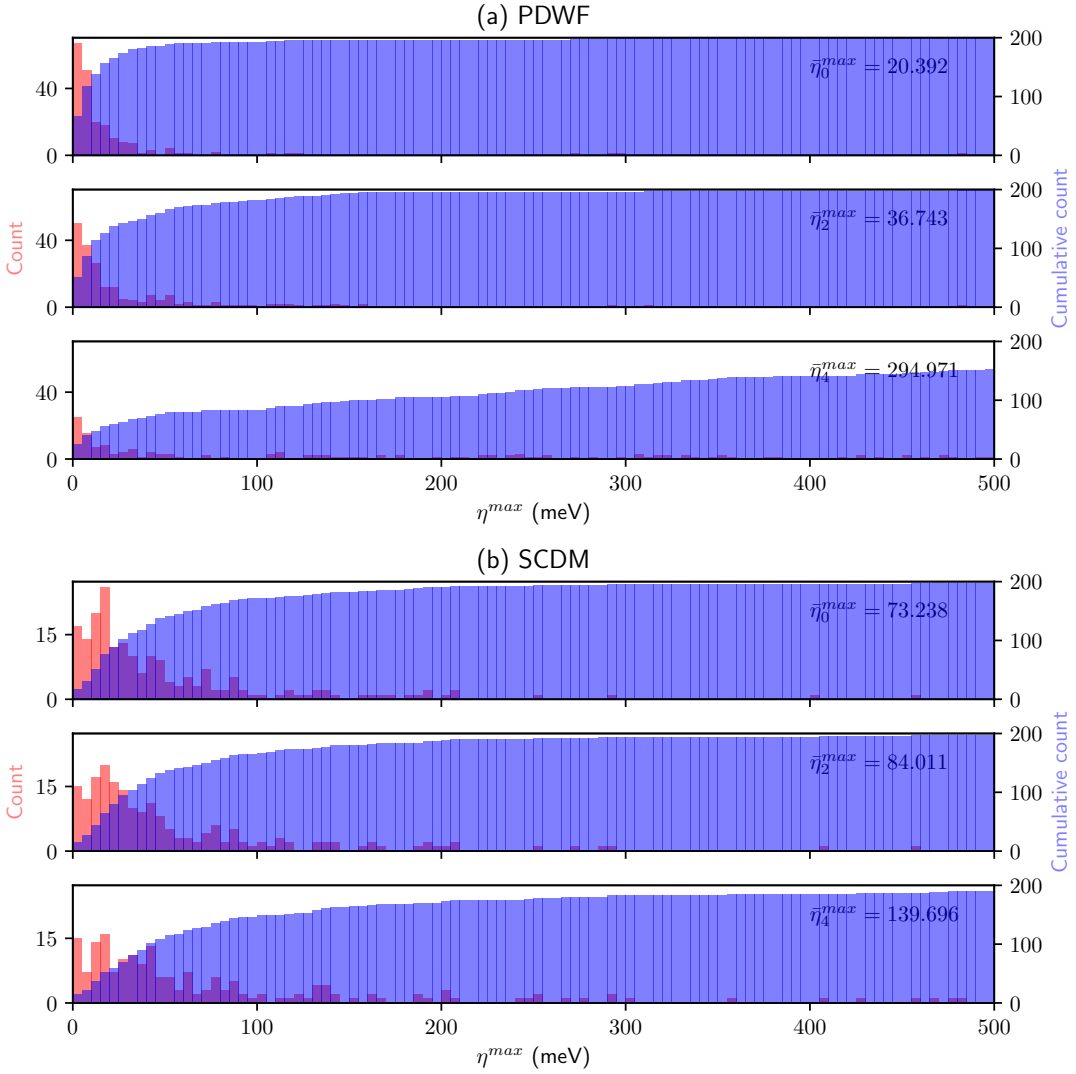



Figure S8: Histograms (red) and cumulative histograms (blue) of band distances $\eta_0^{\max}$, $\eta_2^{\max}$, and $\eta_4^{\max}$ for 200 structures, using (a) PDWF and (b) SCDM. The top, center, and bottom plots for each panel are $\eta_0^{\max}$, $\eta_2^{\max}$ and $\eta_4^{\max}$, respectively. The $\bar{\eta}^{\max}$ at the top right of each panel is the mean value for the 200 structures. This is a zoom-out of Fig. S7.

# S4 MLWF centers

We list in Table S2 the average distance of the WF centers from their nearest neighboring (NN) atom and their next-nearest neighboring (NNN) atom, for the initial WFs (i.e. after disentanglement but before maximal localization) and the final MLWFs (i.e. after maximal localization). The corresponding histograms are shown in Fig. S9. For PDWF, the initial WFs are mostly atom-centered ($d^i_{\mathrm{NN}} = 0.07\,\text{Å}$). The maximal localization pushes the final MLWFs slightly further away ($d^f_{\mathrm{NN}} = 0.43\,\text{Å}$). Inspecting the ratio of $d^{i(f)}_{\mathrm{NN}}/d^{i(f)}_{\mathrm{NNN}}$, both the initial WFs and final MLWFs are still much closer to NN than NNN atoms. For SCDM, both initial WFs and final MLWFs are farther away from NN atoms than PDWF.

Table S2: The average distance of WF center from the NN or NNN atom of the 200 structures for PDWF and SCDM methods. $d_{\mathrm{NN}}$ and $d_{\mathrm{NNN}}$ refer to the distance of the WF center from its NN and NNN atoms, respectively. $d^i$ and $d^f$ are the averages of the initial and the final WF center distances of the 200 structures (in total 6818 WFs), respectively. $d^{i(f)}_{\mathrm{NN}}/d^{i(f)}_{\mathrm{NNN}}$ is the average of the ratio of each WF.

| $d$ (Å) | PDWF | SCDM |
|---|---|---|
| $d^i_{\mathrm{NN}}$ | 0.07 | 0.51 |
| $d^i_{\mathrm{NNN}}$ | 2.36 | 2.11 |
| $d^f_{\mathrm{NN}}$ | 0.43 | 0.53 |
| $d^f_{\mathrm{NNN}}$ | 2.19 | 2.11 |
| $d^i_{\mathrm{NN}}/d^i_{\mathrm{NNN}}$ | 0.03 | 0.28 |
| $d^f_{\mathrm{NN}}/d^f_{\mathrm{NNN}}$ | 0.22 | 0.29 |

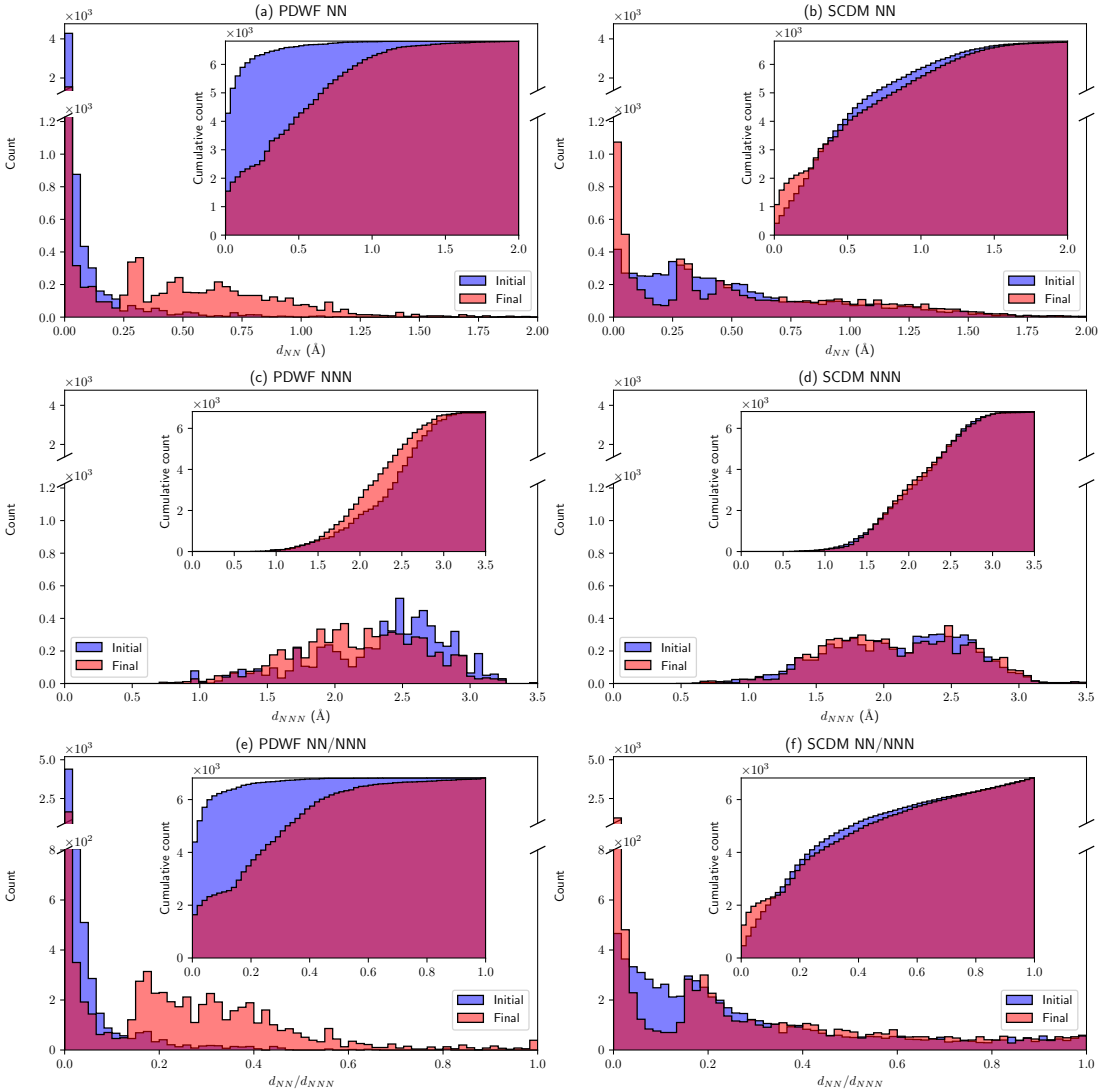



Figure S9: Histograms of the distance of WF centers from their (a) NN atom using PDWF, (b) NN atom using SCDM, (c) NNN atom using PDWF, (d) NNN atom using SCDM; (e) the ratio $d_{\mathrm{NN}}/d_{\mathrm{NNN}}$ using PDWF, and (f) the ratio $d_{\mathrm{NN}}/d_{\mathrm{NNN}}$ using SCDM, of the 200 structures. The insets show the cumulative histogram of each panel. Note that in each histogram the deep red area is the overlap of the initial (red) and the final (blue).

# S5 MLWF spreads

Table S3 and Fig. S10 shows both the initial and final spreads of WFs. The average spreads excluding outliers, i.e., $\Omega^{i(f),\leq 10}$ and $\Omega^{i(f),\leq 20}$ are also listed in Table S3. In all cases, PDWF MLWFs are more localized than SCDM MLWFs.

Table S3: Average of WF spreads of the 200 structures for PDWF and SCDM projections. $\Omega^i$ and $\Omega^f$ are the averages of initial (after disentanglement, before maximal localization) and final (after disentanglement and maximal localization) WF spreads of the 200 structures (in total 6818 WFs), respectively. $\Omega^{i,\leq 10}$ is the average of WFs with $\Omega^i \leq 10\,\text{Å}^2$. $N$ is the number of WFs participating in the averaging.

| Type | PDWF | | SCDM | |
|---|---|---|---|---|
| | $\Omega$ (Å$^2$) | $N$ | $\Omega$ (Å$^2$) | $N$ |
| $\Omega^i$ | 2.72 | 6818 | 30.82 | 6818 |
| $\Omega^f$ | 1.41 | 6818 | 3.54 | 6818 |
| $\Omega^{i,\leq 10}$ | 1.99 | 6626 | 3.83 | 5062 |
| $\Omega^{f,\leq 10}$ | 1.38 | 6808 | 2.91 | 6501 |
| $\Omega^{i,\leq 20}$ | 2.14 | 6708 | 4.68 | 5599 |
| $\Omega^{f,\leq 20}$ | 1.40 | 6814 | 3.31 | 6765 |

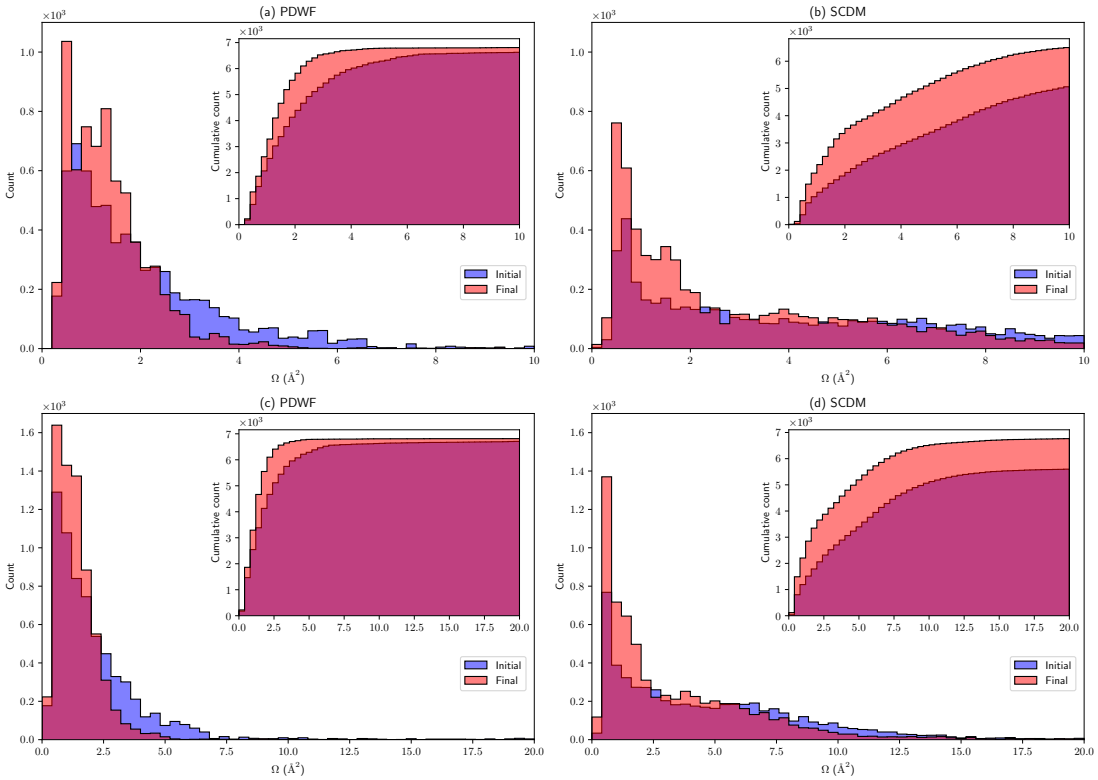



Figure S10: Histogram of WF spreads for 200 structures using (a) PDWF with $\Omega$ in the range 0 $Å^2$ to 10 $Å^2$, (b) SCDM with $\Omega$ in the range 0 $Å^2$ to 10 $Å^2$, (c) PDWF with $\Omega$ in the range 0 $Å^2$ to 20 $Å^2$, and (d) SCDM with $\Omega$ in the range 0 $Å^2$ to 20 $Å^2$. The insets show the cumulative histogram of each panel. Note in each histogram, the deep red area is the overlap of the initial (red) and the final (blue).

# S6 High-throughput Wannierization

Table S4: Average band distance for 21 737 structures from Materials Cloud. $\eta_\nu$ is the average band distance of all the structures below $E_F + \nu$, where $\nu = 0$, 2, or 4 eV. $\eta_\nu^{\leq 20}$ is the average of structures with $\eta_\nu \leq 20$ meV. $\eta_\nu^{\max}$ is the max distance of all the structures. $\eta_\nu^{\max,\leq 100}$ is the average of structures with $\eta_\nu^{\max} \leq 100$ meV. $N$ is the number of structures participating in the averagings.

| Type | $\eta$ (meV) | $N$ |
|---|---|---|
| $\eta_0$ | 2.003 | 21737 |
| $\eta_2$ | 3.685 | 21737 |
| $\eta_4$ | 38.437 | 21737 |
| $\eta_0^{\leq 20}$ | 1.129 | 21445 |
| $\eta_2^{\leq 20}$ | 2.118 | 21259 |
| $\eta_4^{\leq 20}$ | 4.054 | 11911 |
| $\eta_0^{\leq 100}$ | 1.654 | 21703 |
| $\eta_2^{\leq 100}$ | 2.885 | 21650 |
| $\eta_4^{\leq 100}$ | 22.748 | 19100 |
| $\eta_0^{\max}$ | 25.329 | 21737 |
| $\eta_2^{\max}$ | 42.768 | 21737 |
| $\eta_4^{\max}$ | 297.723 | 21737 |
| $\eta_0^{\max,\leq 100}$ | 7.939 | 20980 |
| $\eta_2^{\max,\leq 100}$ | 15.145 | 20217 |
| $\eta_4^{\max,\leq 100}$ | 20.864 | 9769 |
| $\eta_0^{\max,\leq 500}$ | 13.492 | 21567 |
| $\eta_2^{\max,\leq 500}$ | 24.805 | 21453 |
| $\eta_4^{\max,\leq 500}$ | 128.216 | 16593 |

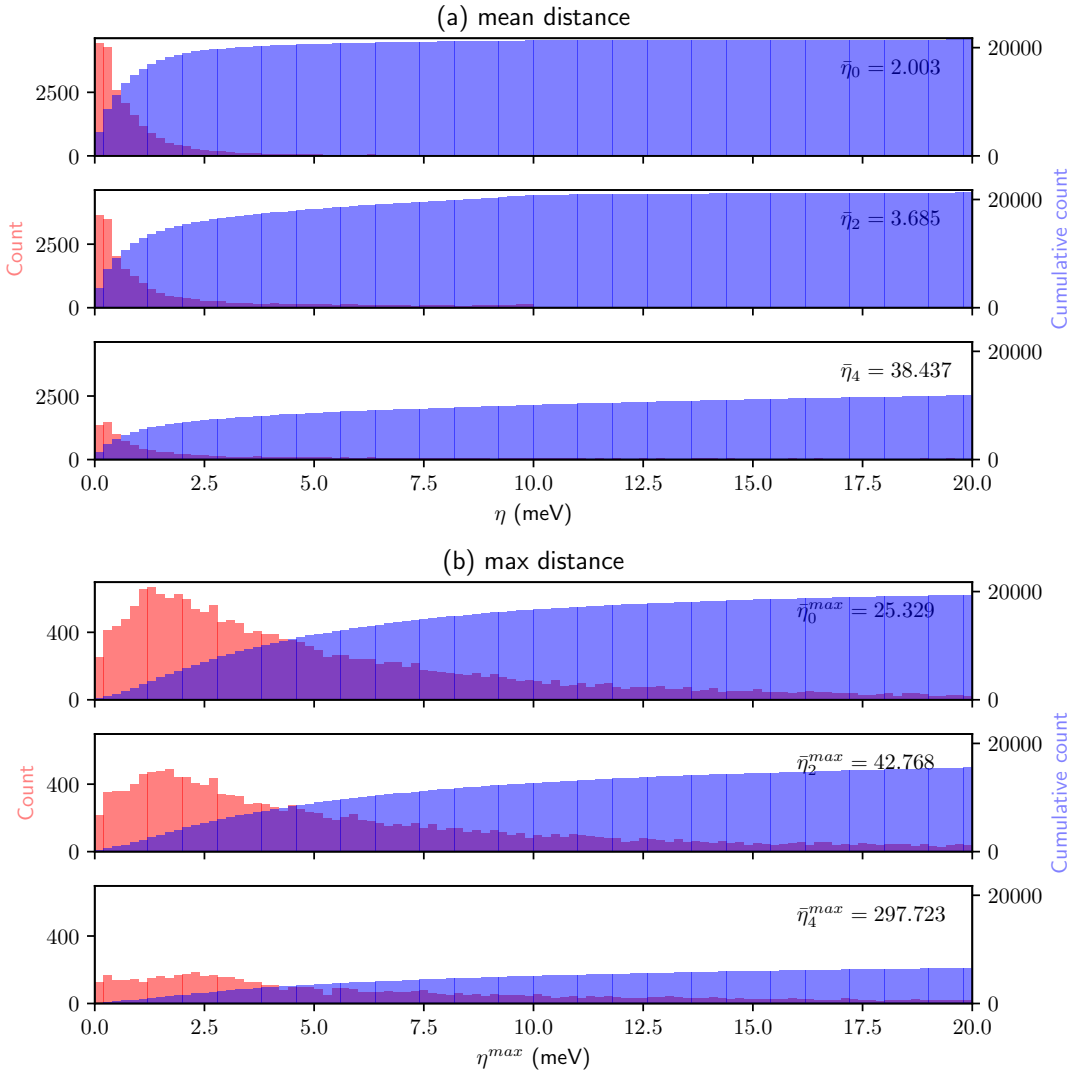



Figure S11: Histograms (red) and cumulative histograms (blue) of band distances of 21 737 structures, for (a) $\eta_0$, $\eta_2$, and $\eta_4$, and (b) $\eta_0^{\max}$, $\eta_2^{\max}$, and $\eta_4^{\max}$. The $\bar{\eta}$ or $\bar{\eta}^{\max}$ at the top right of each panel is the mean value for the 21 737 structures.

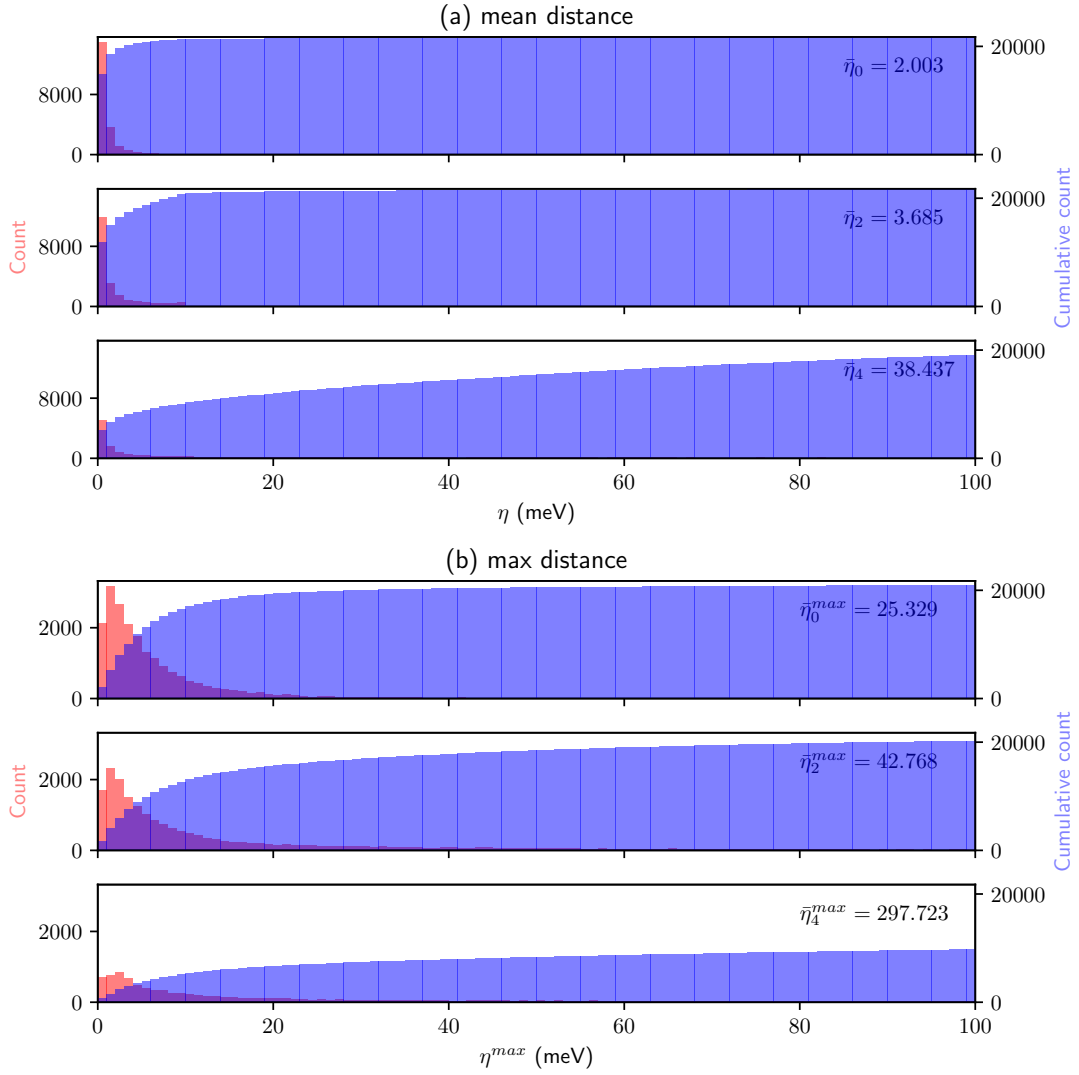



Figure S12: Histograms (red) and cumulative histograms (blue) of band distances of 21 737 structures, for (a) $\eta_0$, $\eta_2$, and $\eta_4$, and (b) $\eta_0^{\max}$, $\eta_2^{\max}$, and $\eta_4^{\max}$. The $\bar{\eta}$ or $\bar{\eta}^{\max}$ at the top right of each panel is the mean value for the 21 737 structures. This is a zoom-out of Fig. S11.

# S7 Additional PAOs

Usually, pseudopotentials are pseudized to accurately reproduce all-electron calculations at specified energies. The targets are often the states below and a few eV above Fermi energy. Most often the pseudopotentials also contains a set of PAOs which normally are good basis vectors that can span the valence bands and a few conduction bands of solids, as indicated by their projectability. However, in some cases where the chemical environment of solid is significantly different from that of atoms, the projectability of states around the Fermi energy on all available PAOs is low. In other cases, one may want to Wannierize higher conduction bands. To tackle these difficulties, we can add additional higher-angular-momentum projectors to satisfy these needs. Take silicon as an example, to Wannierize both valence and conduction bands, one $s$ and three $p$ projectors for each silicon atom are used to generate 8 MLWFs, however, they cannot accurately interpolate bands 5 eV above $E_F$, see Fig. S14a. If 10 additional localized projectors, e.g., five $d$ PAOs on each silicon atom, are introduced, the higher conduction bands can be accurately described (also with a higher inner energy window), see Fig. S14d.

In Fig. S14, the PAOs from the `OpenMX` package [4] (PAO `DFT_DATA19`) are used to generate 18 MLWFs. The `OpenMX` PAOs are the solutions of the Schrödinger equation in a confined potential, thus they are always localized and can be alternatively used as atomic projectors for MLWFs. This is similar to the inclusion of polarization orbitals in the LCAO method[3]. Comparing Fig. S14a and Fig. S14b, the $s$ and $p$ PAOs from the QE pseudopotential and from the `OpenMX` PAOs essentially have the same quality of band interpolation. The inclusion of $d$ PAOs allows raising the maximum inner energy window, thus resulting in a much more accurate interpolation of bands, as shown in Figs. S14c and S14d. Figures S1 and S15 show the MLWF shapes for pseudopotential PAOs and `OpenMX` PAOs, respectively. The ten additional $d$ MLWFs are clearly visible in Fig. S15. When raising the maximum inner energy window to CBM + 10 eV, the MLWFs are mixtures of atomic orbitals and high-energy conduction bands, losing the physical picture of TB atomic orbitals. Instead, in the ED (maximum inner energy window = CBM + 2 eV), PD, or PD+ED cases, the MLWFs still preserve the $s$, $p$, or $d$ characters similar to the original `OpenMX` PAO projectors.

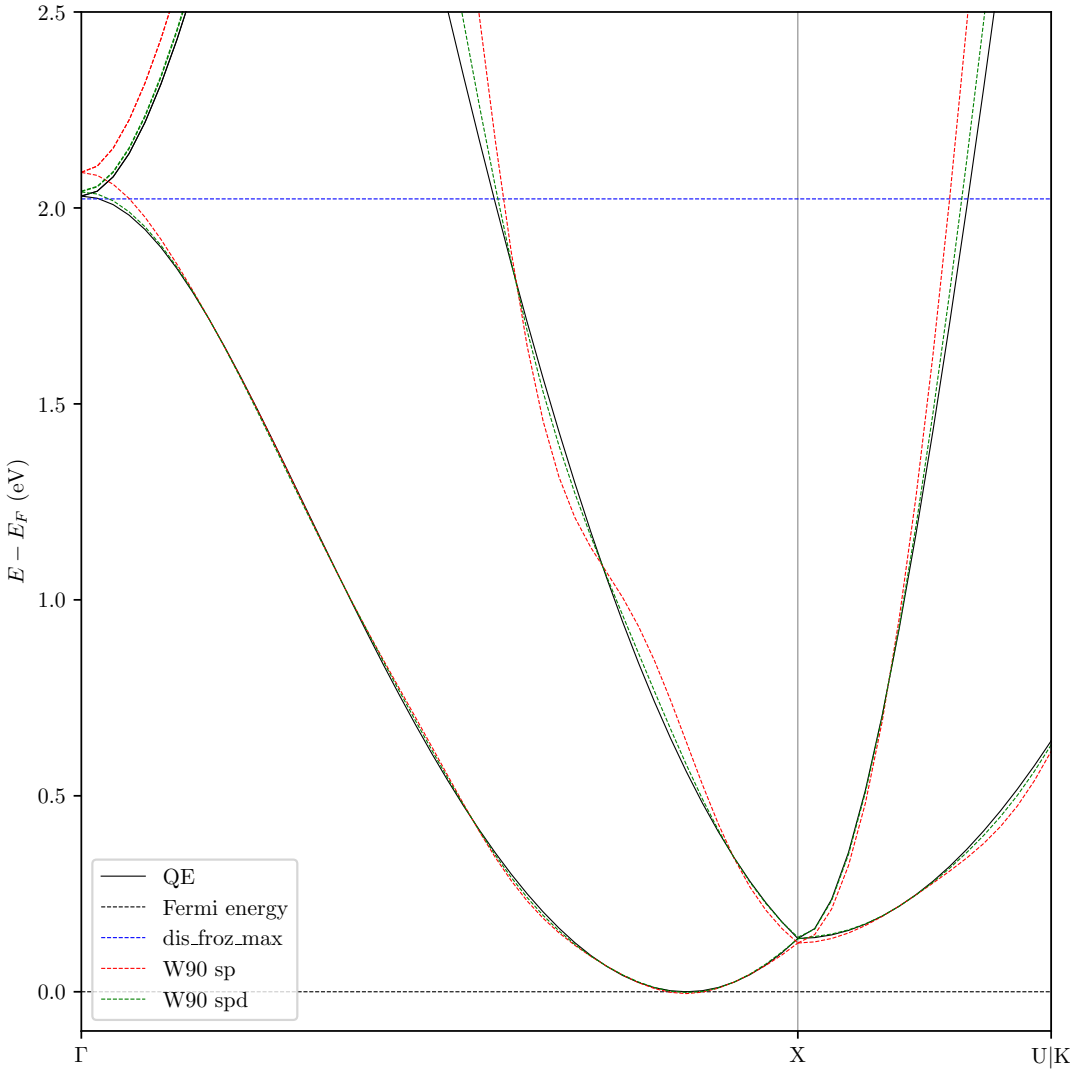



Figure S13: Comparison of QE bands (black lines) and Wannier-interpolated bands using `OpenMX` $s, p$ projections (red dashed lines) and `OpenMX` $s, p, d$ projections (green dashed lines). Results using QE $s, p$ projections are not shown since they exactly overlap with that from `OpenMX` $s, p$ projections. The MLWFs are obtained using `OpenMX` PAOs and ED with the maximum of the inner energy window (blue dashed line) set to CBM + 2 eV (actually slightly larger than CBM + 2 eV since in the `AiiDA` workflow the CBM is automatically computed based on the eigenenergies only on the regular $k-$point mesh of the non-self-consistent calculation, that does not include the exact $k-$point where the CBM is located). The CBM (horizontal black dashed line) is at zero. Note that the interpolation quality can be further improved by increasing the $k-$point sampling density.

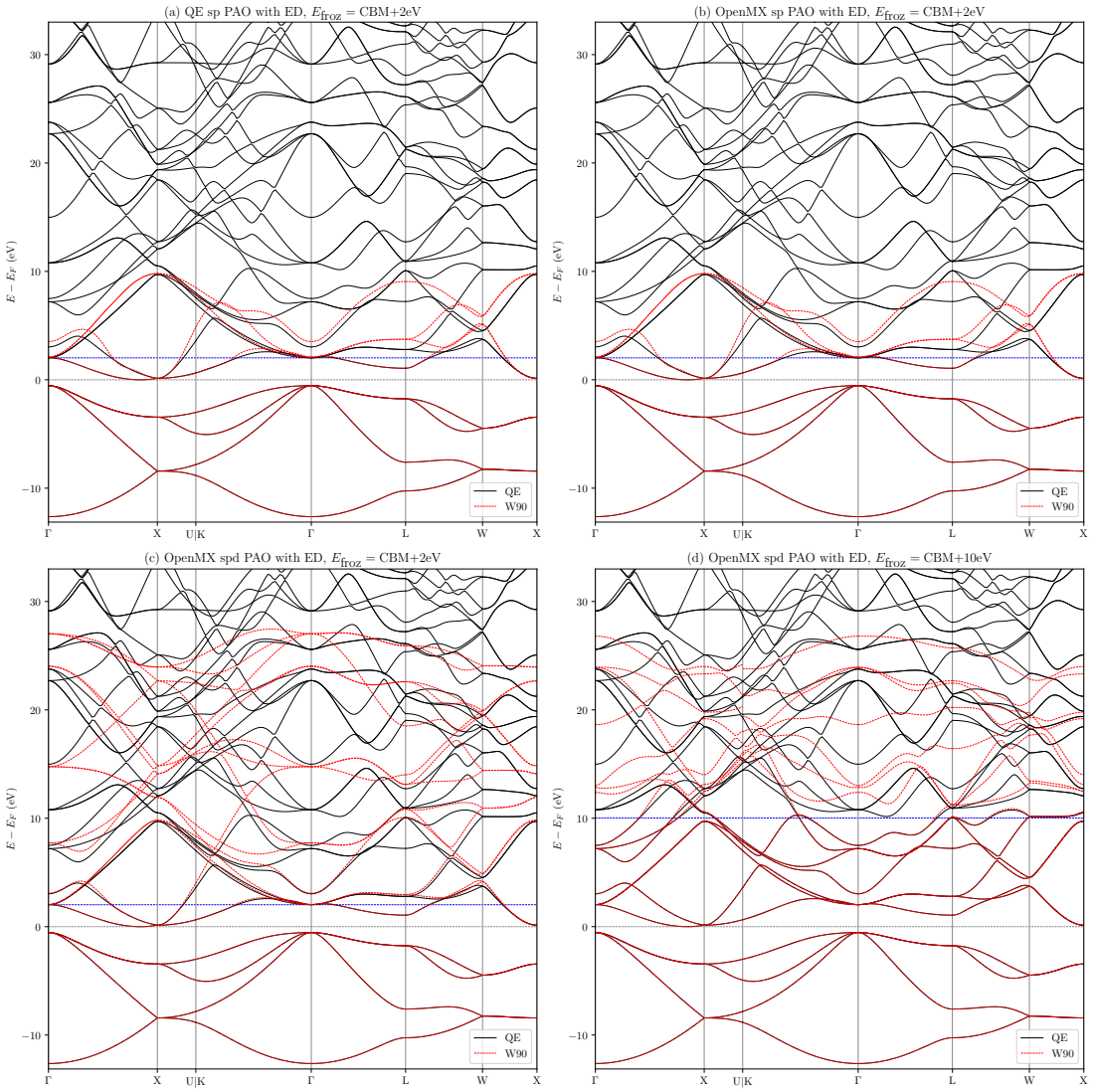



Figure S14: Comparisons between QE bands (black lines) and Wannier-interpolated bands (red dashed lines) using (a) QE pseudopotential PAOs with ED, where the maximum inner energy window is set as CBM + 2 eV, (b) `OpenMX` $s, p$ PAOs with ED, where the maximum inner energy window is set as CBM + 2 eV, (c) `OpenMX` $s, p, d$ PAOs with ED, where the maximum inner energy window is set as CBM + 2 eV, and (d) `OpenMX` $s, p, d$ PAOs with ED, where the maximum inner energy window is set as CBM + 10 eV. The Fermi energy $E_F$ (horizontal black dashed line) is at zero. The horizontal blue dashed line denotes the maximum inner energy window.

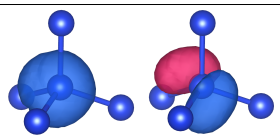
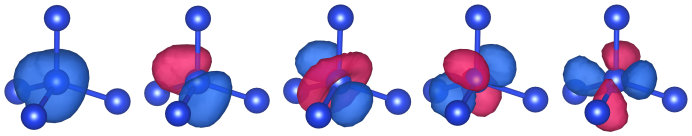
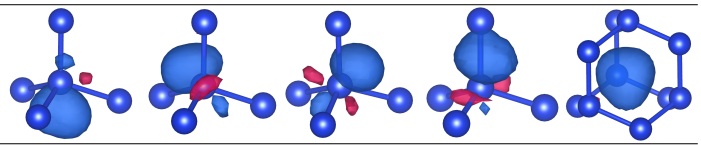
| | | | | | | |
|---|---|---|---|---|---|---|
| | |  | | | | |
| | multiplicity | 2 | 6 | | | |
| **sp ED** | $d_{WFC}$(Å) | 0.000 | 0.000 | | | |
| | $\Omega_{WF}$(Å$^2$) | 1.849 | 2.546 | | | |
| **sp PD** | $d_{WFC}$(Å) | 0.000 | 0.000 | | | |
| | $\Omega_{WF}$(Å$^2$) | 1.060 | 1.256 | | | |
| **sp PD+ED** | $d_{WFC}$(Å) | 0.000 | 0.000 | | | |
| | $\Omega_{WF}$(Å$^2$) | 1.844 | 2.550 | | | |
| | |  | | | | |
| | multiplicity | 2 | 6 | 2 | 2 | 6 |
| | character | $s$ | $p_x, p_y, p_z$ | $d_{z^2}$ | $d_{x^2-y^2}$ | $d_{xy}, d_{xz}, d_{yz}$ |
| **spd ED** | $d_{WFC}$(Å) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}$(Å$^2$) | 1.101 | 1.411 | 1.451 | 1.451 | 1.557 |
| **spd PD** | $d_{WFC}$(Å) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}$(Å$^2$) | 1.121 | 1.278 | 1.352 | 1.352 | 1.327 |
| **spd PD+ED** | $d_{WFC}$(Å) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| | $\Omega_{WF}$(Å$^2$) | 1.101 | 1.412 | 1.454 | 1.454 | 1.556 |
| | |  | | | | |
| **spd ED CBM + 10 eV** | $d_{WFC}$(Å) | 0.905 | 0.722 | 0.752 | 0.995 | 1.793 |
| | $\Omega_{WF}$(Å$^2$) | 1.082 | 0.928 | 1.141 | 1.235 | 1.459 |
| | $d_{WFC}$(Å) | 0.807 | 0.77 | 0.738 | 0.952 | 1.877 |
| | $\Omega_{WF}$(Å$^2$) | 0.985 | 1.055 | 1.053 | 1.214 | 1.428 |
| | $d_{WFC}$(Å) | 0.835 | 0.798 | 0.749 | | |
| | $\Omega_{WF}$(Å$^2$) | 1.103 | 0.988 | 1.125 | | |
| | $d_{WFC}$(Å) | 0.917 | 0.735 | 0.752 | | |
| | $\Omega_{WF}$(Å$^2$) | 1.112 | 0.932 | 1.043 | | |
| | $d_{WFC}$(Å) | 0.827 | 0.787 | | | |
| | $\Omega_{WF}$(Å$^2$) | 1.110 | 1.022 | | | |

Figure S15: Silicon MLWF shapes, centers, and spreads for `OpenMX` $s$+$p$ or `OpenMX` $s$+$p$+$d$ PAOs as starting projections, with ED, PD, and PD+ED disentanglements, where for ED and PD+ED the maximum of the inner energy window is set at CBM + 2 eV. In addition, we also show the results for ED disentanglement when the maximum of the inner energy window is set as CBM + 10 eV. In this latter case, all the 18 MLWFs are listed (and roughly categorized into five groups) since their $d_{\mathrm{WF}}$, $\Omega_{\mathrm{WF}}$, and shapes are different; as discussed in main text Section II B, including the higher-energy states breaks the atomic-like picture of these WFs.

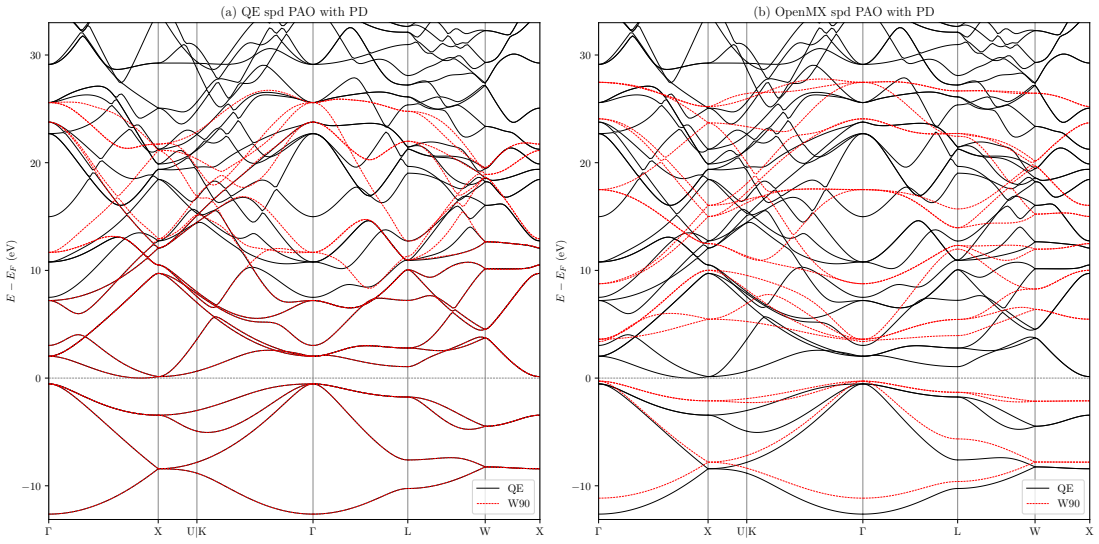



Figure S16: Comparisons between QE bands (black lines) and Wannier-interpolated bands (red dashed lines) using (a) a newly generated custom pseudopotential including $3d$ PAOs with PD, (b) `OpenMX` $s, p, d$ PAOs with PD. The Fermi energy $E_F$ (horizontal black dashed line) is at zero.

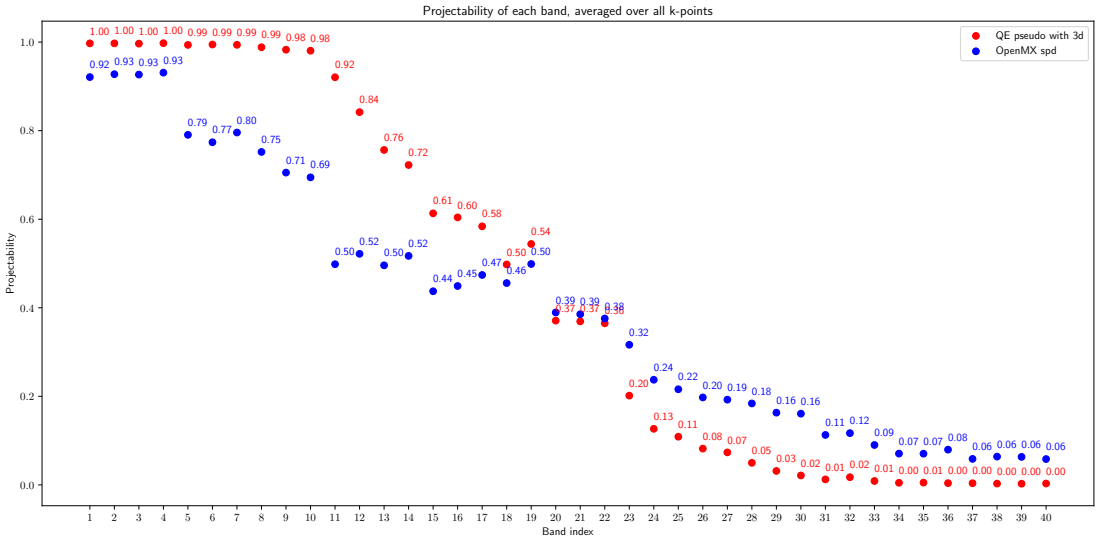



Figure S17: Band projectabilities using the orbitals from our newly generated custom pseudopotential including $3d$ PAOs (red) and `OpenMX` $s, p, d$ PAOs (blue).

# References

[1] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. D. Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch. QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. *J. Phys.: Condens. Matter*, 21(39):395502, sep 2009.

[2] P. Giannozzi, O. Baseggio, P. Bonfà, D. Brunato, R. Car, I. Carnimeo, C. Cavazzoni, S. de Gironcoli, P. Delugas, F. F. Ruffino, A. Ferretti, N. Marzari, I. Timrov, A. Urru, and S. Baroni. Quantum ESPRESSO toward the exascale. *J. Chem. Phys.*, 152(15):154105, apr 2020.

[3] P. C. Hariharan and J. A. Pople. The influence of polarization functions on molecular orbital hydrogenation energies. *Theor. Chim. Acta*, 28(3):213–222, 1973.

[4] T. Ozaki and H. Kino. Numerical atomic basis orbitals from H to Kr. *Phys. Rev. B*, 69(19):195113, may 2004.

[5] G. Pizzi, V. Vitale, R. Arita, S. Blügel, F. Freimuth, G. Géranton, M. Gibertini, D. Gresch, C. Johnson, T. Koretsune, J. Ibañez-Azpiroz, H. Lee, J.-M. Lihm, D. Marchand, A. Marrazzo, Y. Mokrousov, J. I. Mustafa, Y. Nohara, Y. Nomura, L. Paulatto, S. Poncé, T. Ponweiser, J. Qiao, F. Thöle, S. S. Tsirkin, M. Wierzbowska, N. Marzari, D. Vanderbilt, I. Souza, A. A. Mostofi, and J. R. Yates. Wannier90 as a community code: new features and applications. *J. Phys.: Condens. Matter*, 32(16):165902, jan 2020.

# S8 Band structure and Hamiltonian decay

In this section, we show on each page the band structures, band distances, and Hamiltonian decay for each of the 200 structures.

On each page, the left (right) column shows the band structure comparison between `Quantum ESPRESSO`, labeled QE, and Wannier-interpolated bands from PDWF (SCDM) method. The Fermi energy $E_F$ is at zero. The horizontal blue dashed line denotes the `dis_froz_max` in the PDWF method (note in the PDWF method some high-projectability states which are higher than the `dis_froz_max` are also frozen, but they are not explicitly shown in the figure). The title shows the structural formula and a description of the calculation, and the UUID of the corresponding `AiiDA` calculations for the QE band structure (PW) and Wannier-interpolated bands (W90). In general, there are two types of description: (a) "exclude semicore": the semicore states are excluded from Wannierization, this is the default setting; (b) "INCLUDE semicore": the semicore states are included in Wannierization, since the semicore states overlap with valence states, Wannierization quality would be worse if the semicore states were excluded.

The table at the bottom left shows the band distances between the band structures. All the $\eta$ are in meV units. The last column of the table shows the Hamiltonian decay $\tau$ in Å units.

Finally, the bottom figure shows the Hamiltonian decay and its logarithmic fitting for both PDWF and SCDM methods. Note since the minimal-distance replica selection method is used in the Wannier interpolation [5], when plotting the figures, the $\mathbf{R}$ vector (shown on the x axis) already contains the translation vector $\mathbf{T}$, which is chosen to minimize the distance between two WF centers $\mathbf{r}_m$ (of $|w_{m\mathbf{0}}\rangle$) and $\mathbf{r}_n$ (of $|w_{n\mathbf{R}}\rangle$):

$$\arg\min_{\mathbf{T}} |\mathbf{r}_m - (\mathbf{r}_n + \mathbf{R} + \mathbf{T})| \,. \tag{1}$$

## S8.1 List of 200 structures (Hill formula, in alphabetic order)


1. $Ag_2Hf_2$ ..... 30
2. $Ag_2Sc$ ..... 31
3. $Ag_2Ti_4$ ..... 32
4. $Ag_2Y$ ..... 33
5. $Ag_4Sc_2$ ..... 34
6. AgMg ..... 35
7. AgSc ..... 36
8. AgY ..... 37
9. $Al_{12}Ni_4$ ..... 38
10. $Al_{18}Co_4$ ..... 39
11. $Al_{24}W_6$ ..... 40
12. $Al_2Mo_6$ ..... 41
13. $Al_2Nb_6$ ..... 42
14. $Al_2Os$ ..... 43
15. $Al_3Nb$ ..... 44
16. $Al_3Ta$ ..... 45
17. $Al_4Mn_2O_8$ ..... 46
18. $Al_4O_8Zn_2$ ..... 47
19. $Al_4Sc_2$ ..... 48
20. $Al_4Y_2$ ..... 49
21. $Al_8Zr_4$ ..... 50
22. AlCo ..... 51
23. AlFe ..... 52
24. $AlHfNi_2$ ..... 53
25. AlIr ..... 54
26. $AlRe_2$ ..... 55
27. $Ar_2$ ..... 56
28. $As_2Ni_2$ ..... 57
29. $As_4O_{16}Y_4$ ..... 58
30. $As_8Si_4Zn_4$ ..... 59
31. AsB ..... 60
32. $Au_2Hf_2$ ..... 61
33. $Au_2Nb$ ..... 62
34. $Au_2Pb_4$ ..... 63
35. $Au_2Sc$ ..... 64
36. $Au_2Y$ ..... 65
37. $Au_4V_2$ ..... 66
38. AuMn ..... 67
39. $B_{16}Mg_4$ ..... 68
40. $B_2Cr$ ..... 69
41. $B_2Hf$ ..... 70
42. $B_2Mn$ ..... 71
43. $B_2Ta$ ..... 72
44. $B_2Ti$ ..... 73
45. $B_2Y$ ..... 74
46. $B_4Co_4$ ..... 75
47. $B_4Ni_4$ ..... 76
48. $B_4Re_2$ ..... 77
49. $B_4V_6$ ..... 78
50. $B_6Si$ ..... 79
51. $B_8H_{16}O_{16}$ ..... 80
52. BaS ..... 81
53. BaTe ..... 82
54. $BeO_4S$ ..... 83
55. $Bi_2Na_6$ ..... 84
56. $Bi_4Cl_{12}$ ..... 85
57. BiNa ..... 86
58. $Br_{18}W_3$ ..... 87
59. $Br_2Fe$ ..... 88
60. $Br_2Ti$ ..... 89
61. $Br_2V$ ..... 90
62. $Br_4Ca_2$ ..... 91
63. $Br_6Ni_3$ ..... 92
64. $Br_6Zr_2$ ..... 93
65. BrLi ..... 94
66. BrNa ..... 95
67. $C_2Cd_2O_6$ ..... 96
68. $C_2Cu_2O_6$ ..... 97
69. $C_2N_2Na_2$ ..... 98
70. $C_3Ag_3N_3$ ..... 99
71. $C_4Mg_2$ ..... 100
72. $C_4O_{12}Sr_4$ ..... 101
73. $C_6Mg_4$ ..... 102
74. $CBe_2$ ..... 103
75. $CTa_2$ ..... 104
76. CTi ..... 105
77. $Ca_4Cr_4O_{12}$ ..... 106
78. $Ca_4Mg_8$ ..... 107
79. $CaI_2$ ..... 108
80. CaO ..... 109
81. $CdCl_2$ ..... 110
82. $Cl_2O_2Ti_2$ ..... 111
83. $Cl_2Ti$ ..... 112
84. $Cl_2V$ ..... 113
85. $Cl_4Li_4O_{16}$ ..... 114
86. $Cl_6Ni_3$ ..... 115
87. $Cl_6Rh_2$ ..... 116
88. $Cl_8Hf_2$ ..... 117
89. $Cl_8Sr_4$ ..... 118
90. $Co_2F_4$ ..... 119
91. $Co_2O_8W_2$ ..... 120
92. $Co_4S_8$ ..... 121
93. $Co_4Sc_8$ ..... 122
94. CoHf ..... 123
95. $CoSi_2$ ..... 124
96. $Cr_2F_4$ ..... 125
97. $Cr_6Ga_2$ ..... 126
98. $Cr_6Si_2$ ..... 127
99. $Cs_4O_4$ ..... 128
100. CsH ..... 129
101. $Cu_3Pt$ ..... 130
102. $Cu_4P_8$ ..... 131
103. $Cu_4Sb_2$ ..... 132
104. $Cu_4Sc_2$ ..... 133
105. $Cu_4Te_2$ ..... 134
106. $F_2Ti$ ..... 135
107. $F_2Xe$ ..... 136
108. $F_4H_2K_2$ ..... 137
109. $F_4Ni_2$ ..... 138
110. $F_4Sn$ ..... 139
111. $F_8V_2$ ..... 140
112. FLi ..... 141
113. FNa ..... 142
114. $Fe_4N$ ..... 143
115. FeO ..... 144
116. FeTi ..... 145
117. $Ga_2Mo_6$ ..... 146
118. $Ga_4Y_4$ ..... 147
119. GaRu ..... 148
120. $Ge_4Ir_4$ ..... 149
121. $Ge_4Pt_4$ ..... 150
122. $Ge_4Ru_4$ ..... 151
123. $H_8O_{16}W_4$ ..... 152
124. HK ..... 153
125. HLi ..... 154
126. He ..... 155
127. $Hf_{10}Si_6$ ..... 156
128. $Hf_2I_6$ ..... 157
129. $Hf_4Ni_4$ ..... 158
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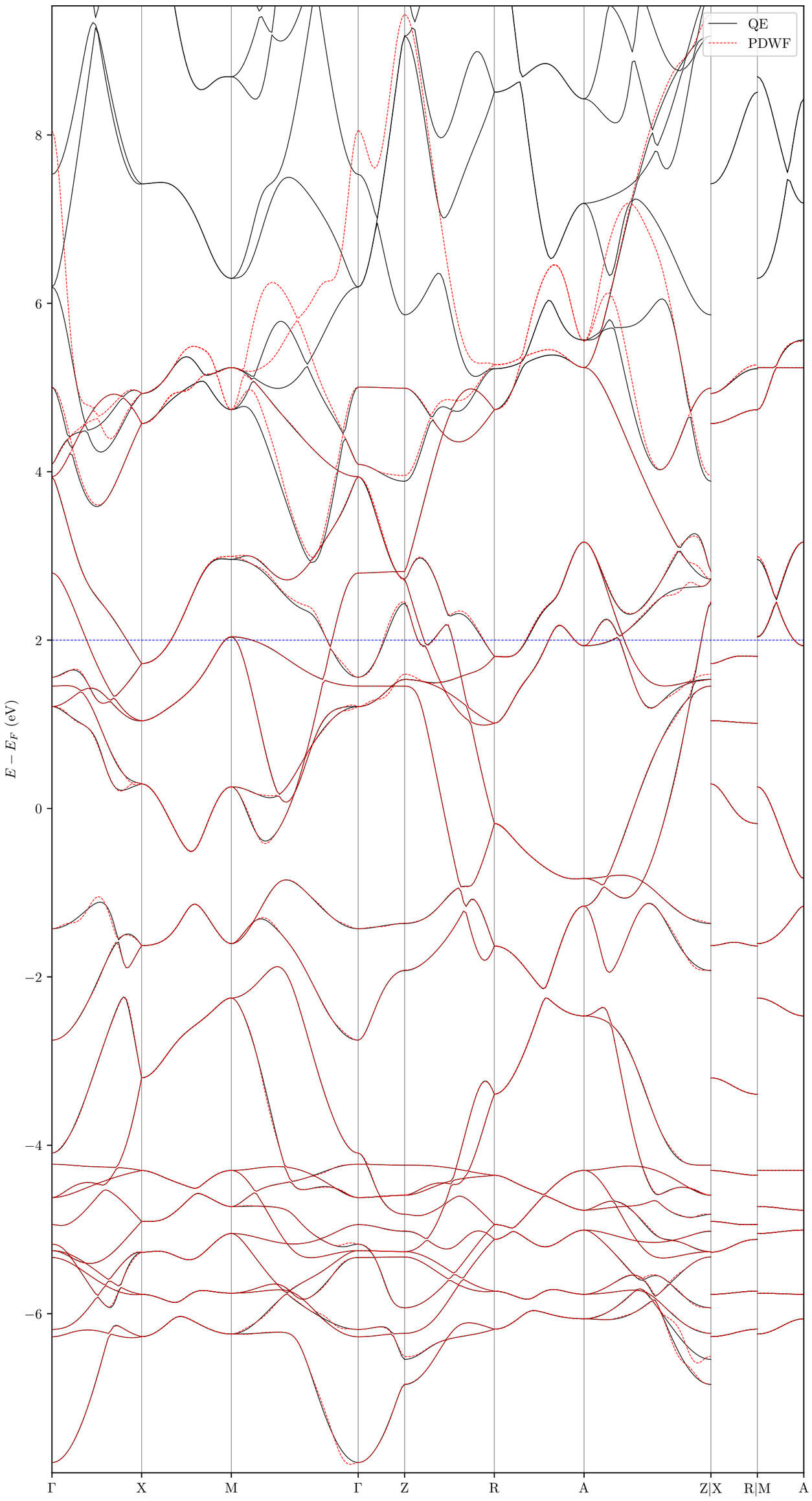
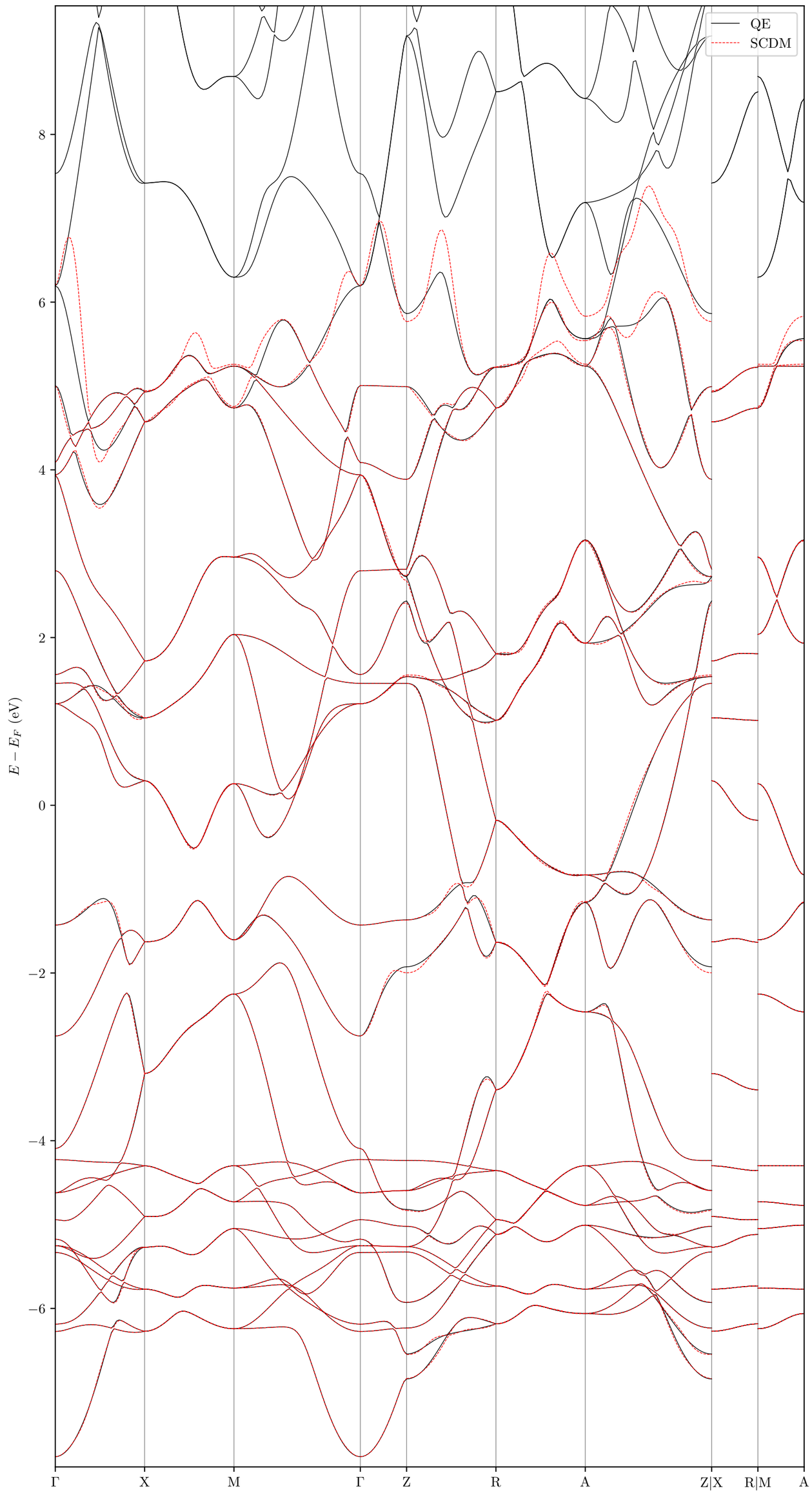


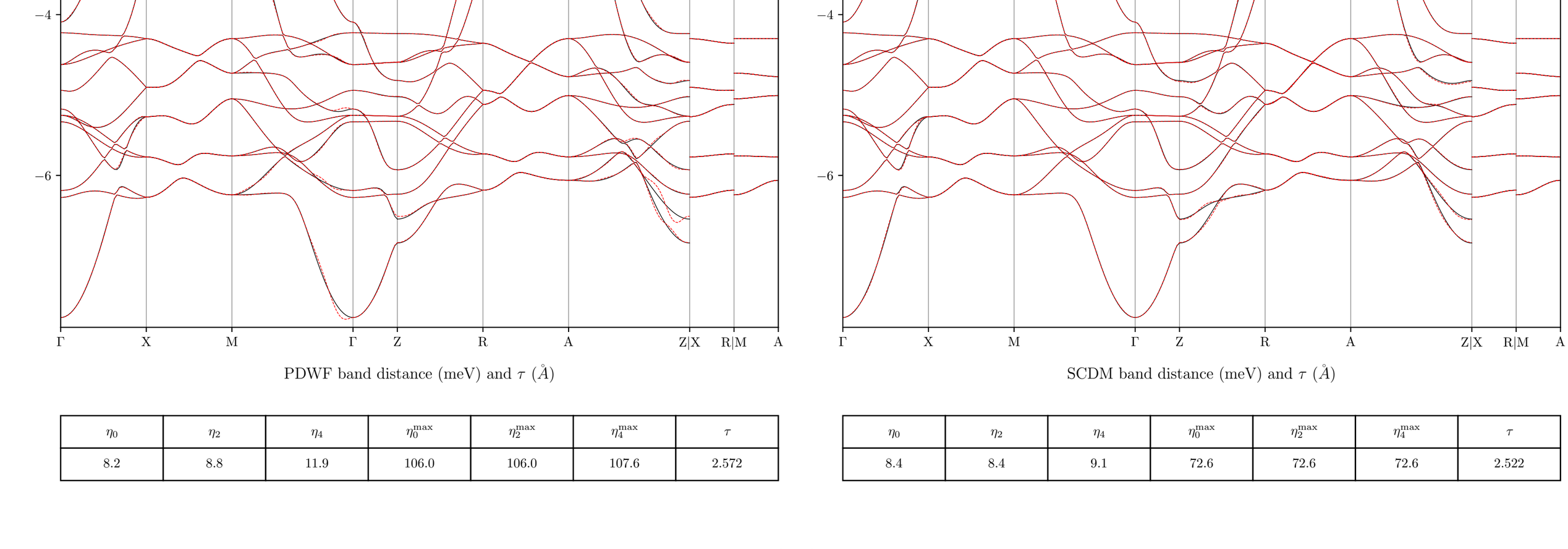

PDWF band distance (meV) and $\tau$ ($\AA$)

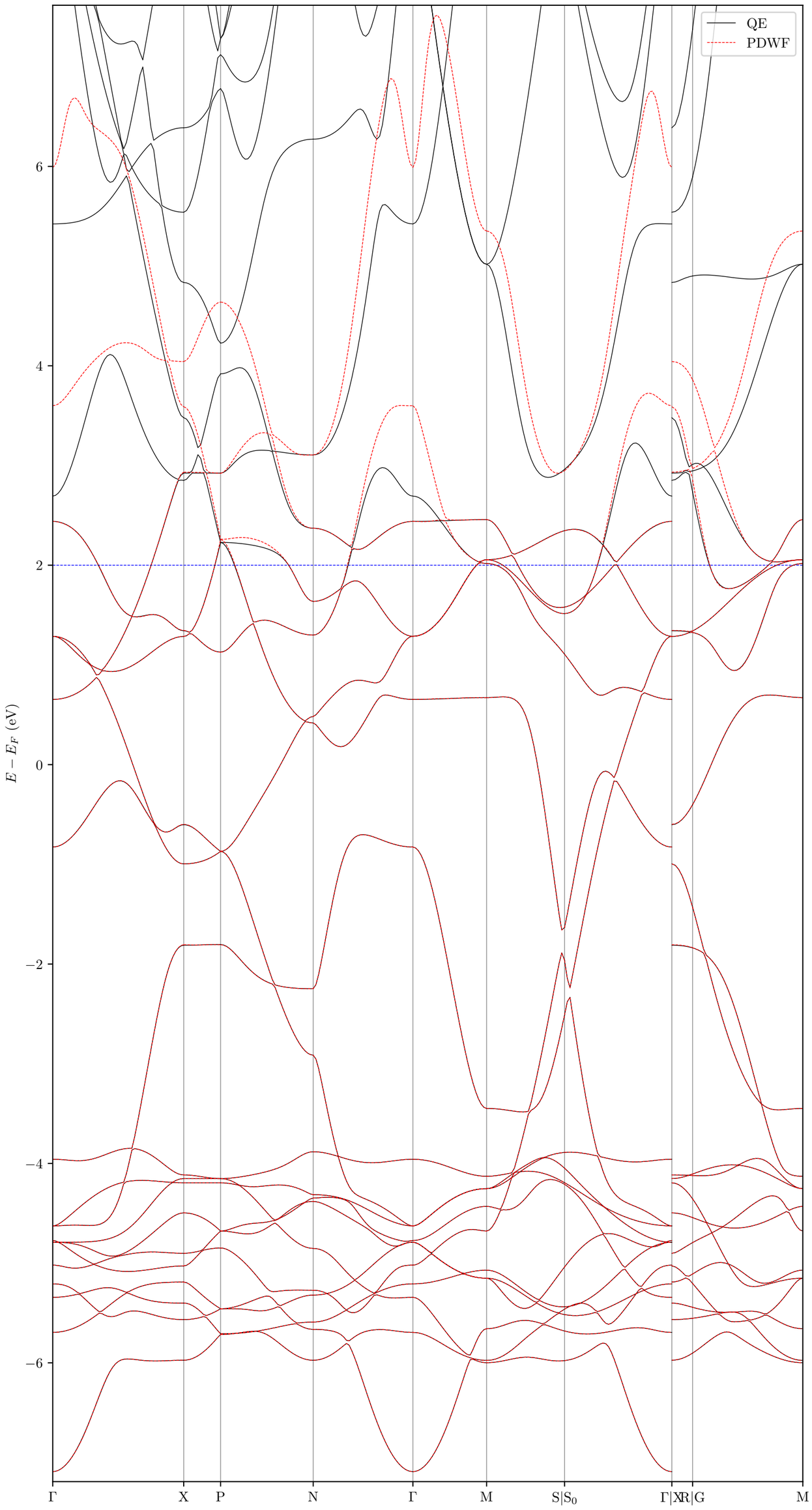
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.2 | 8.8 | 11.9 | 106.0 | 106.0 | 107.6 | 2.572 |




SCDM band distance (meV) and $\tau$ ($\AA$)

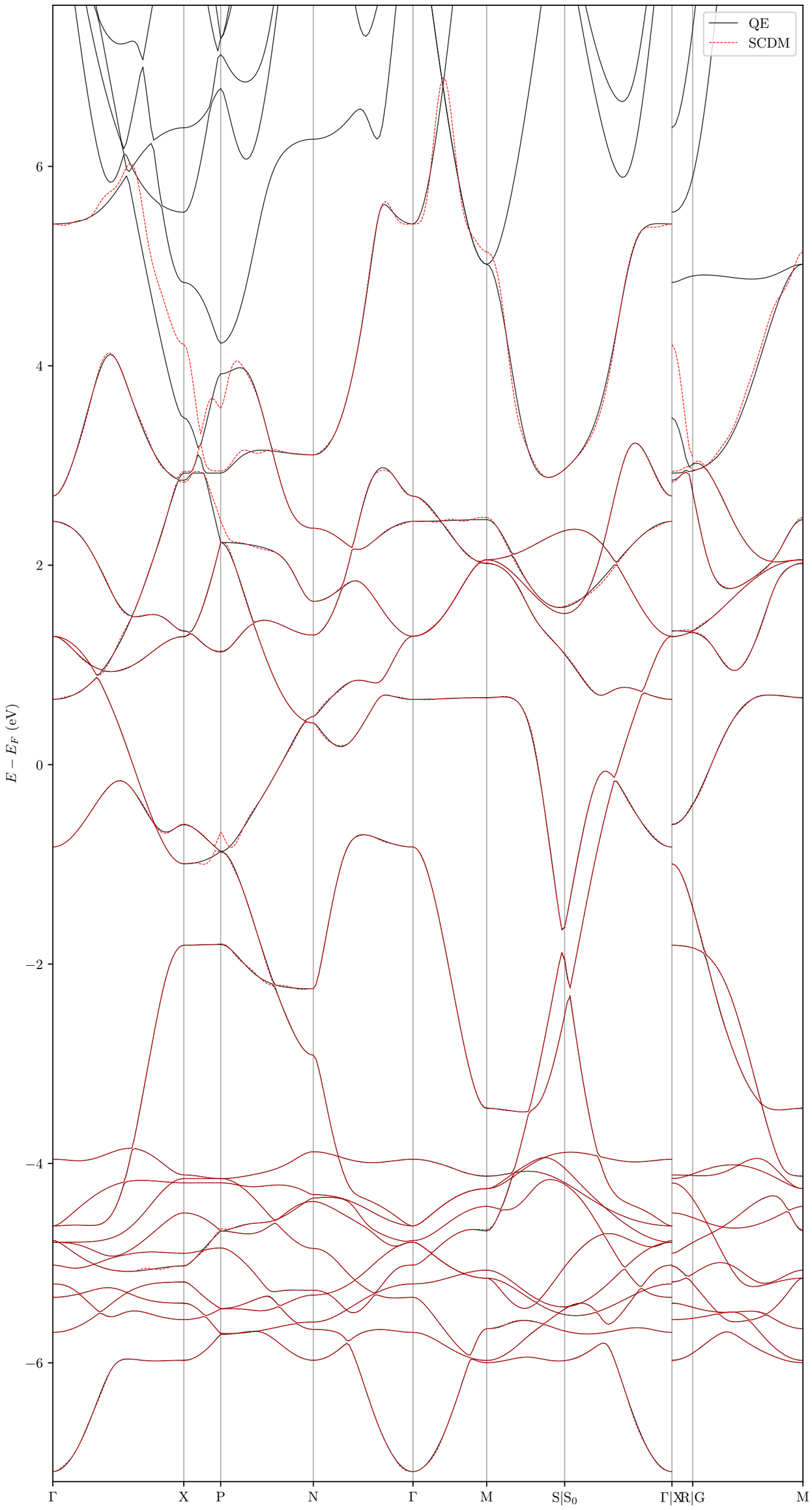
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.4 | 8.4 | 9.1 | 72.6 | 72.6 | 72.6 | 2.522 |





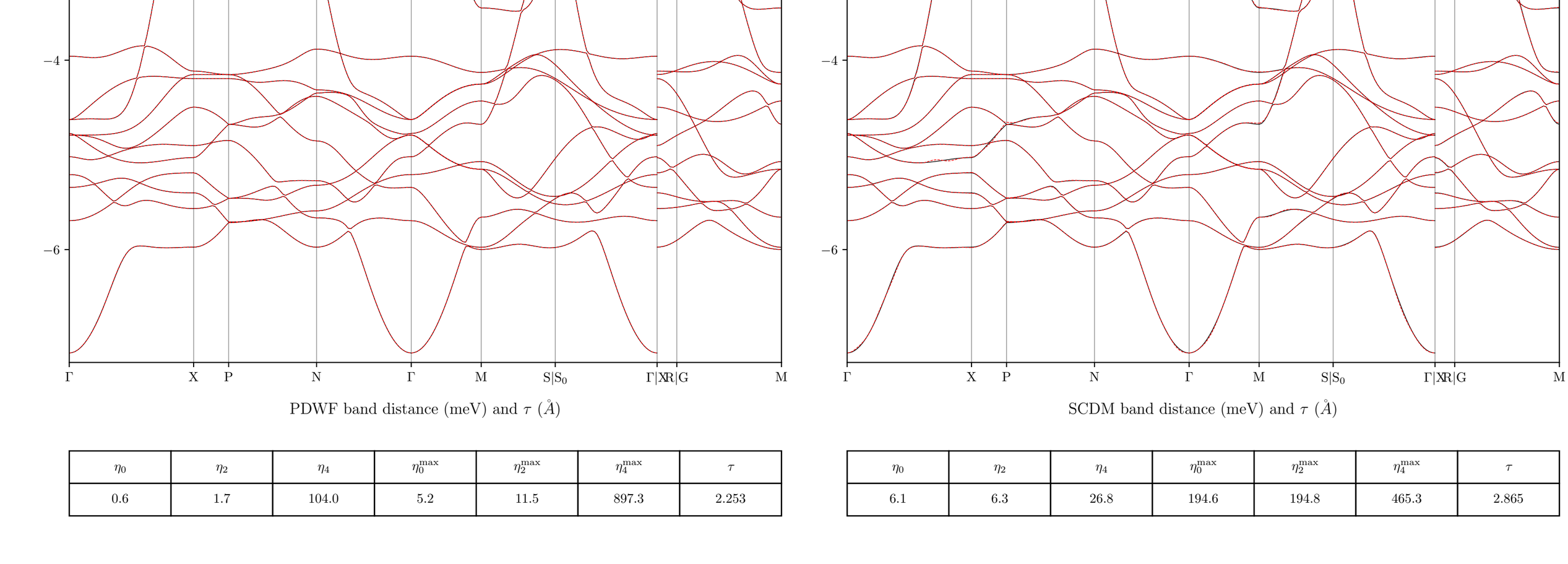

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

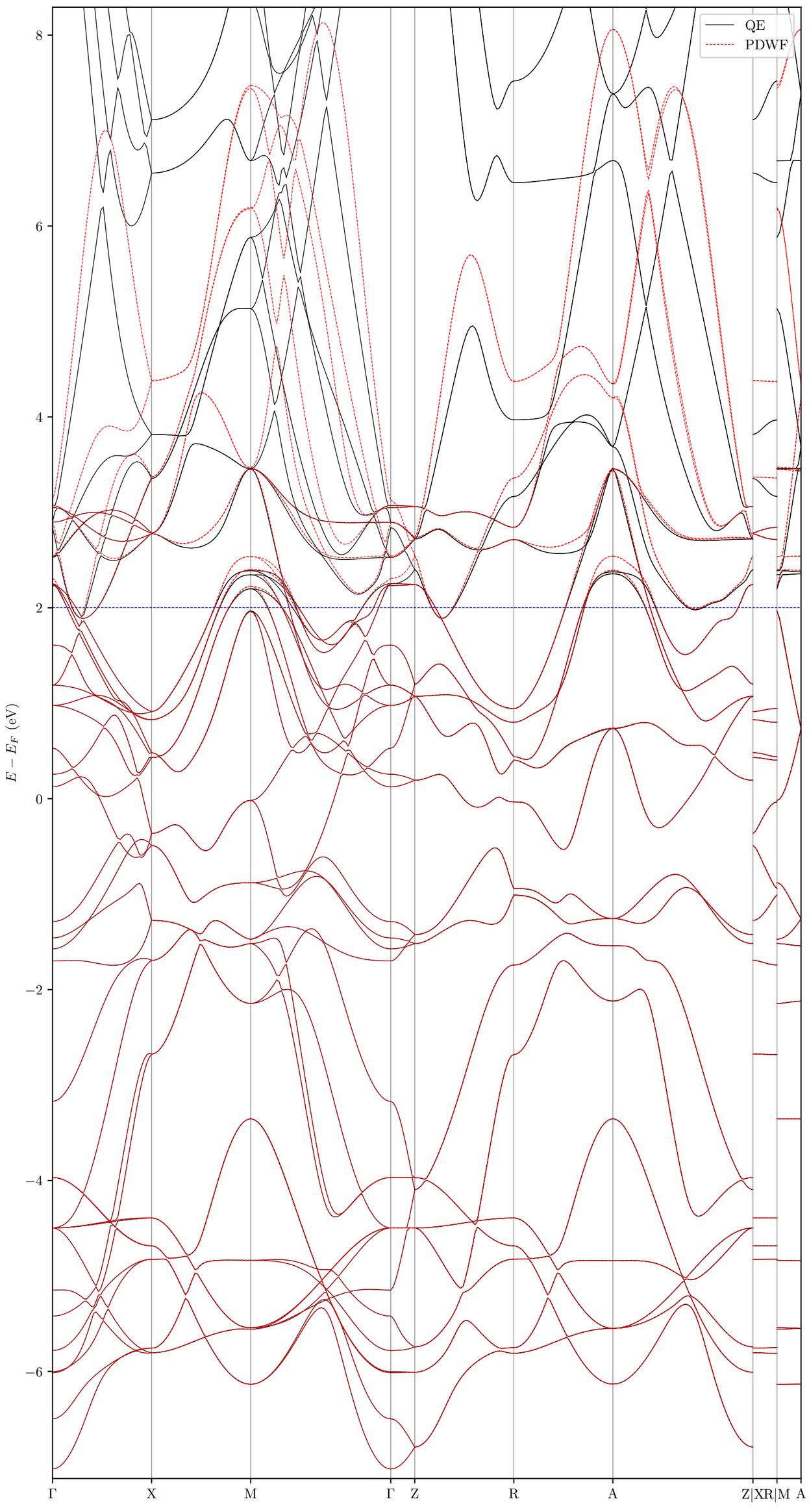
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 1.7 | 104.0 | 5.2 | 11.5 | 897.3 | 2.253 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

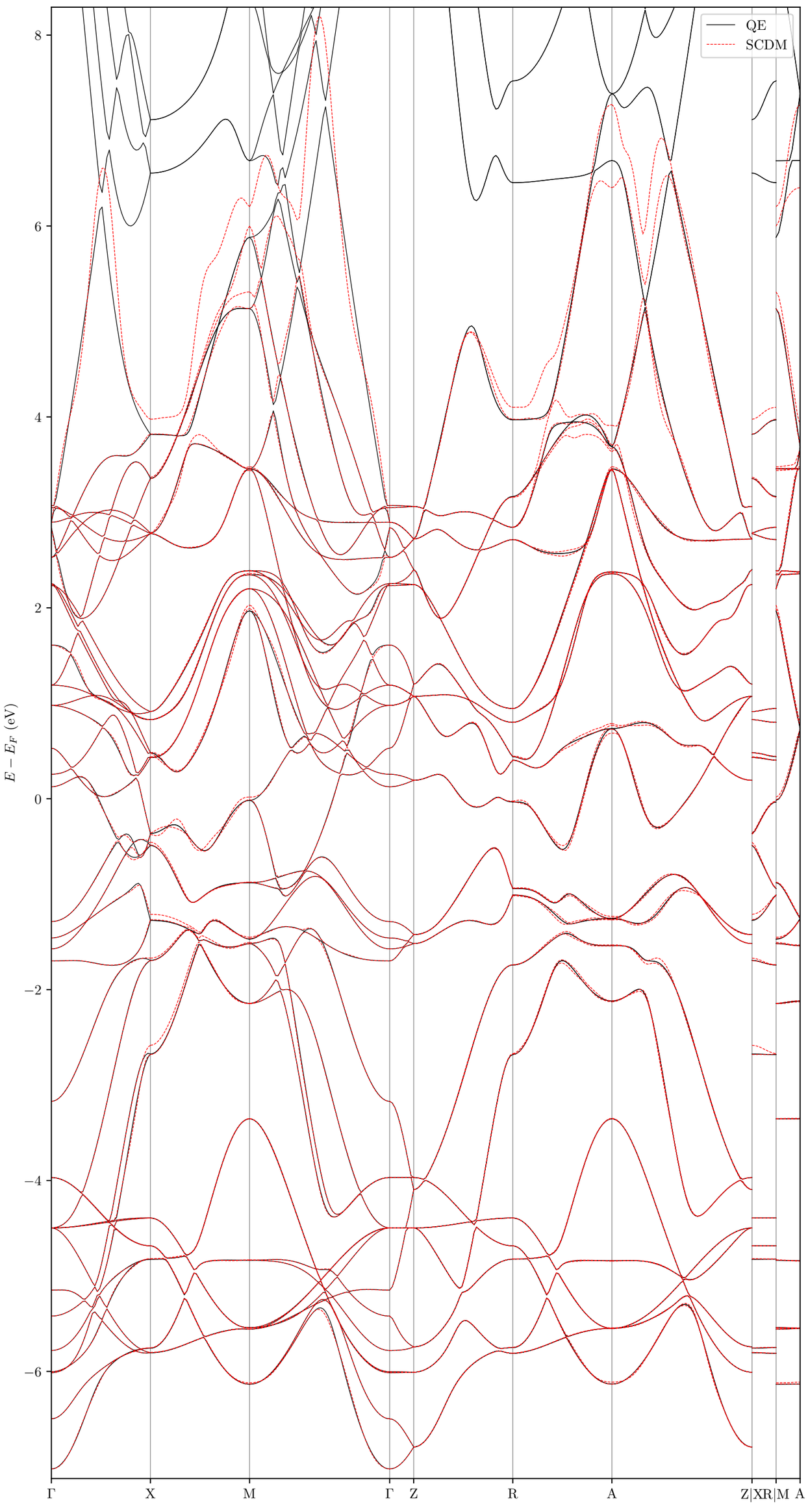
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.1 | 6.3 | 26.8 | 194.6 | 194.8 | 465.3 | 2.865 |





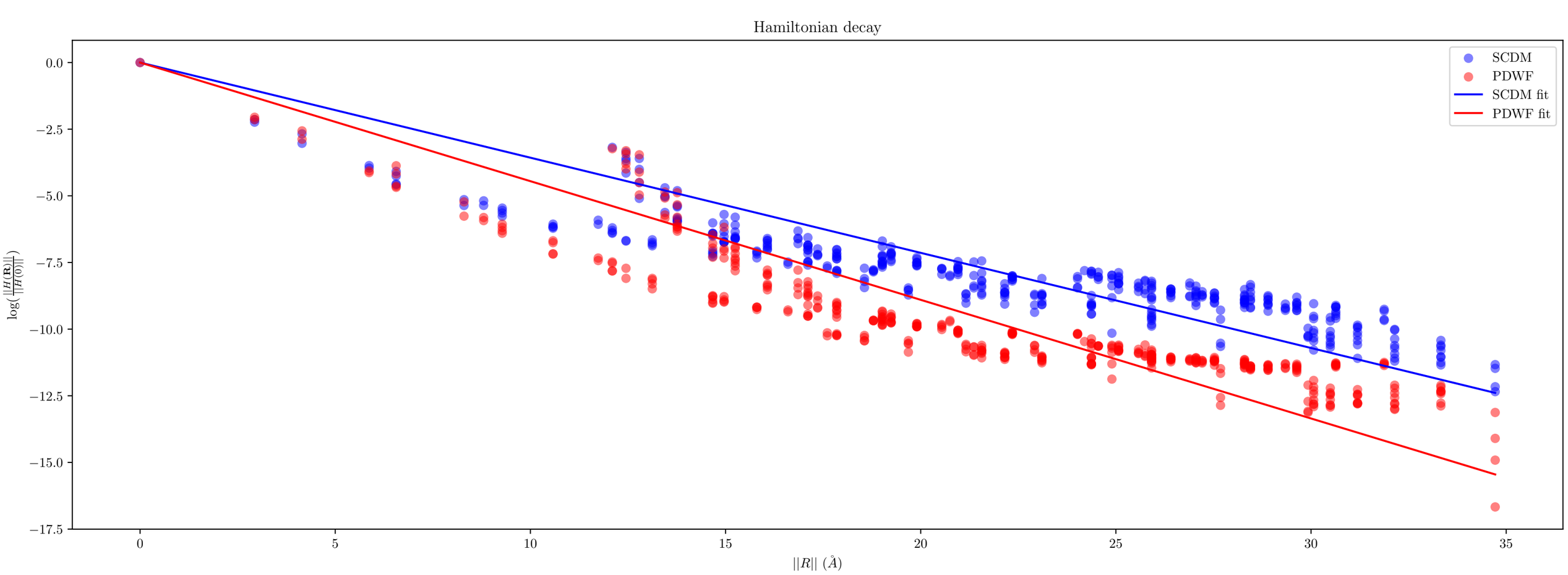

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 3.3 | 61.1 | 3.7 | 23.3 | 510.1 | 2.247 |

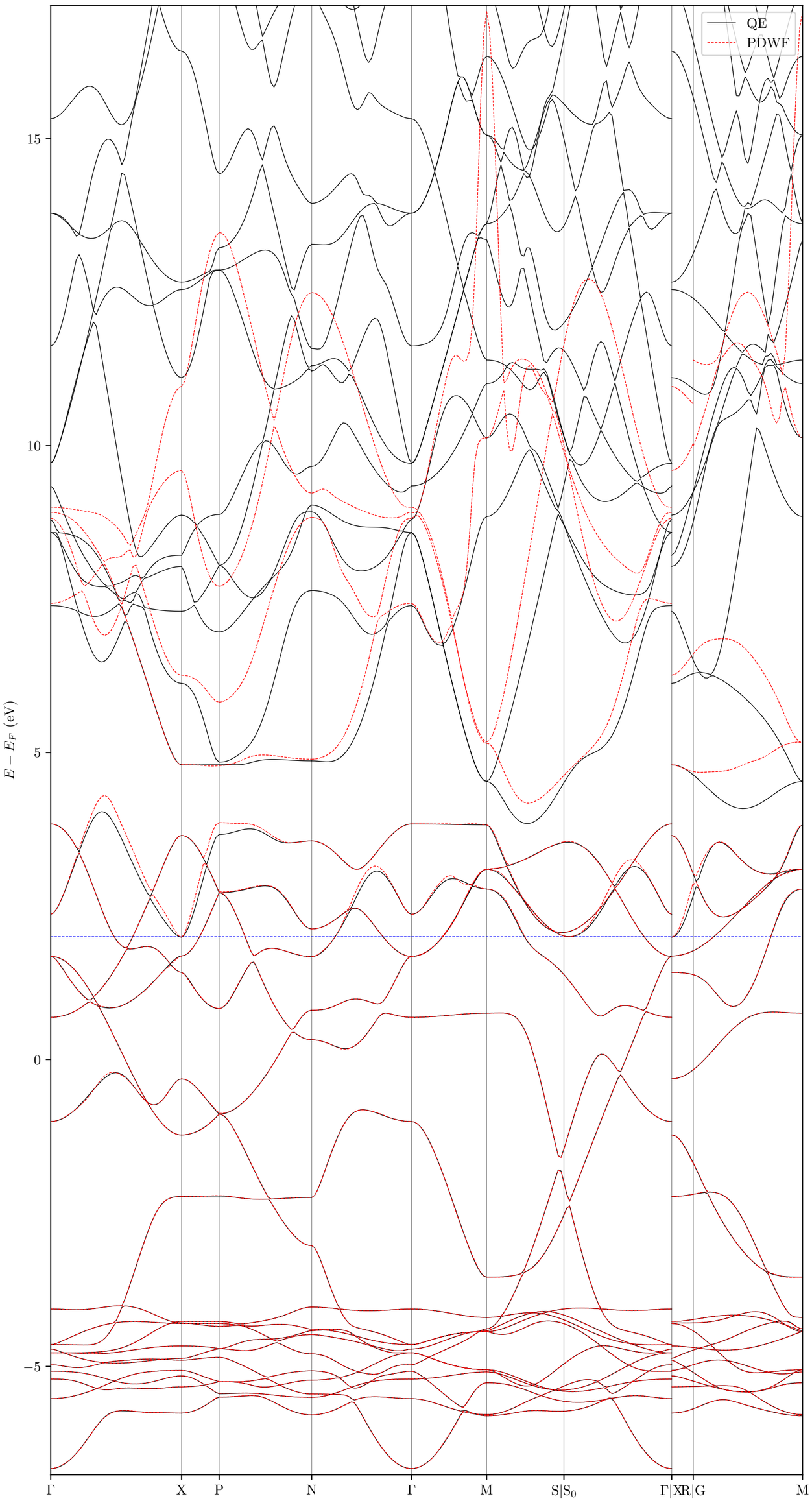



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 10.4 | 10.4 | 16.7 | 91.6 | 91.6 | 185.0 | 2.802 |



Ag2Y exclude semicore
PW=b0c80941-8e0f-4e60-a879-722d2391f408
W90=1cdcdb0e-7b36-4114-89e2-96d3feb1d63a




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.3 | 3.0 | 23.0 | 32.5 | 35.0 | 237.6 | 2.687 |

Ag2Y exclude semicore
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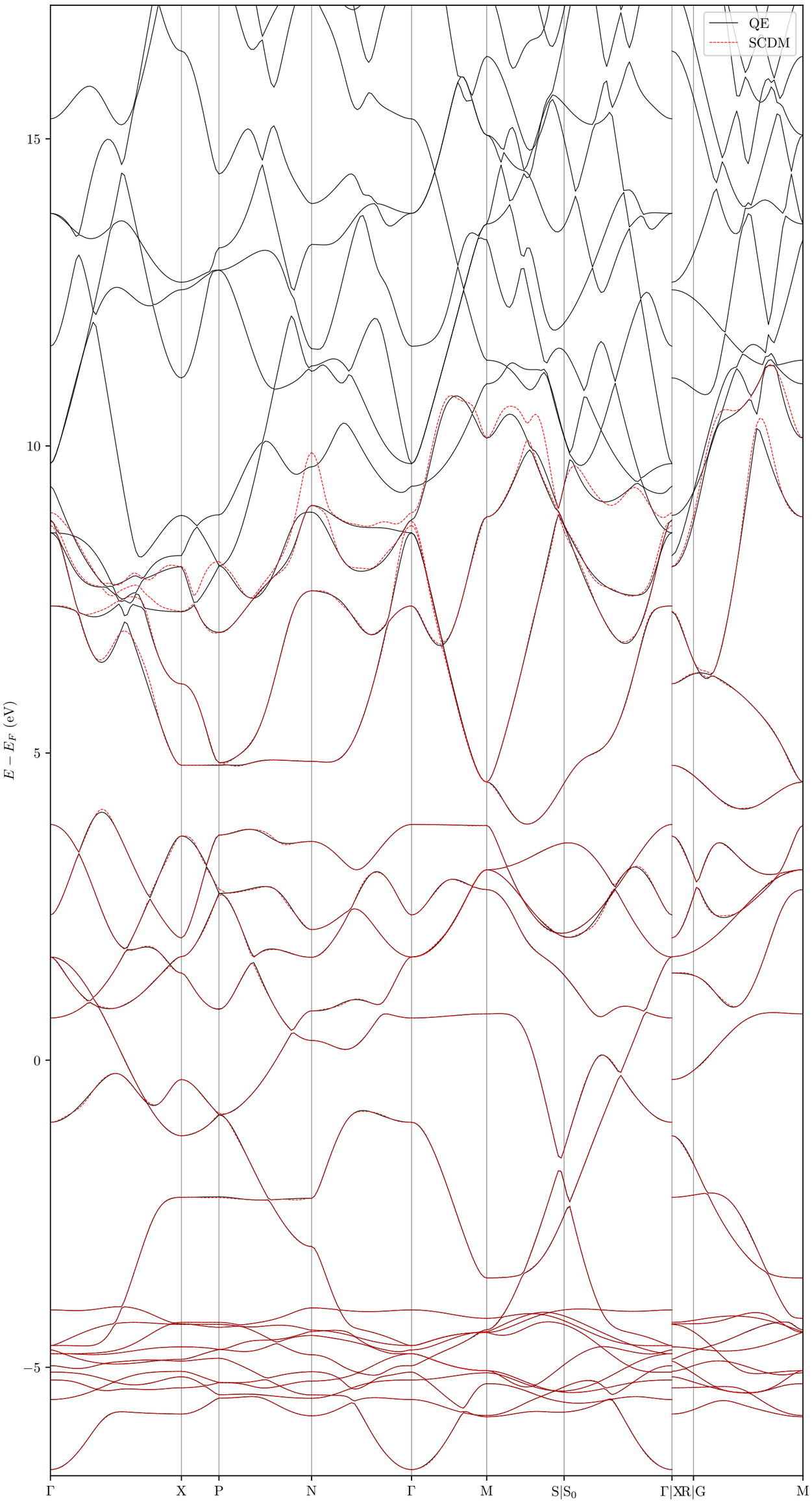
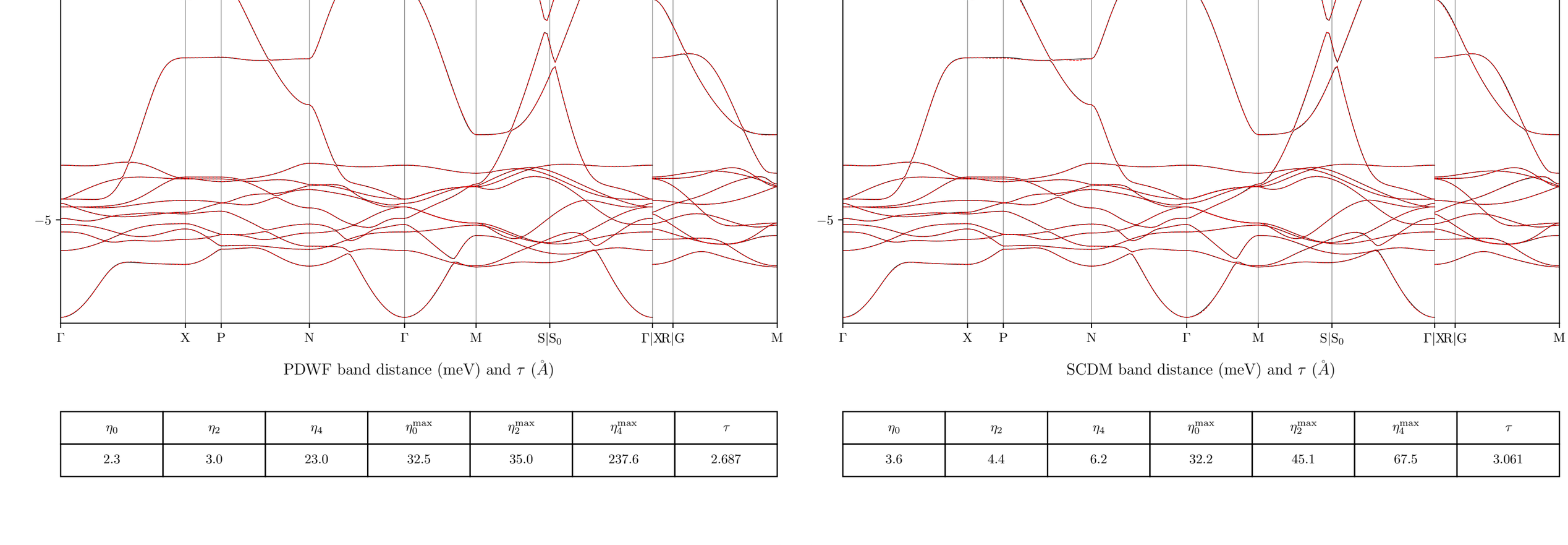
W90=1970717c-fc3a-4f87-bf11-12bd3bb71cef



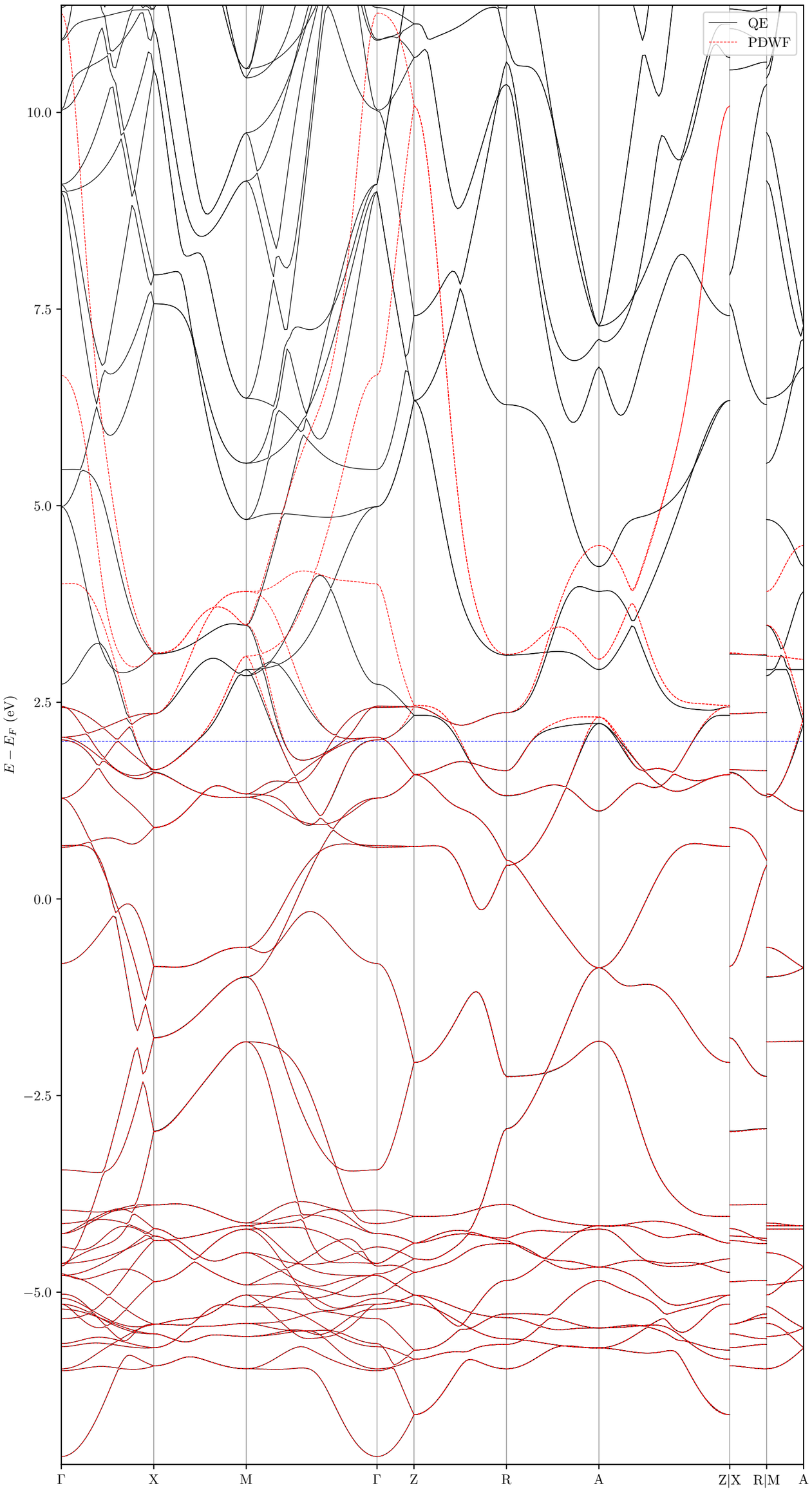

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.6 | 4.4 | 6.2 | 32.2 | 45.1 | 67.5 | 3.061 |

Hamiltonian decay



Ag4Sc2 exclude semicore
PW=e1e17472-cc96-4903-bae9-b4d19ab9d239
W90=8e593b1c-0ed0-498c-8cb7-5faff3b8a935




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.4 | 3.8 | 96.3 | 13.1 | 24.9 | 1020.0 | 1.839 |

Ag4Sc2 exclude semicore
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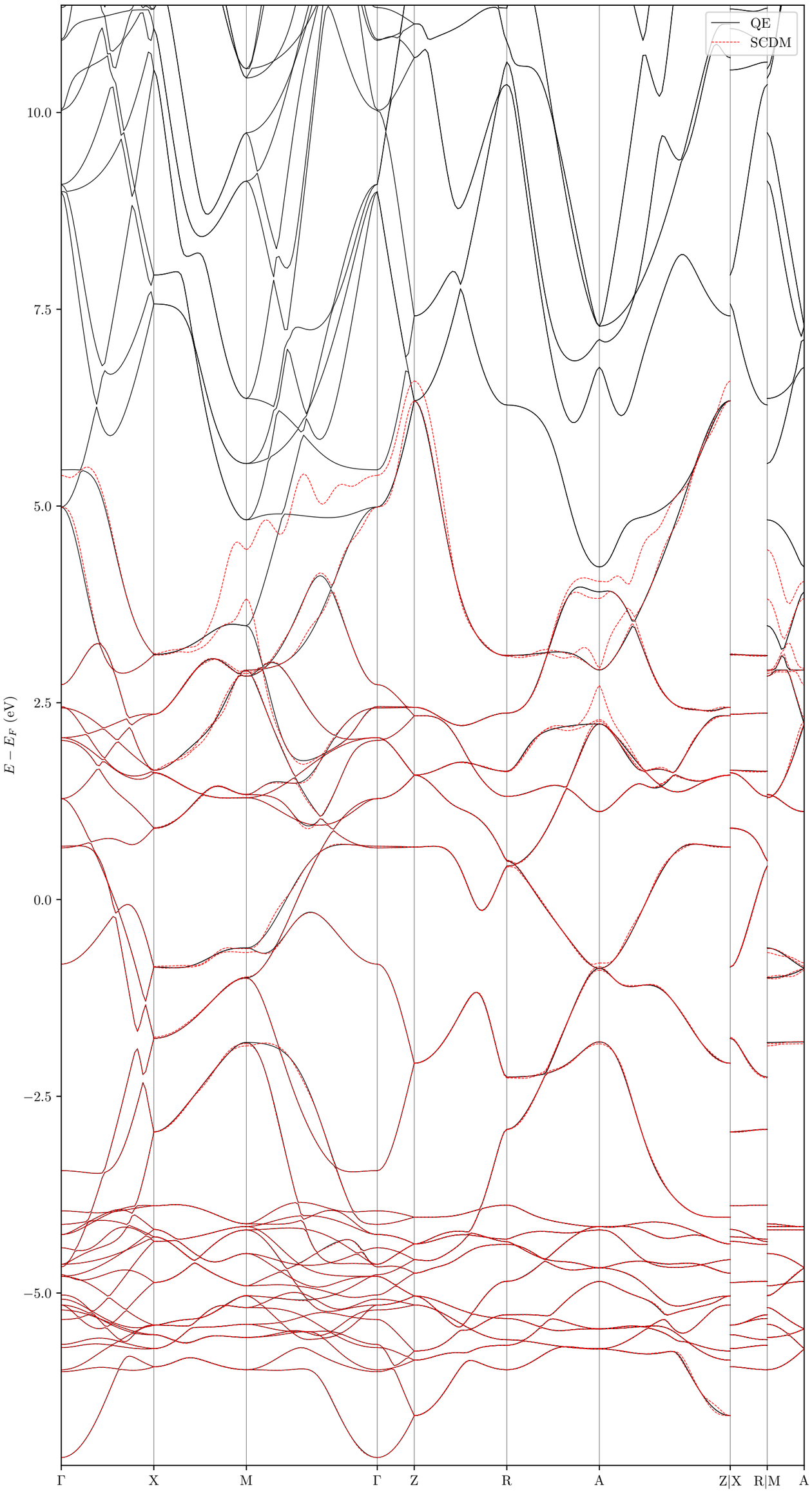
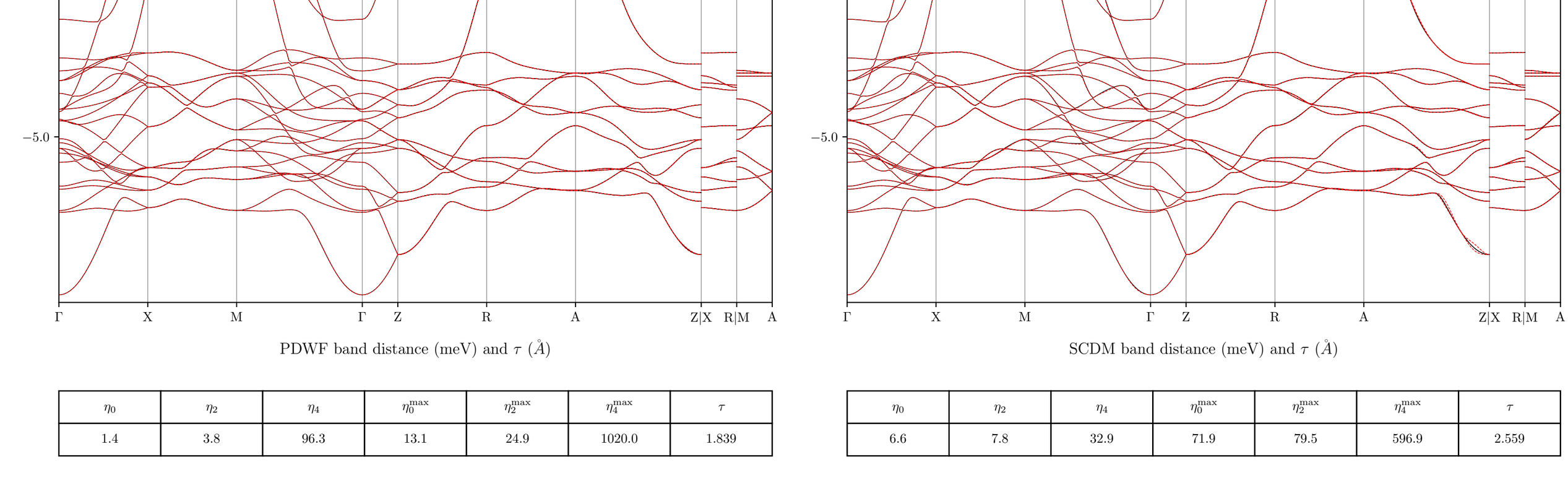
W90=effcdd96-c01e-44fa-aee2-6ff6d515177a



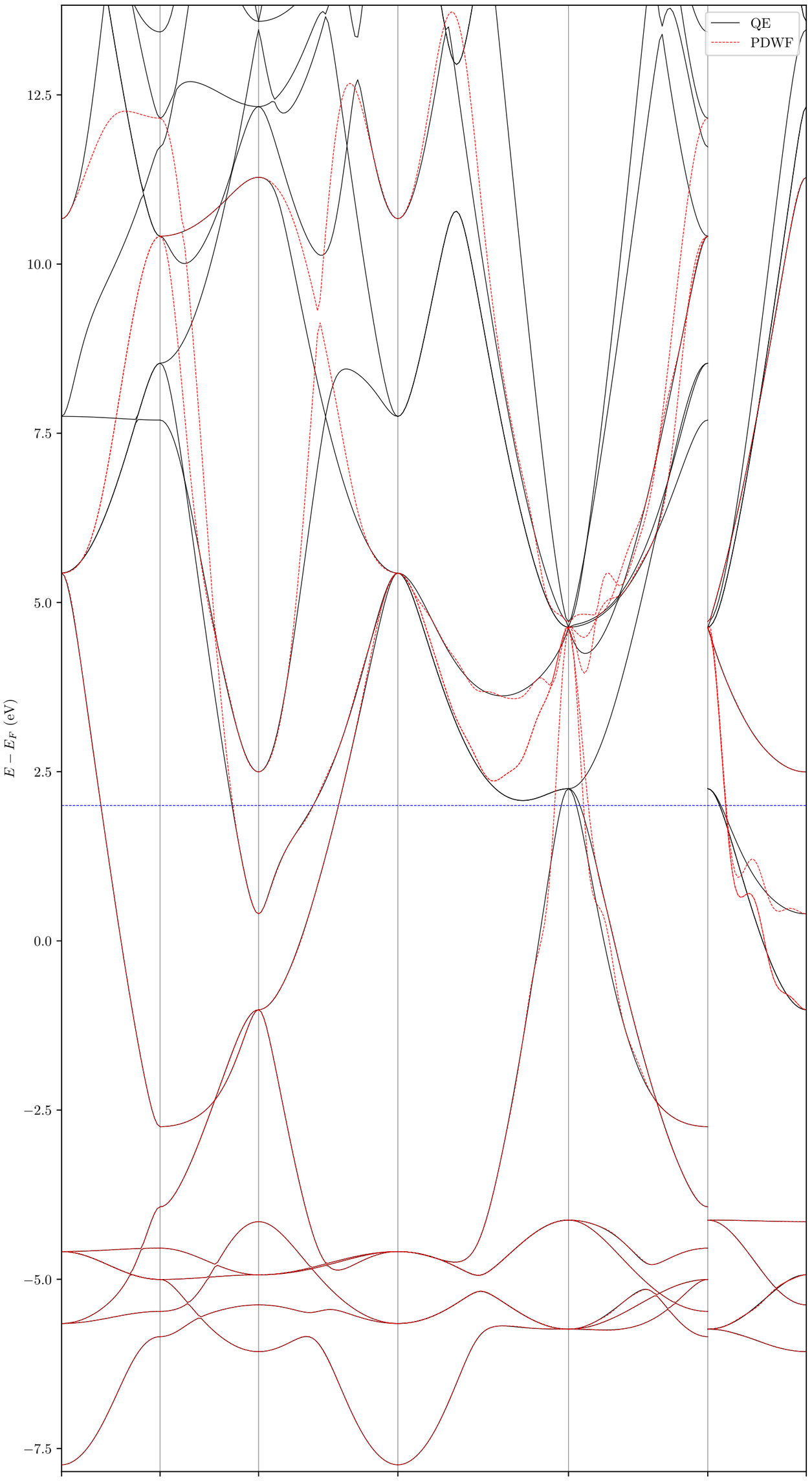

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.6 | 7.8 | 32.9 | 71.9 | 79.5 | 596.9 | 2.559 |

Hamiltonian decay



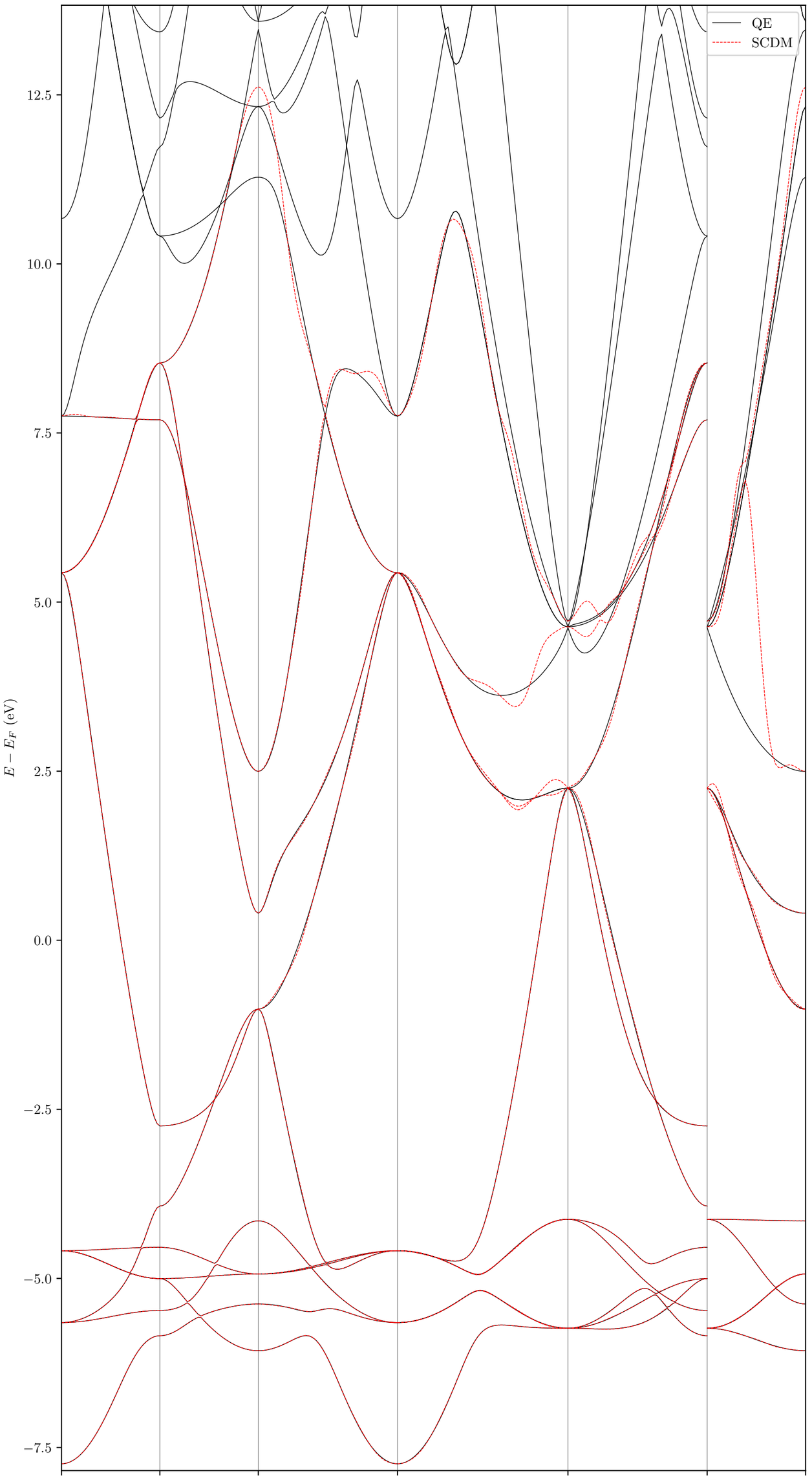
AgMg exclude semicore
PW=10a44a28-6440-4132-acff-a0900876dbea
W90=1f2dd721-9b1b-4380-89e6-cac563d5ab6d




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 18.3 | 54.7 | 226.5 | 299.4 | 501.7 | 1635.0 | 2.114 |

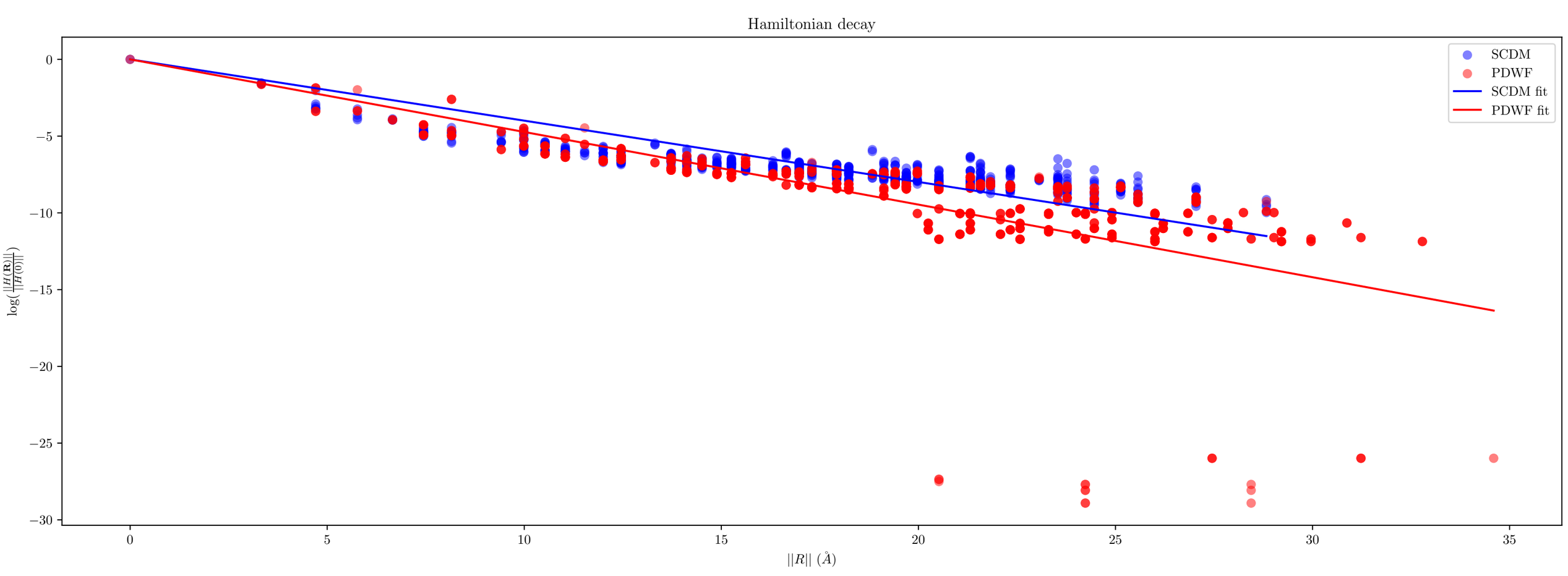
AgMg exclude semicore
PW=10a44a28-6440-4132-acff-a0900876dbea
W90=1fb20ce6-3299-44a6-a5d3-f8523af2651b



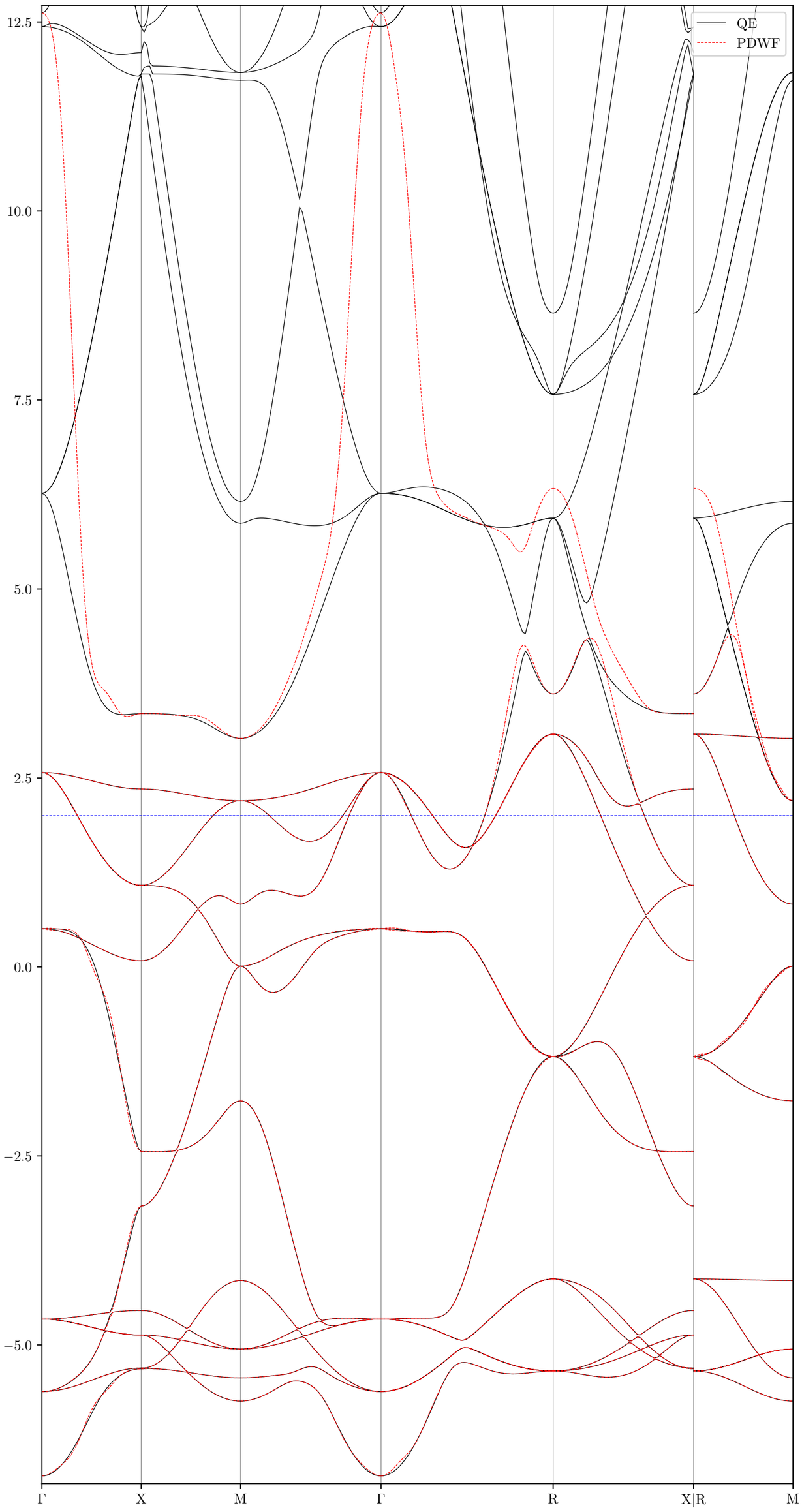

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.5 | 13.1 | 37.7 | 70.9 | 107.9 | 798.2 | 2.504 |

Hamiltonian decay



AgSc exclude semicore
PW=d0f0f226-f935-44aa-9a05-6c3ff0d42f3d
W90=8afd336d-febb-4b74-91a7-3f84376dca6c




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 9.6 | 9.0 | 32.3 | 119.2 | 119.2 | 332.7 | 2.266 |

AgSc exclude semicore
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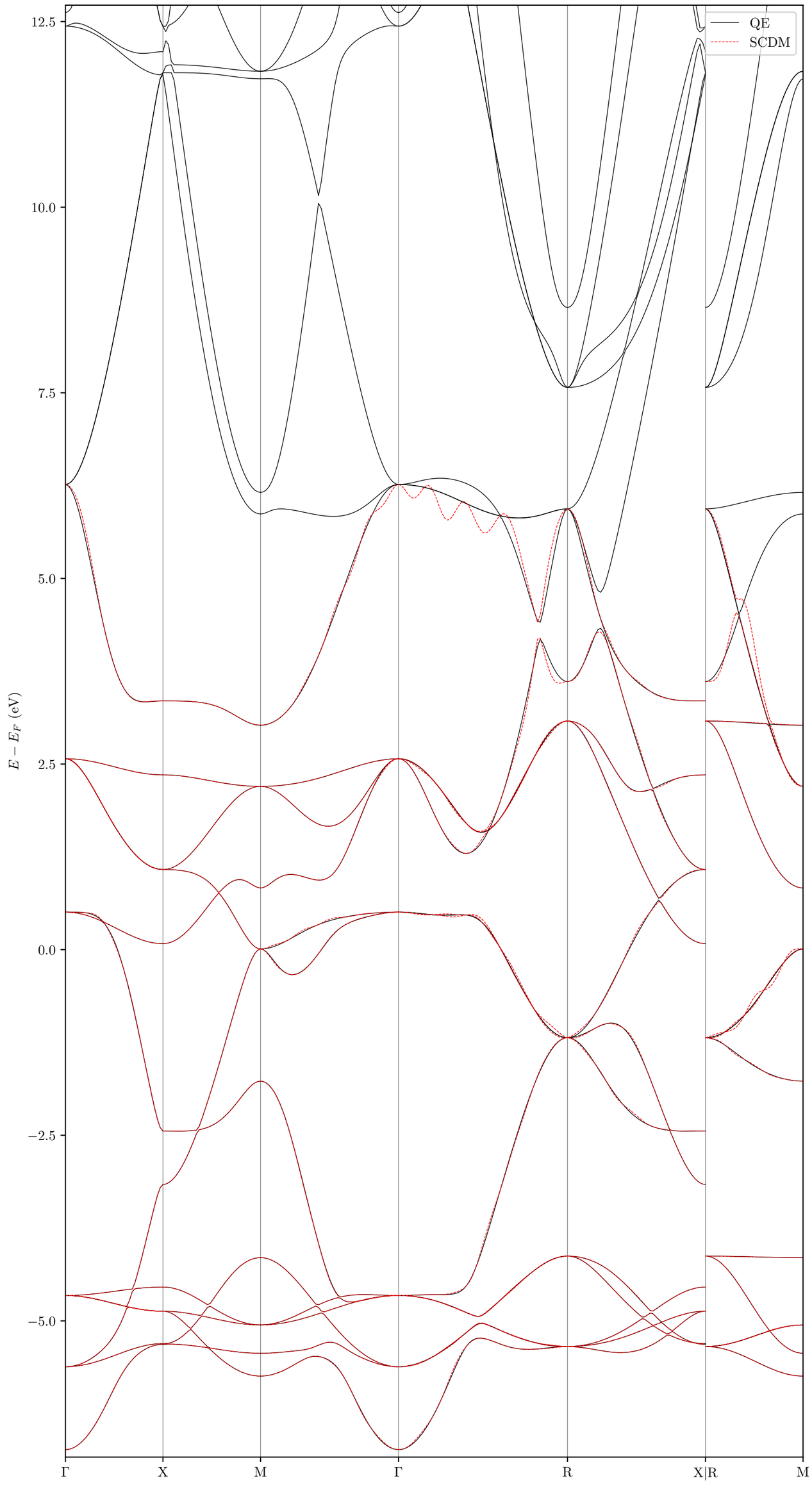
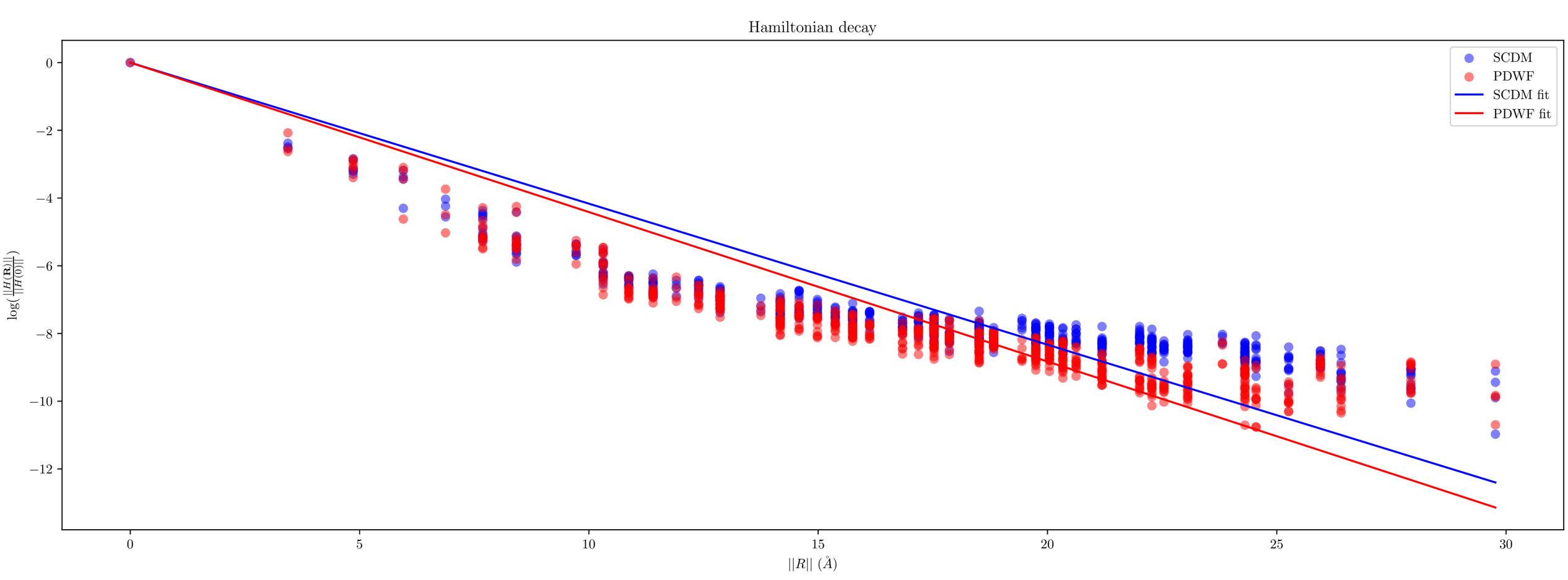
W90=54acc0be-e4fd-41fe-8701-12764888873c

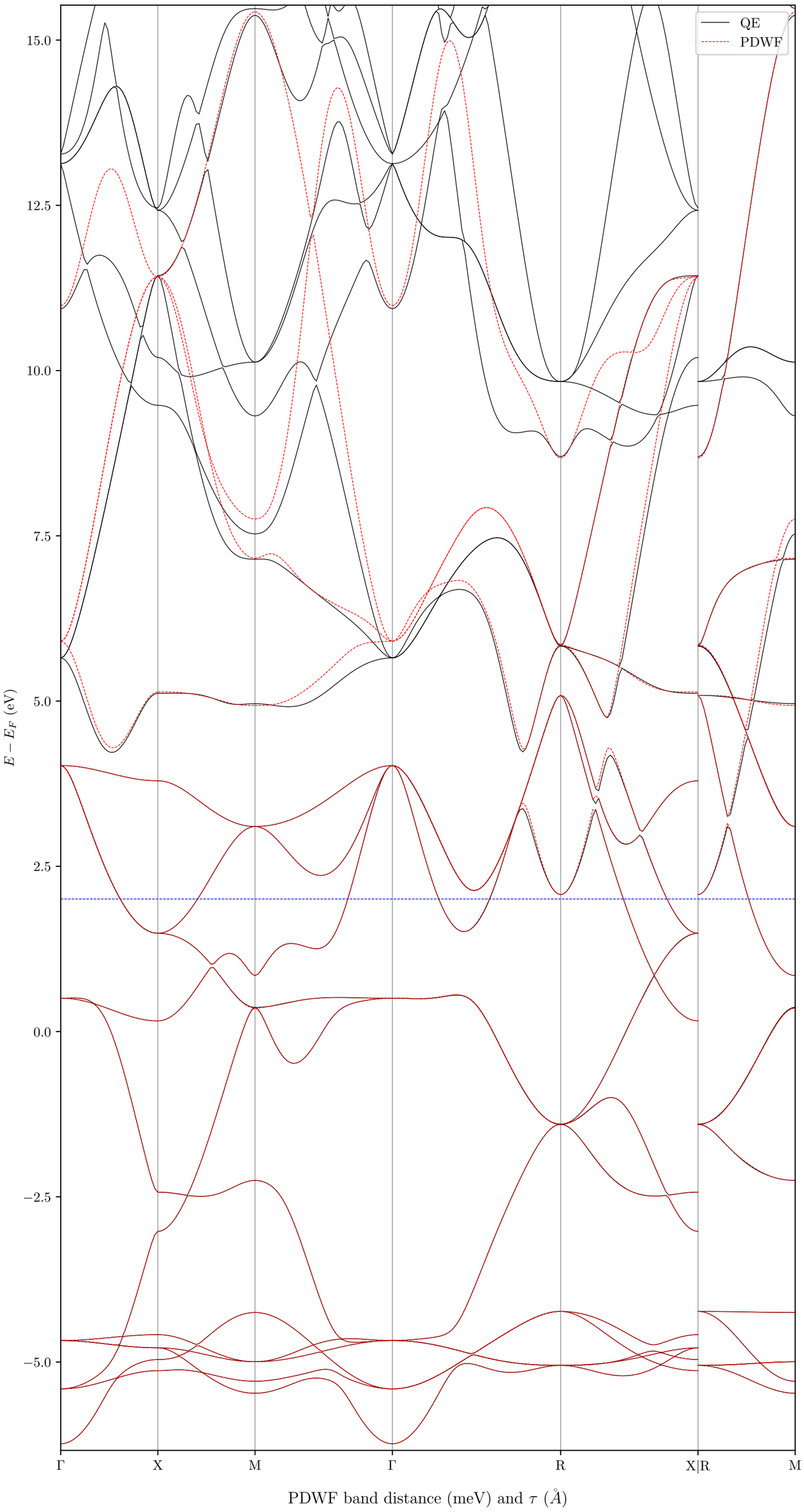



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 9.4 | 9.4 | 15.5 | 85.4 | 85.5 | 240.6 | 2.401 |

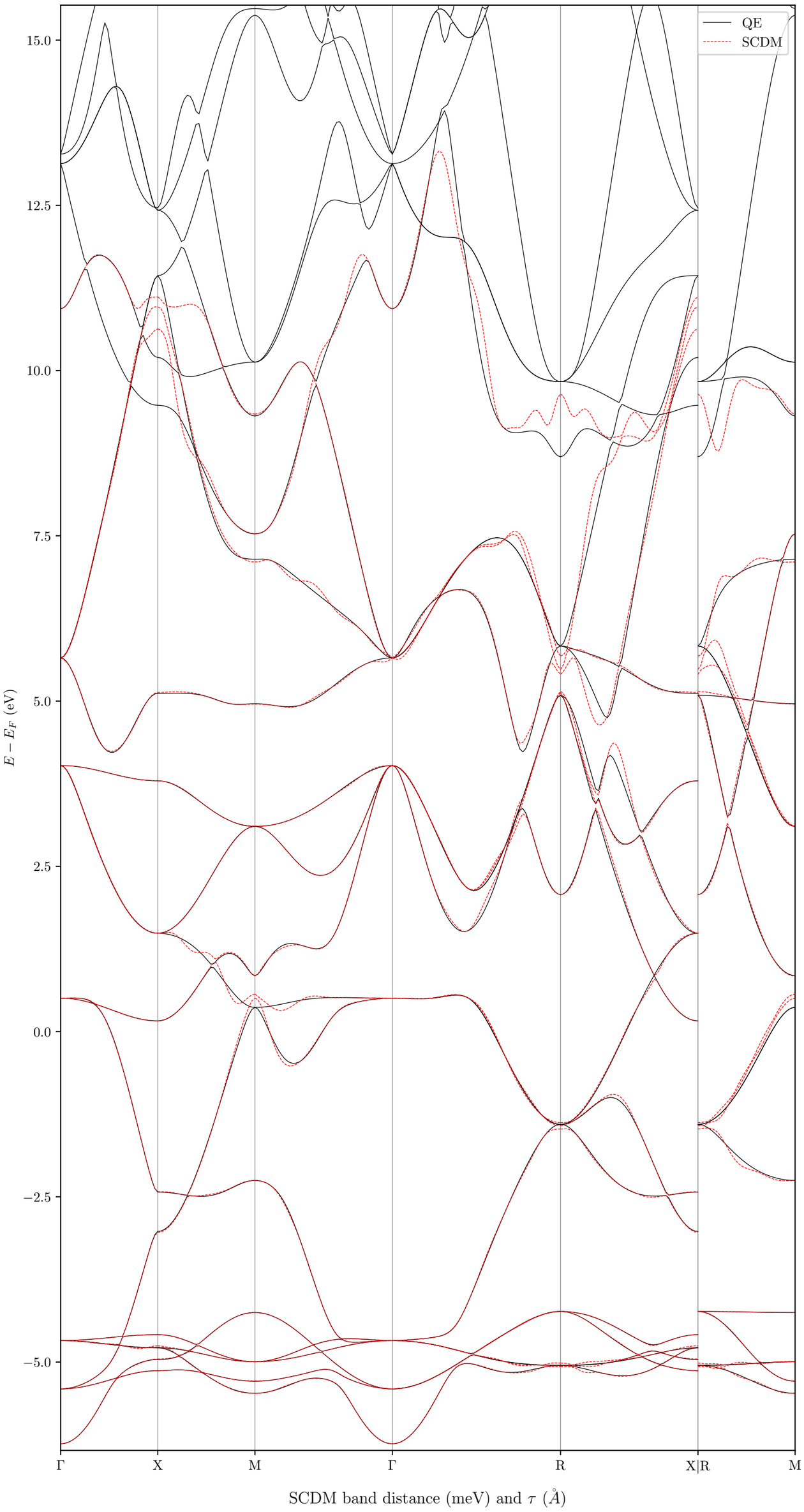
Hamiltonian decay





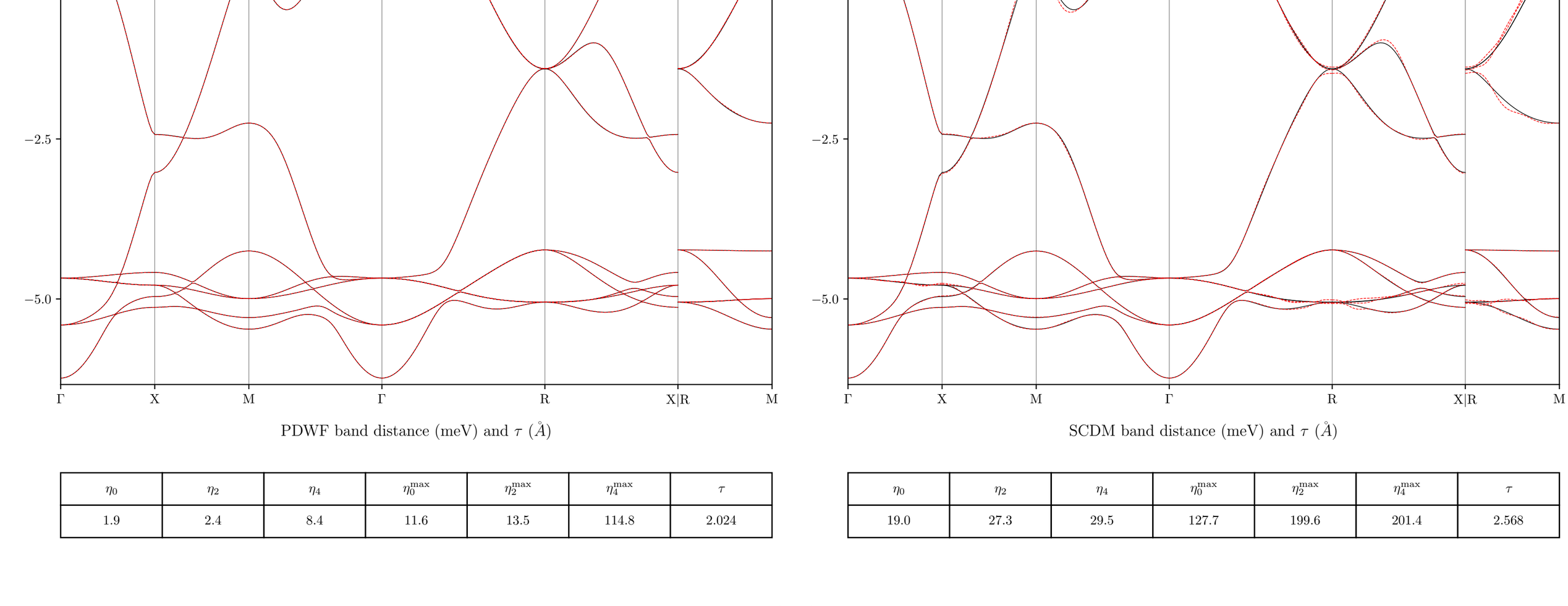

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.9 | 2.4 | 8.4 | 11.6 | 13.5 | 114.8 | 2.024 |

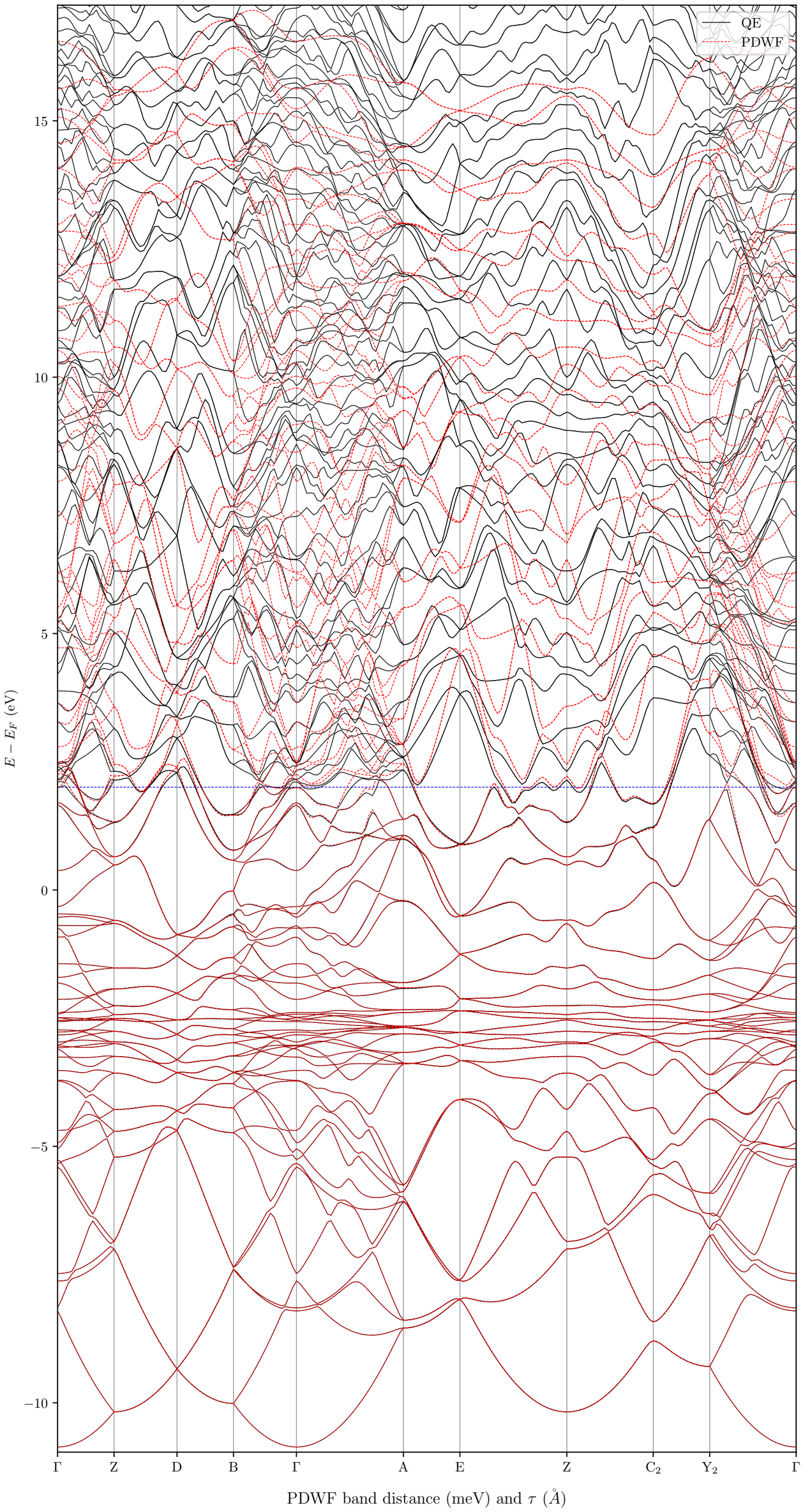



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 19.0 | 27.3 | 29.5 | 127.7 | 199.6 | 201.4 | 2.568 |



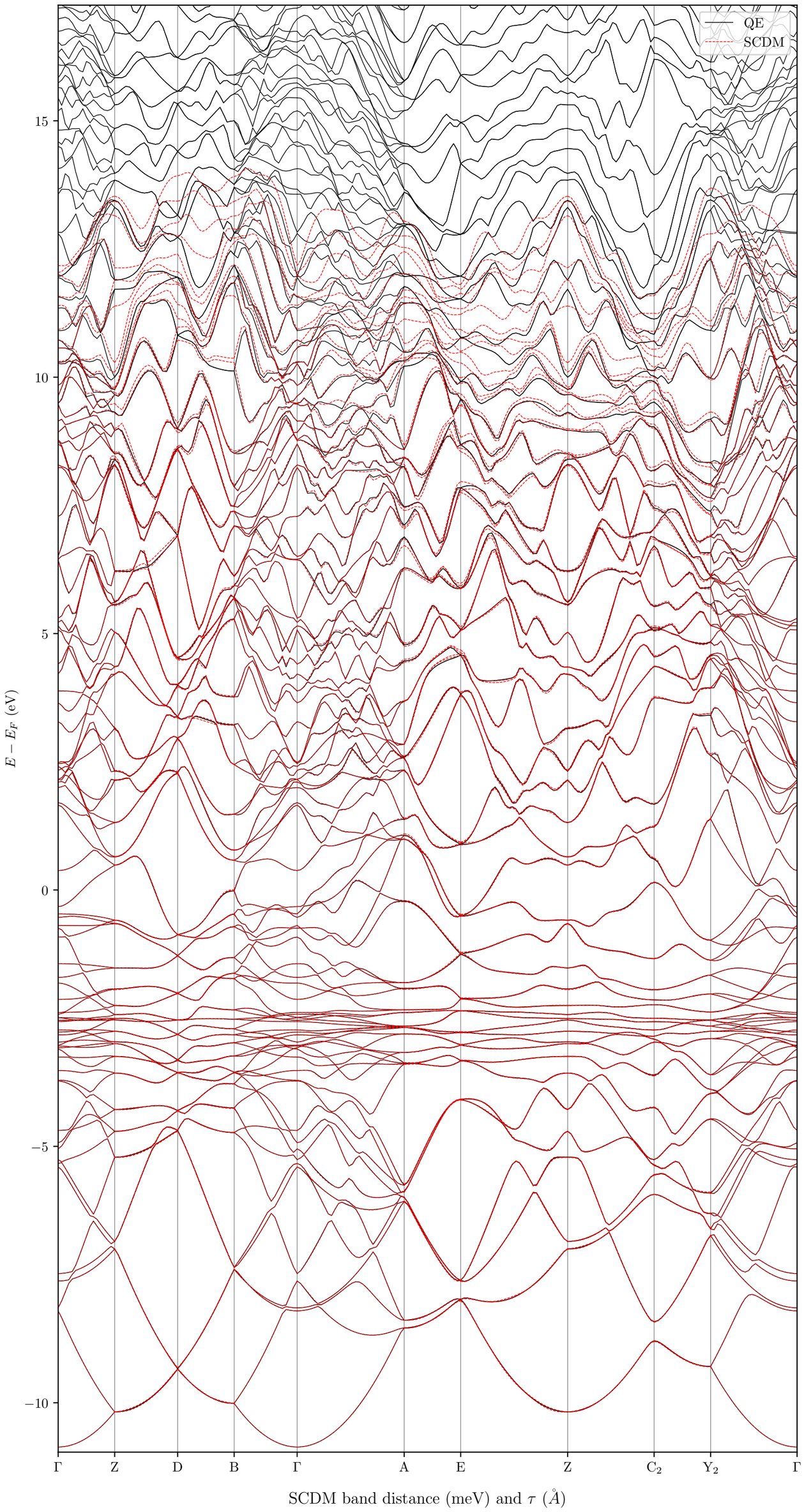
Al12Ni4 exclude semicore
PW=6e4fafe6-e27c-4934-b58a-f867c983db36
W90=29acf50d-bec3-4179-8303-1ceb75b2c296




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.4 | 9.4 | 107.3 | 25.5 | 156.0 | 585.9 | 2.710 |

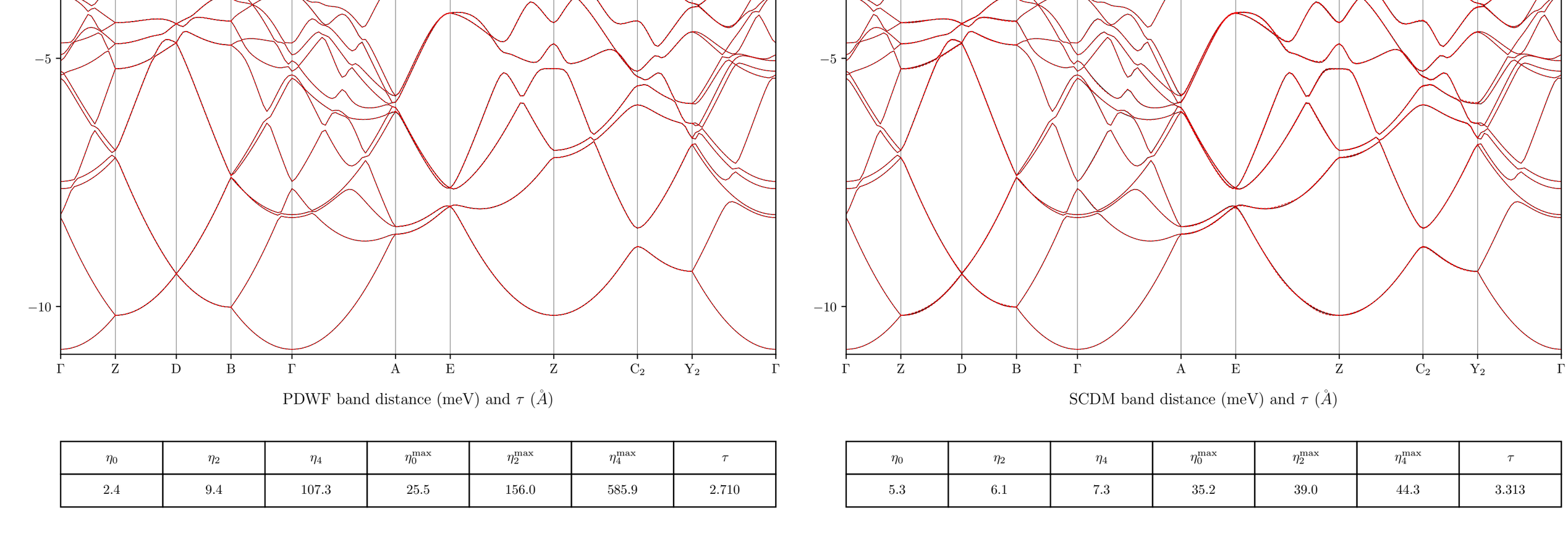
Al12Ni4 exclude semicore
PW=6e4fafe6-e27c-4934-b58a-f867c983db36
W90=1e75622d-6870-4925-bfd8-756df6fa31ae



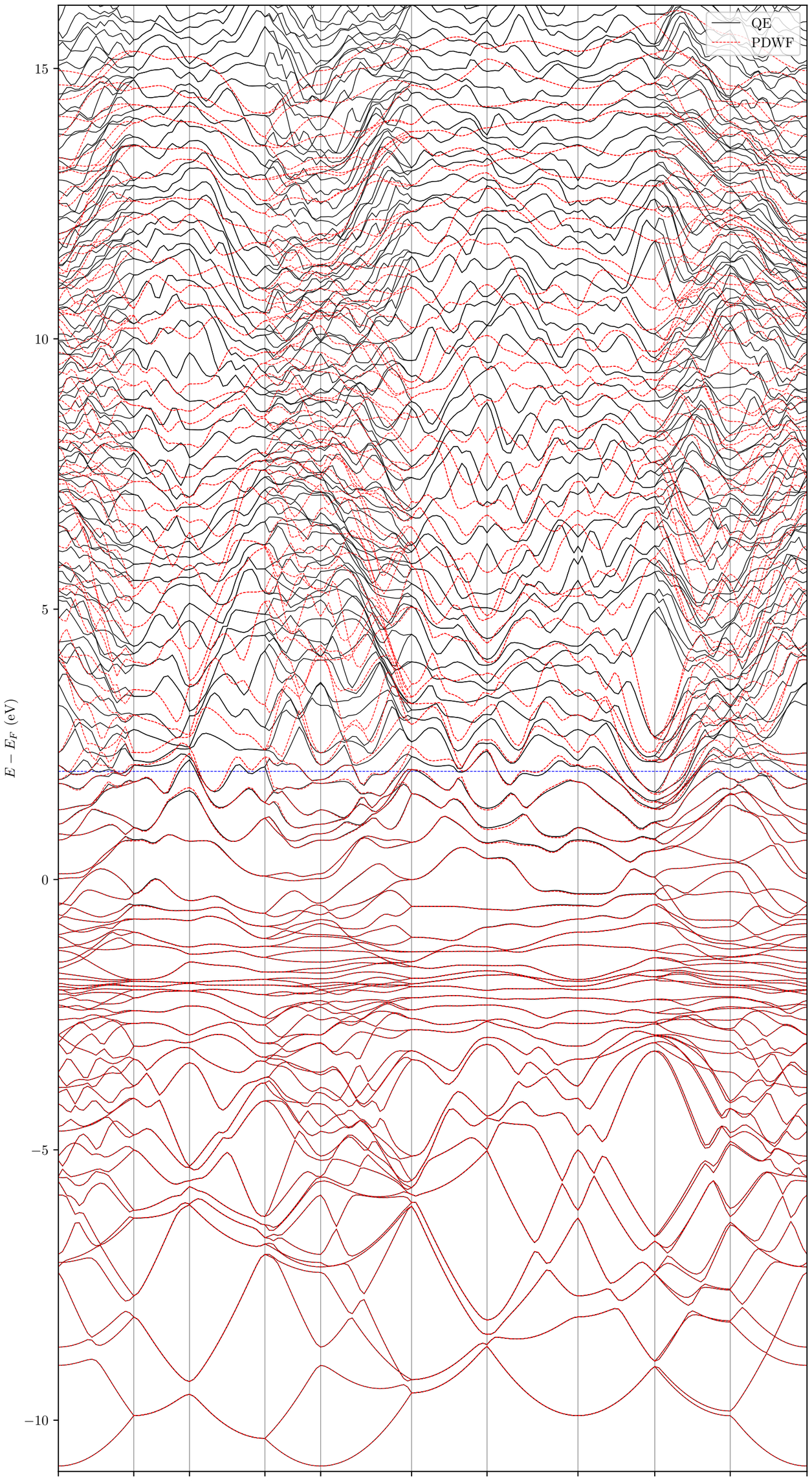

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.3 | 6.1 | 7.3 | 35.2 | 39.0 | 44.3 | 3.313 |

Hamiltonian decay



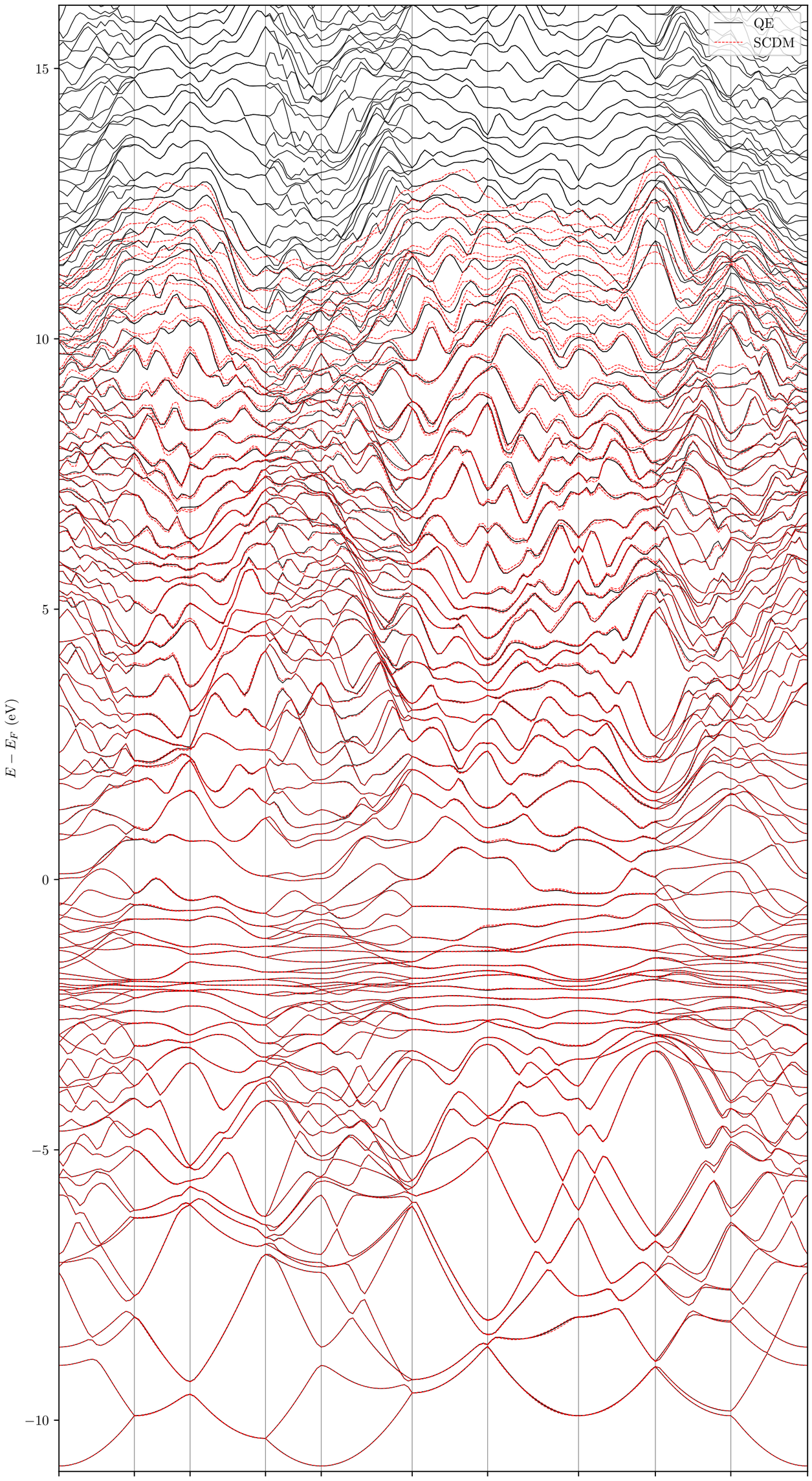
Al18Co4 exclude semicore
PW=a5f2af16-cdc9-4b4e-9aea-07139c9c009f
W90=96633496-49c0-4fc1-929c-c3ad2da0a33e




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.1 | 9.9 | 122.5 | 15.7 | 96.3 | 686.7 | 2.751 |

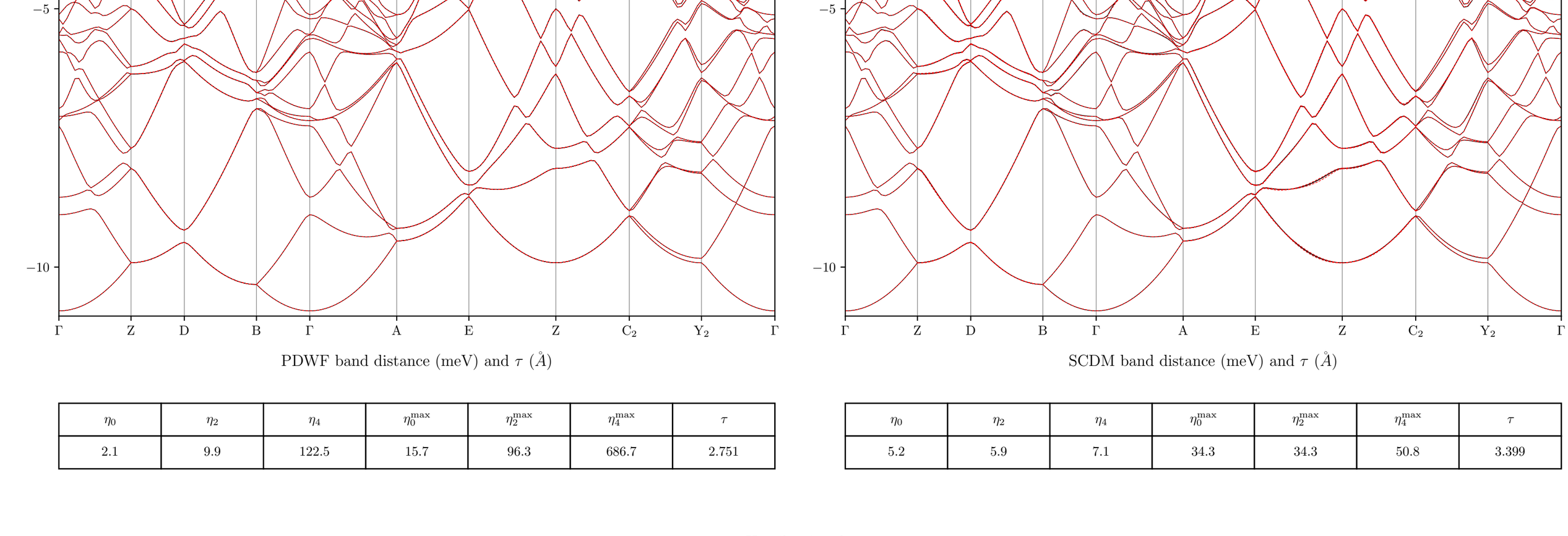
Al18Co4 exclude semicore
PW=a5f2af16-cdc9-4b4e-9aea-07139c9c009f
W90=ac6f8c26-36d9-4bc6-ae38-dffeb3d7ff33



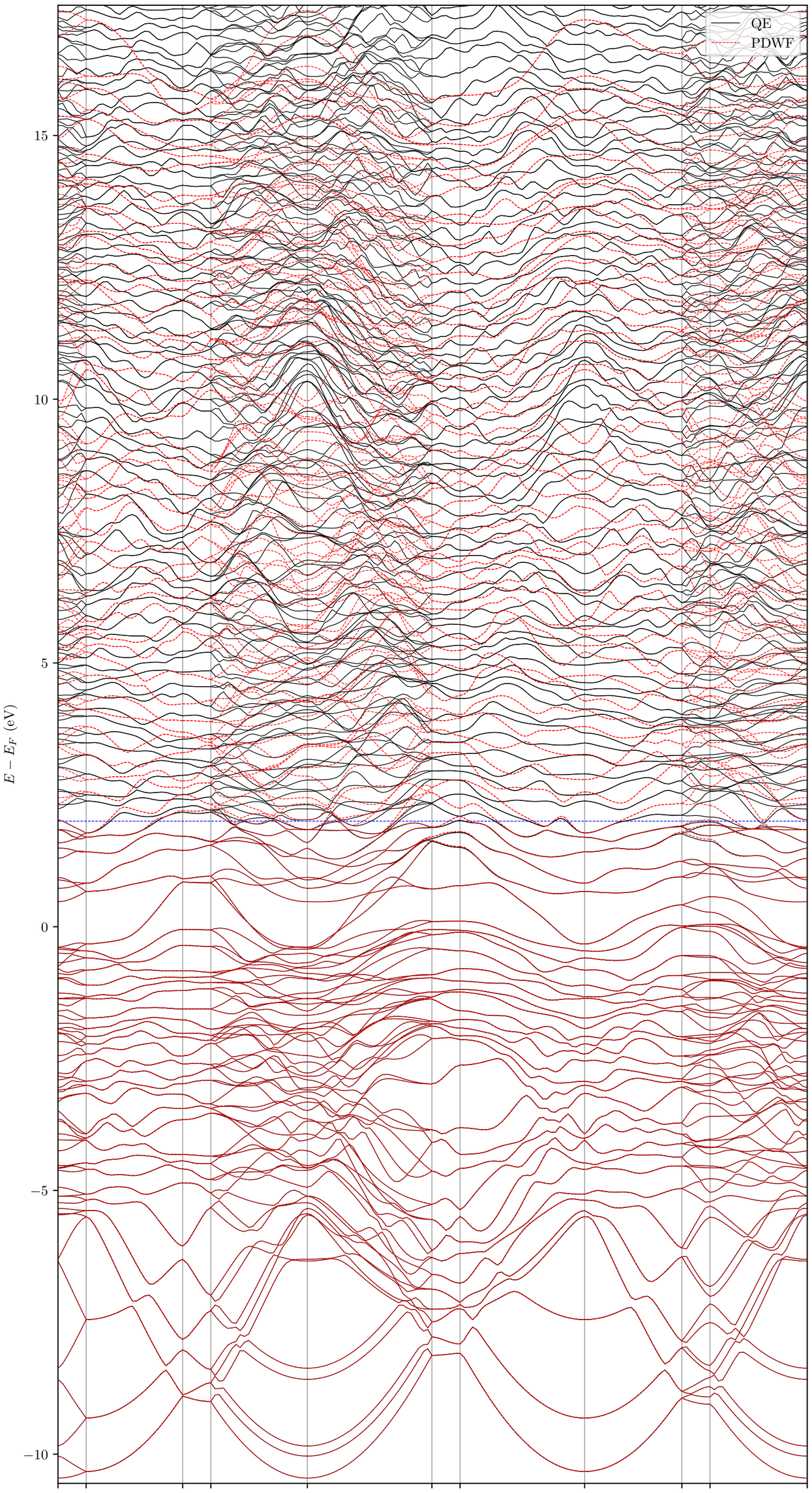

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.2 | 5.9 | 7.1 | 34.3 | 34.3 | 50.8 | 3.399 |

Hamiltonian decay



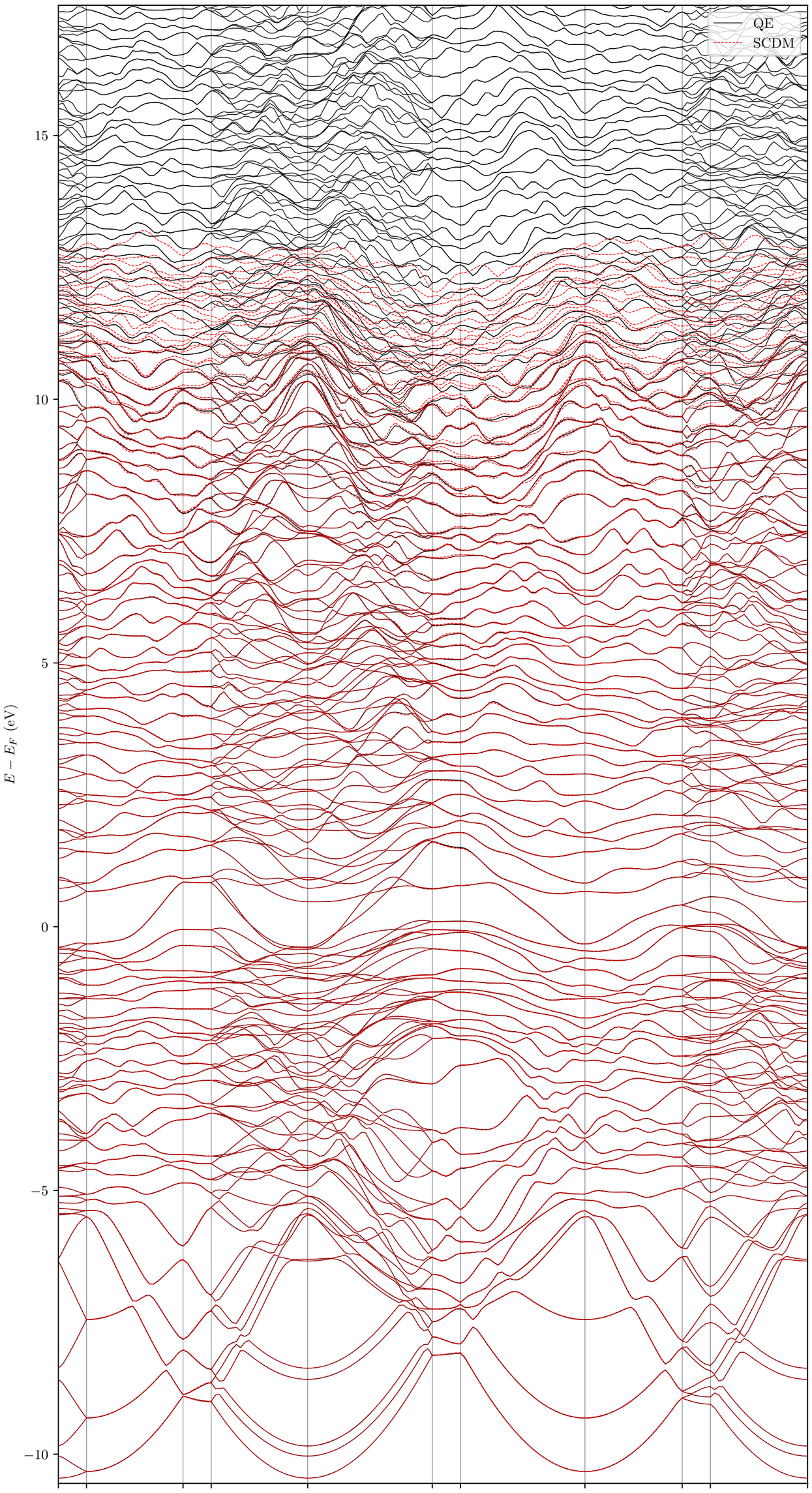
Al24W6 exclude semicore
PW=ddfd66fc-ade4-4304-8139-b9420f55354b
W90=f9bcdcb3-ce58-4501-9c1f-51049c7d5893




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.9 | 7.7 | 166.4 | 5.6 | 37.9 | 636.6 | 2.753 |

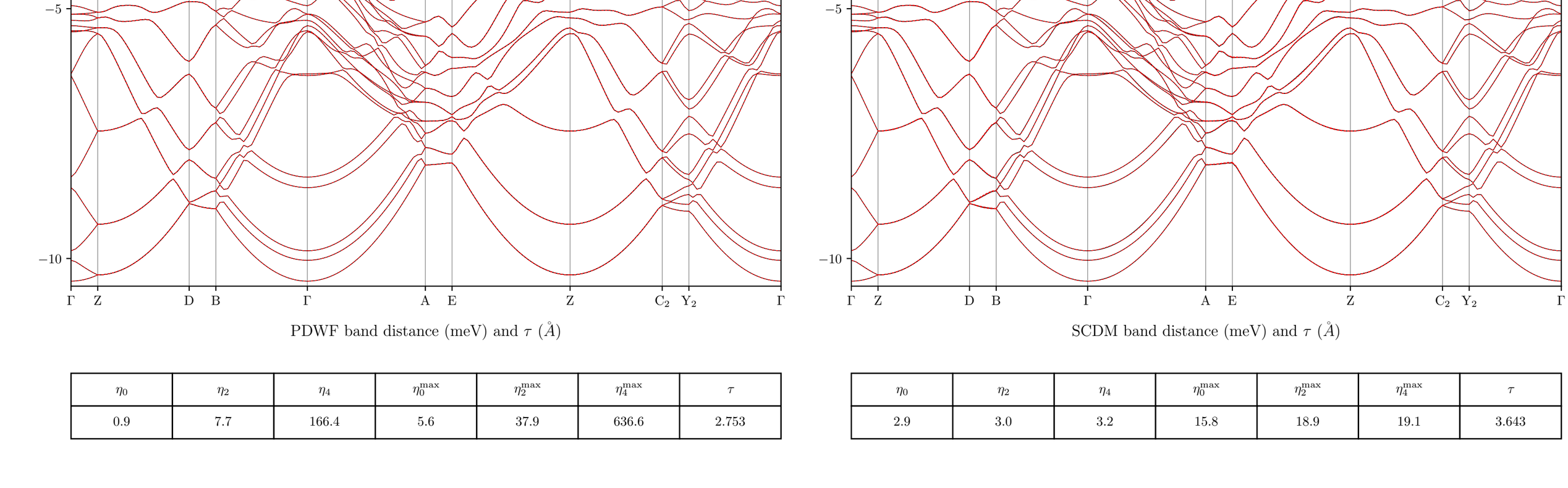
Al24W6 exclude semicore
PW=ddfd66fc-ade4-4304-8139-b9420f55354b
W90=0fe997db-27af-401c-8451-4c5d6fba8de6



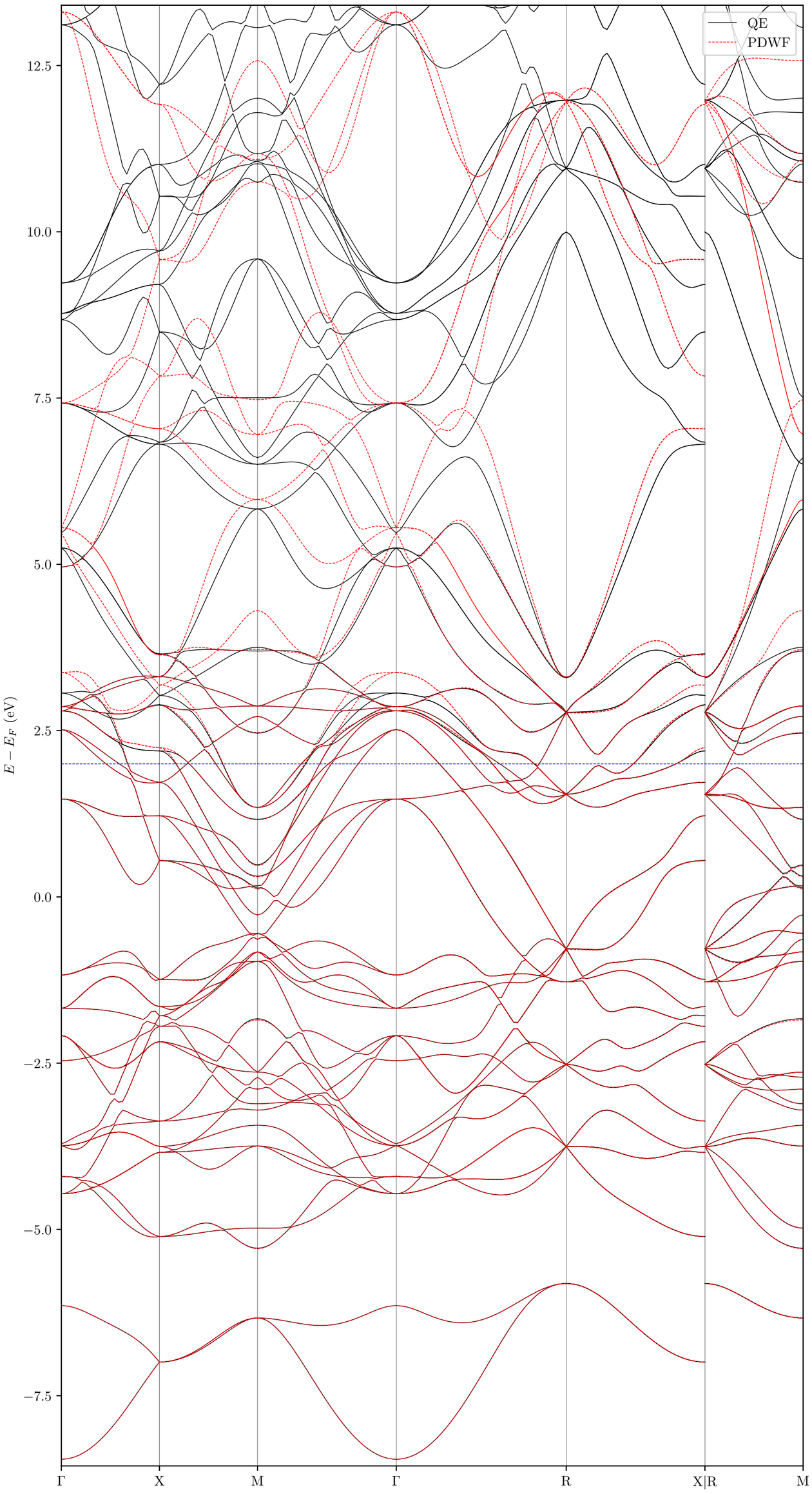

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.9 | 3.0 | 3.2 | 15.8 | 18.9 | 19.1 | 3.643 |

Hamiltonian decay



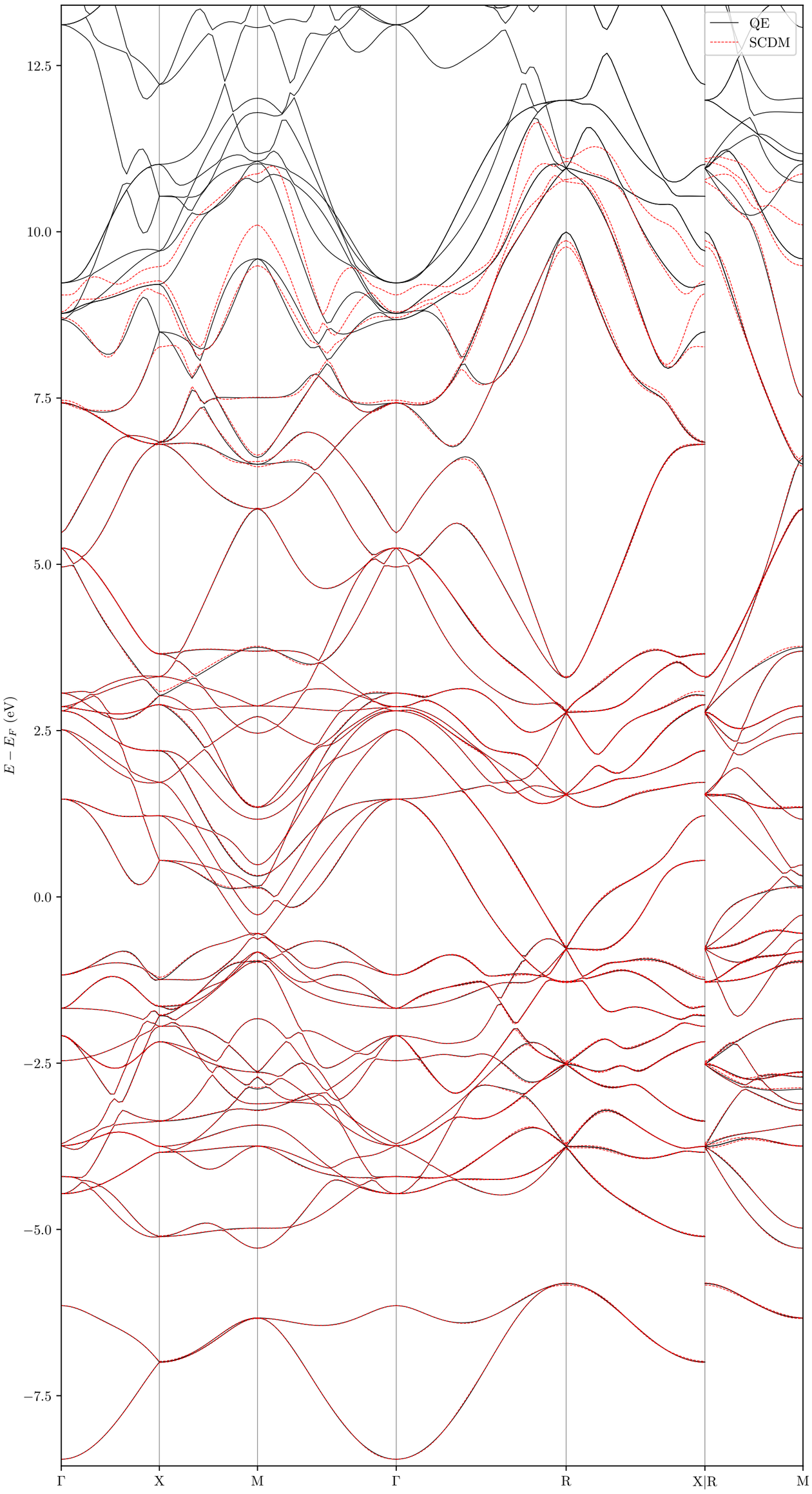
Al2Mo6 exclude semicore
PW=2c4ec42e-27e6-43e4-a0c4-a58874442084
W90=050f34a6-8866-4db7-936d-a68635a1fff0




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.4 | 3.1 | 37.8 | 18.3 | 18.3 | 309.5 | 2.313 |

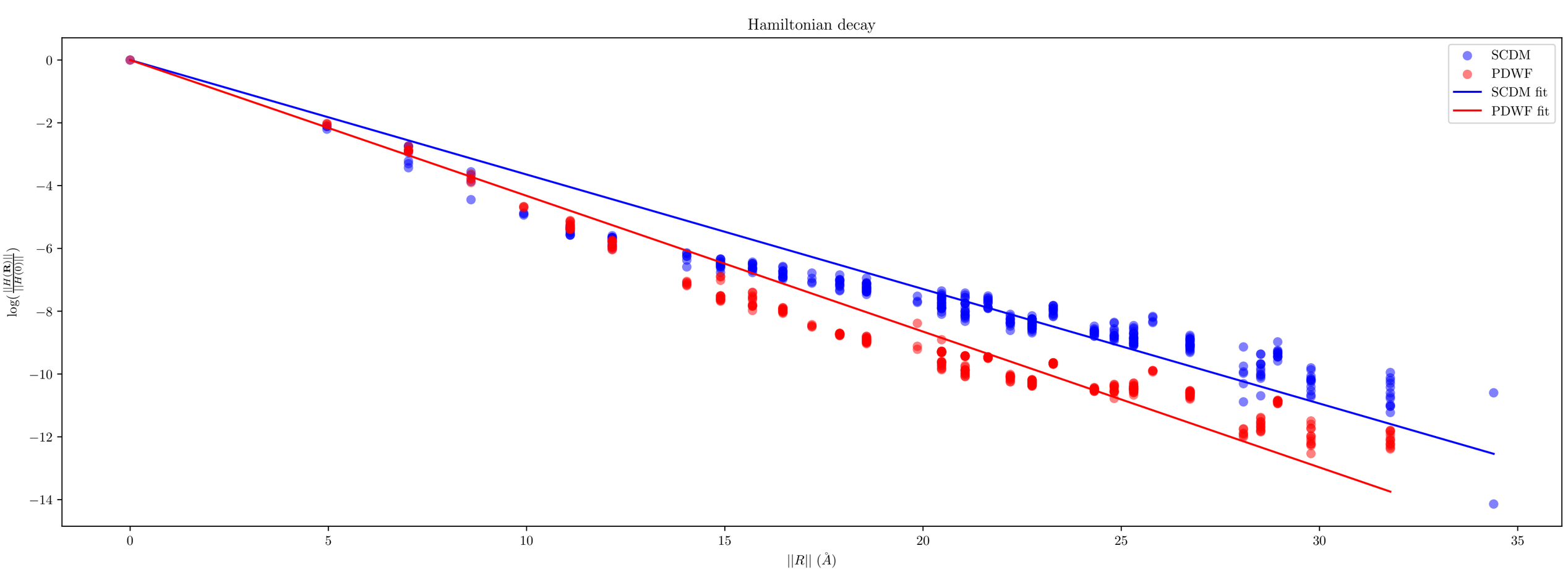
Al2Mo6 exclude semicore
PW=2c4ec42e-27e6-43e4-a0c4-a58874442084
W90=2d6d9153-460e-4de6-b2f1-6b21b029e5fc

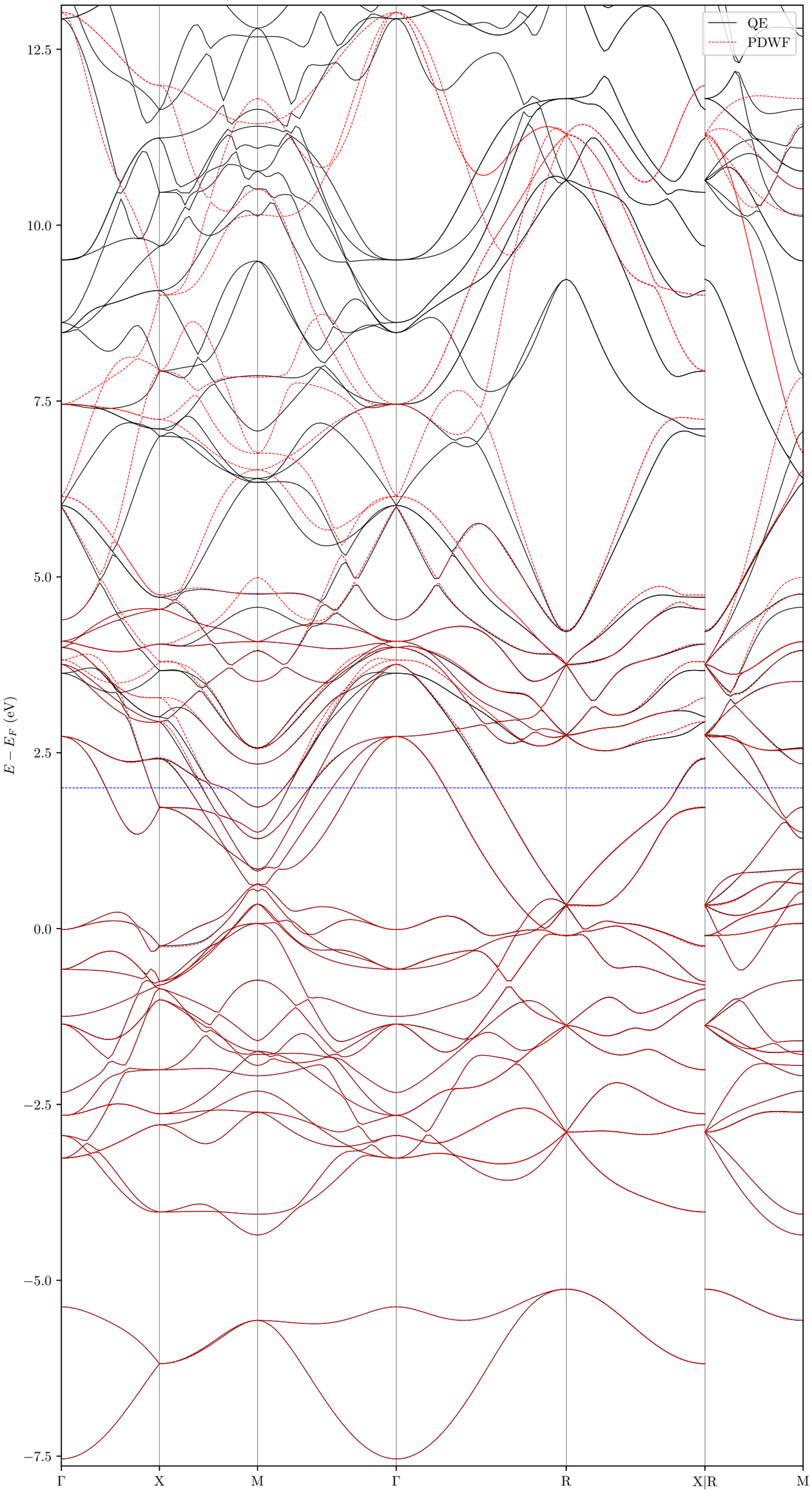



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.9 | 7.5 | 7.8 | 47.6 | 47.6 | 58.7 | 2.742 |

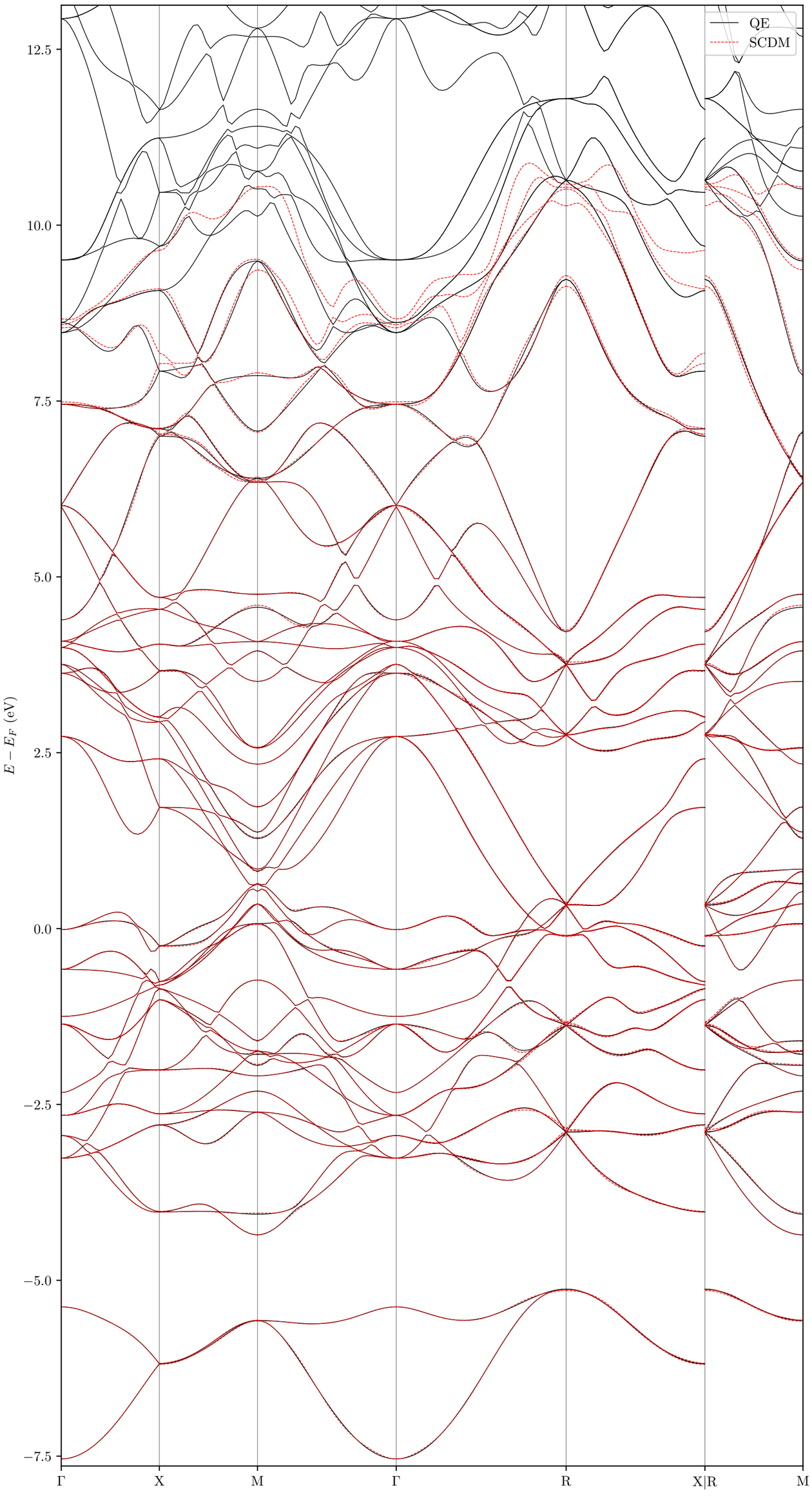
Hamiltonian decay





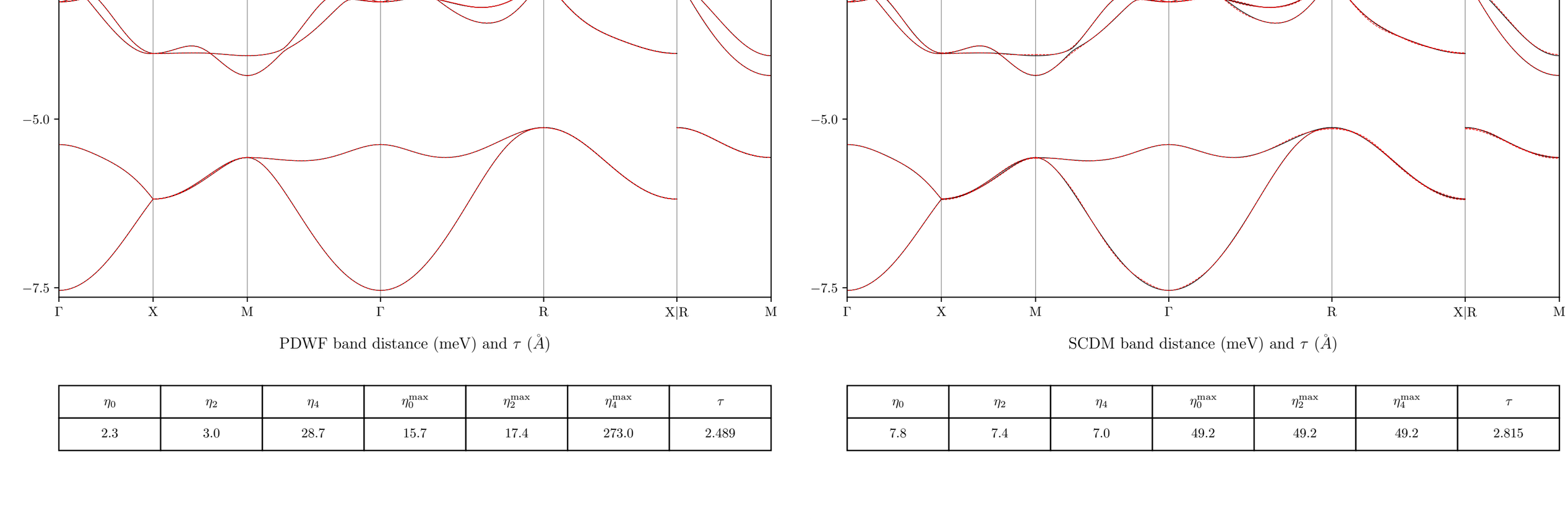

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

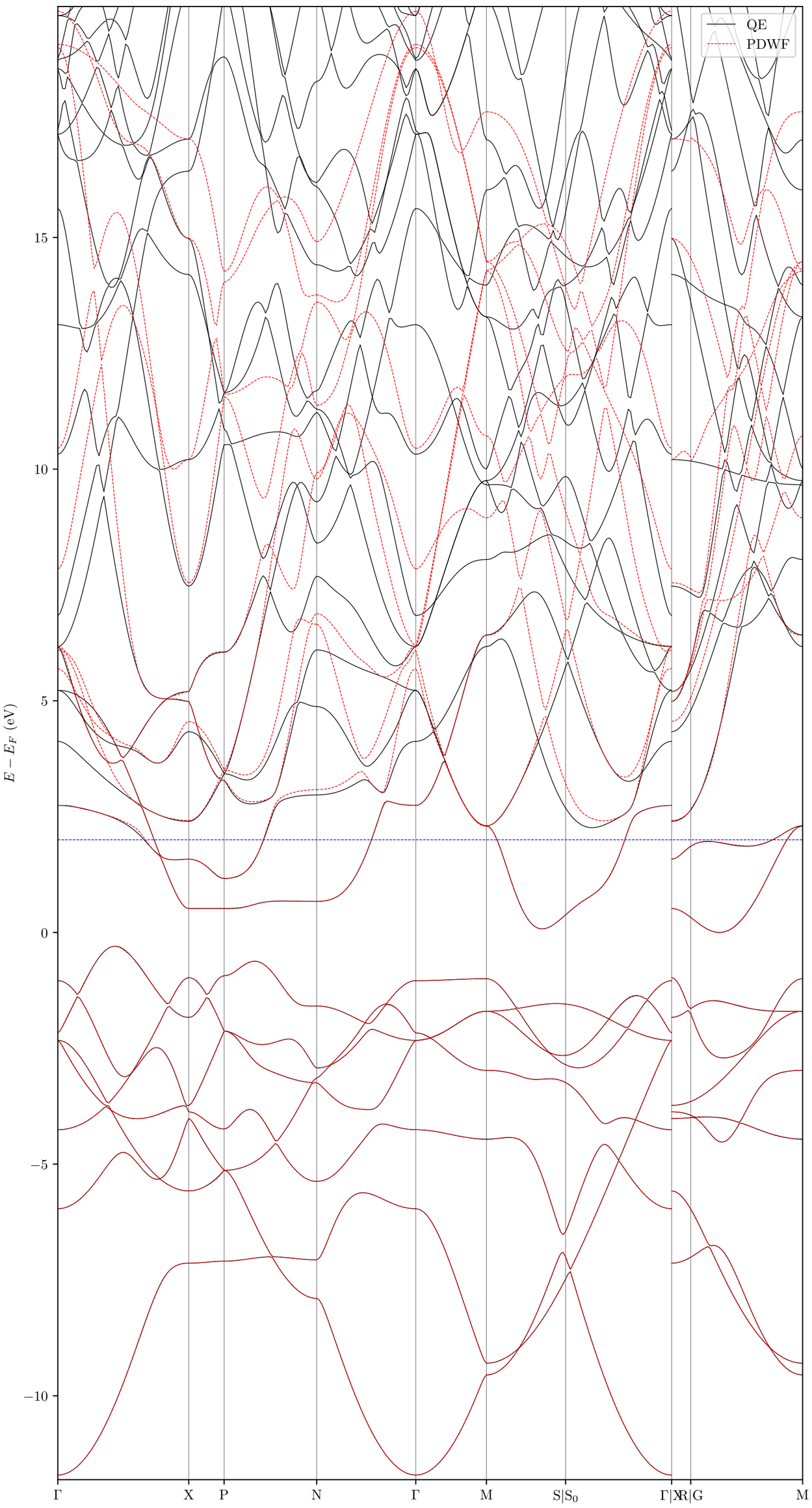
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.3 | 3.0 | 28.7 | 15.7 | 17.4 | 273.0 | 2.489 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

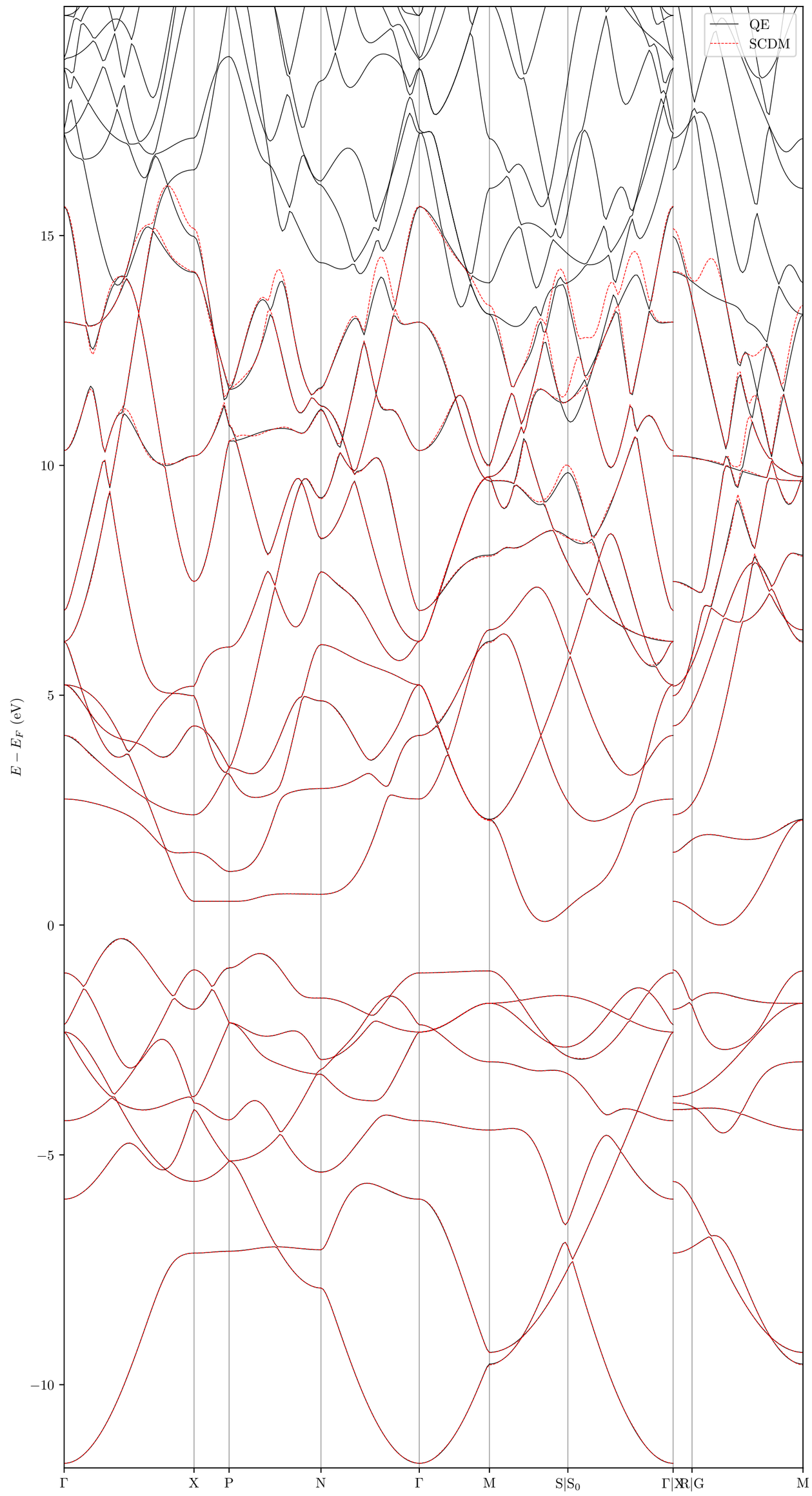
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.8 | 7.4 | 7.0 | 49.2 | 49.2 | 49.2 | 2.815 |





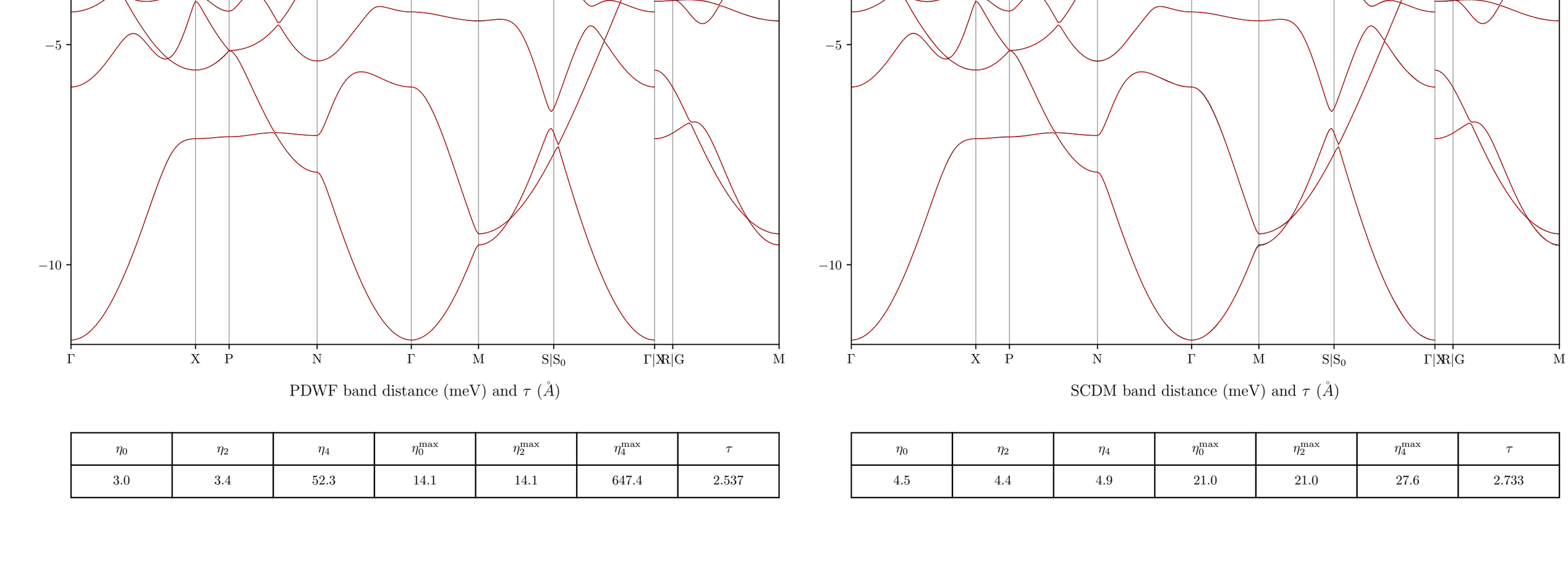

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.0 | 3.4 | 52.3 | 14.1 | 14.1 | 647.4 | 2.537 |

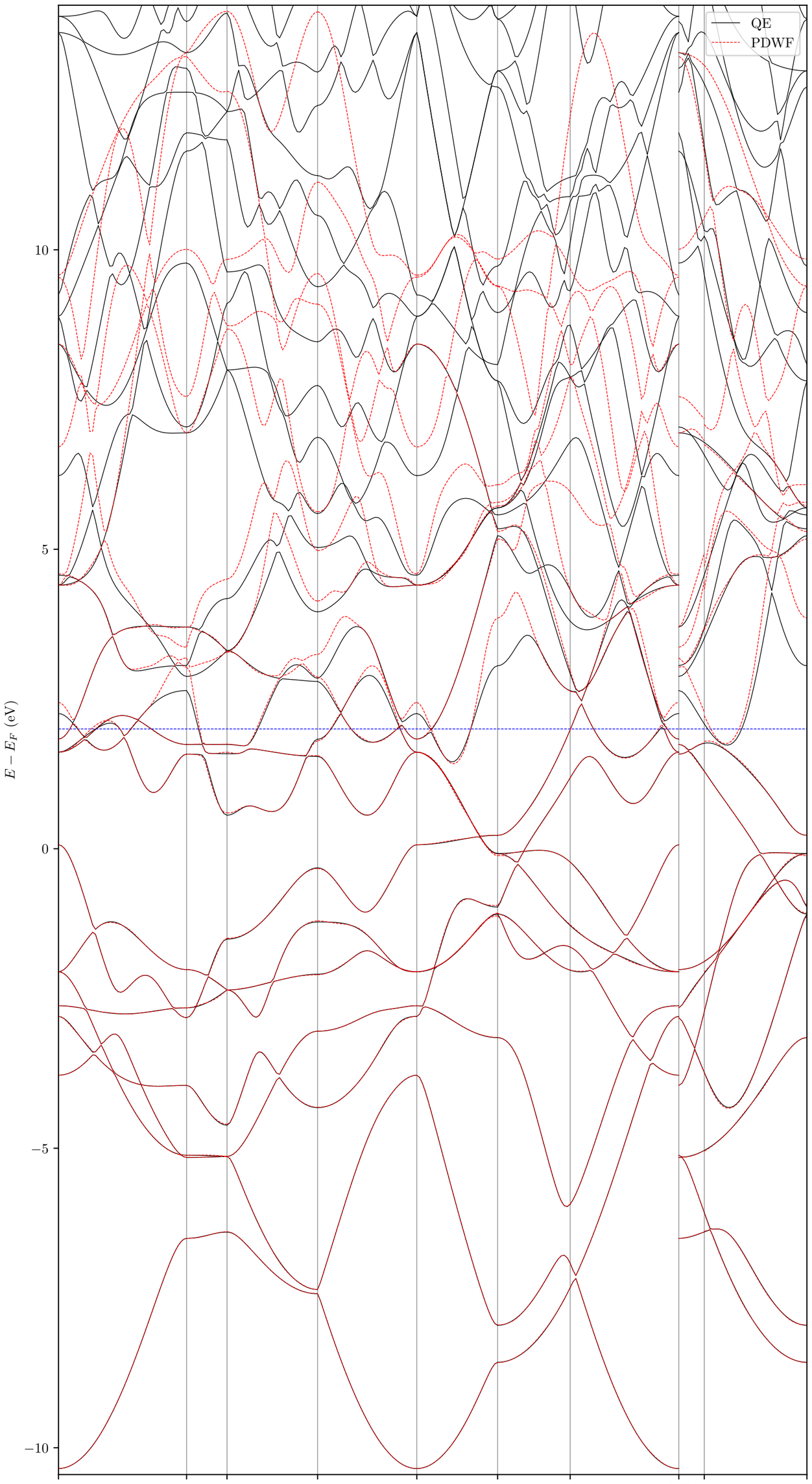



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.5 | 4.4 | 4.9 | 21.0 | 21.0 | 27.6 | 2.733 |



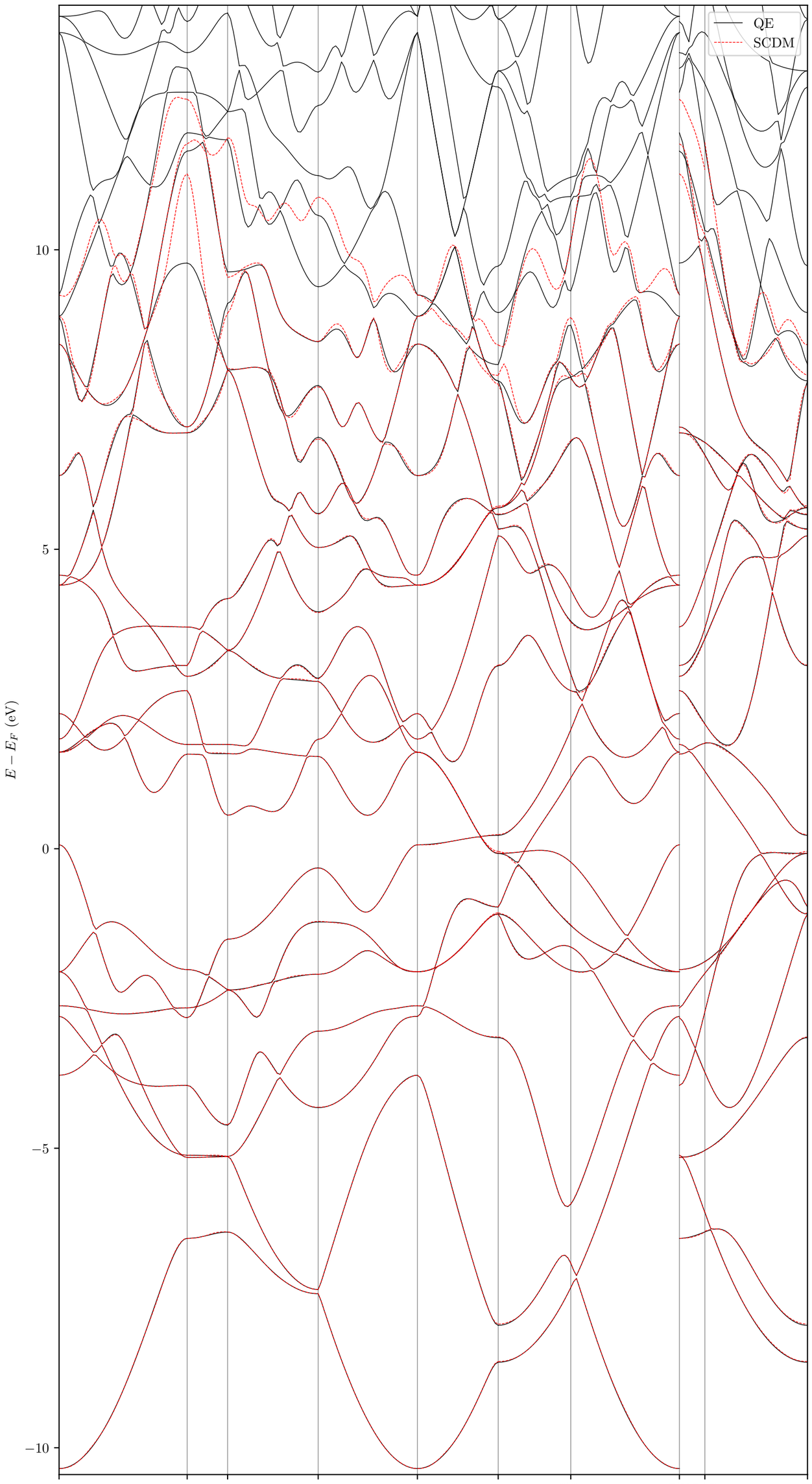
Al3Nb exclude semicore
PW=2bd21fa5-f7e7-4277-93dc-c3c655547e2c
W90=adf5f633-200f-421c-bcf0-e2de743bcb76




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.1 | 9.6 | 86.3 | 30.1 | 57.4 | 714.8 | 2.659 |

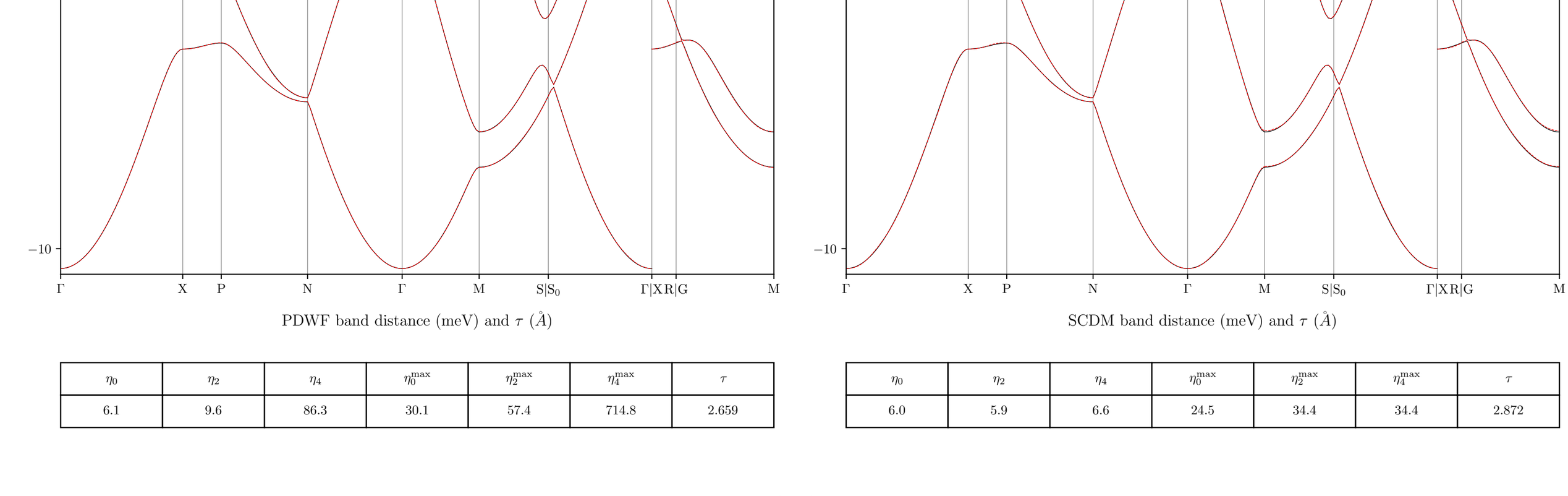
Al3Nb exclude semicore
PW=2bd21fa5-f7e7-4277-93dc-c3c655547e2c
W90=29c4ea77-516b-4422-9396-6275efb0ca09



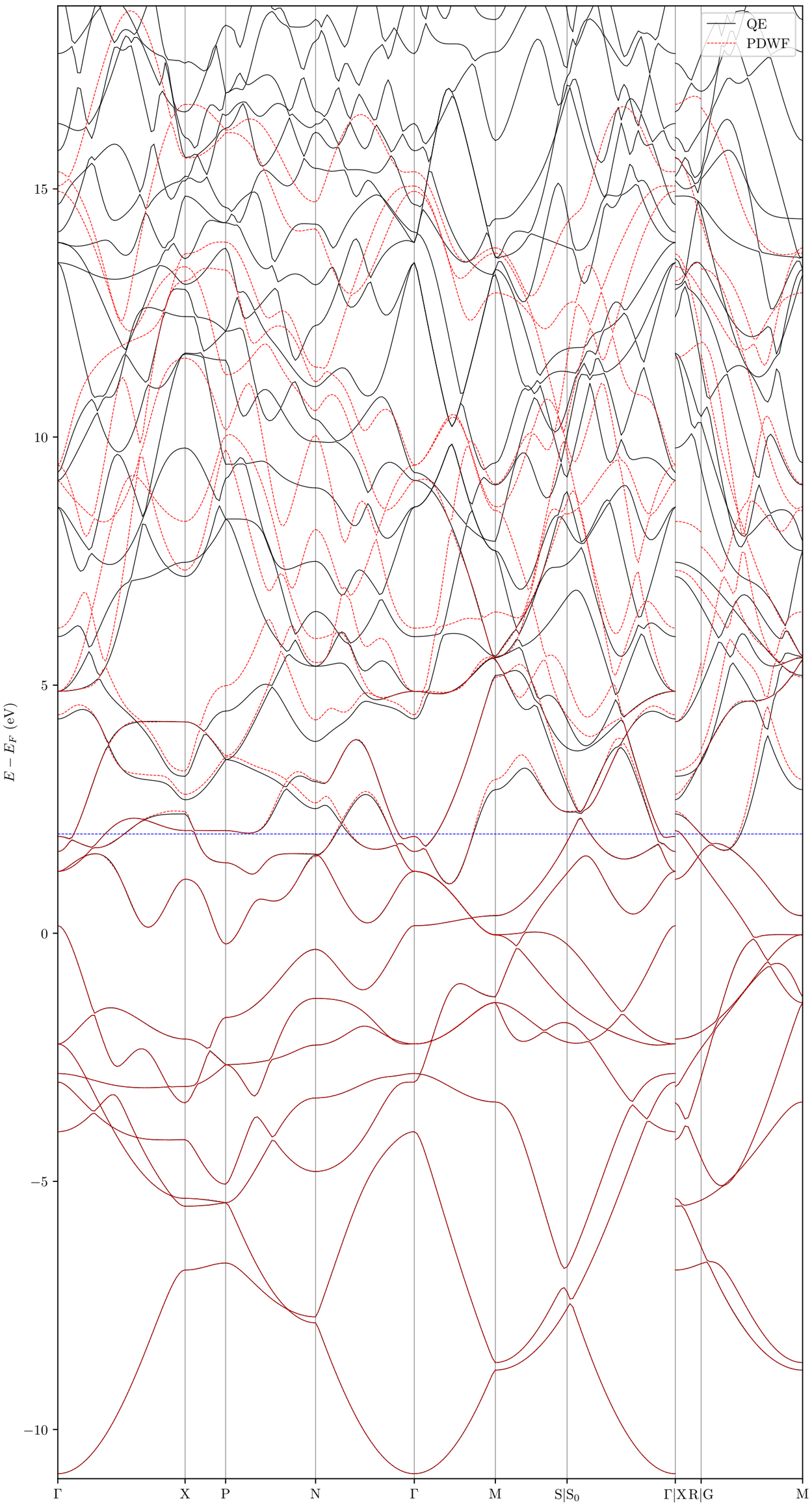

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.0 | 5.9 | 6.6 | 24.5 | 34.4 | 34.4 | 2.872 |

Hamiltonian decay



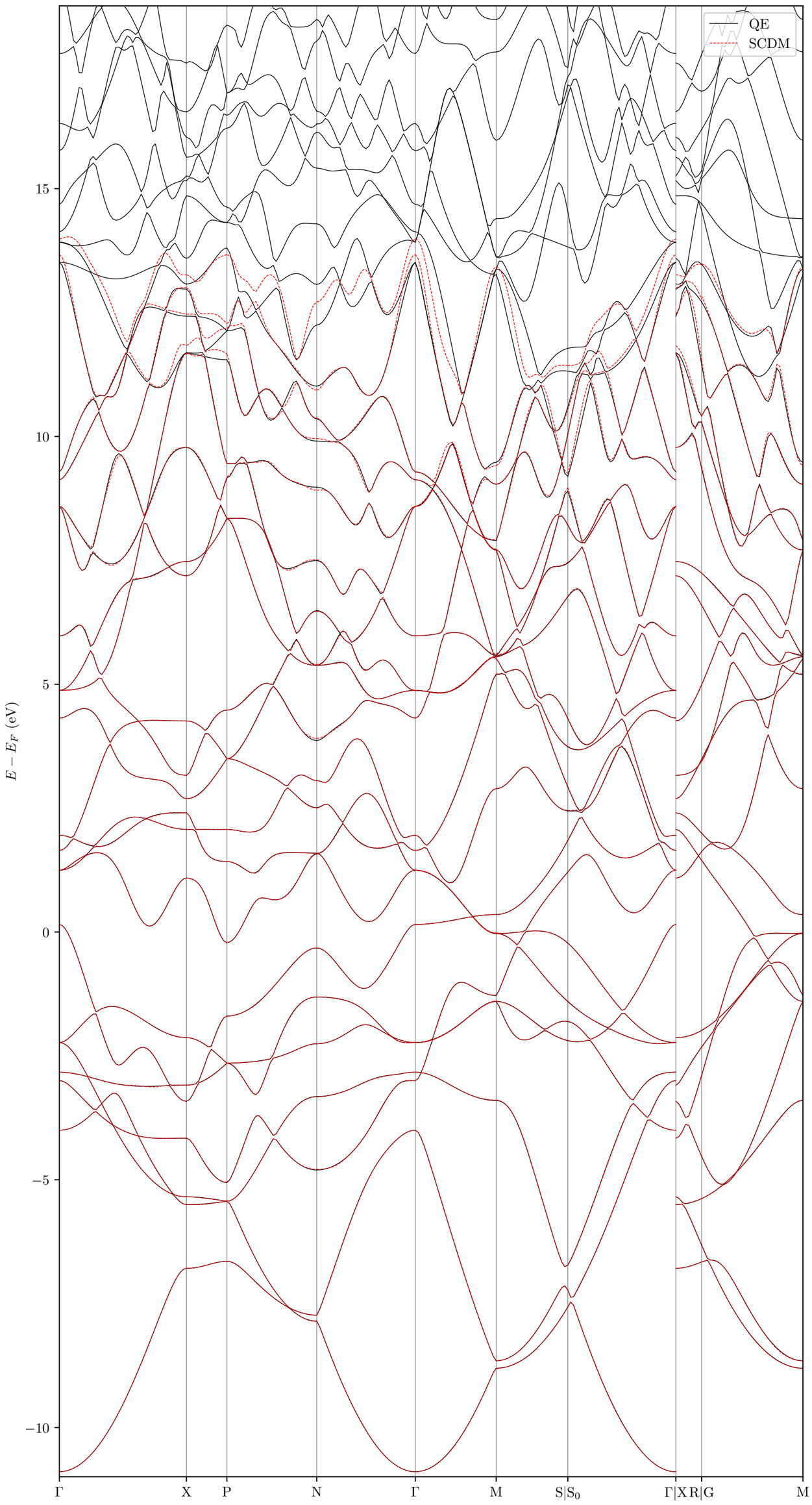
Al3Ta exclude semicore
PW=5e78af73-68b2-4255-a82f-064d85b67006
W90=29af2cd7-a54f-4b9d-a95e-e4df3fd9c424




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.8 | 4.9 | 50.3 | 13.9 | 46.6 | 473.0 | 2.514 |

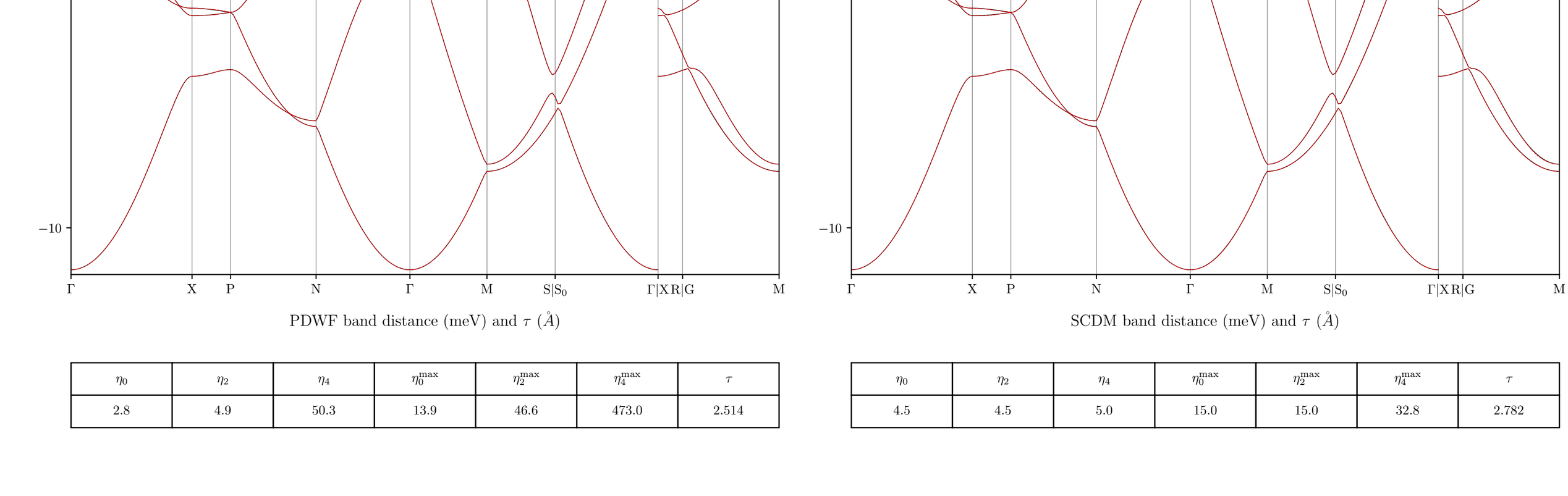
Al3Ta exclude semicore
PW=5e78af73-68b2-4255-a82f-064d85b67006
W90=57991e17-595c-4692-9f31-50995863e911

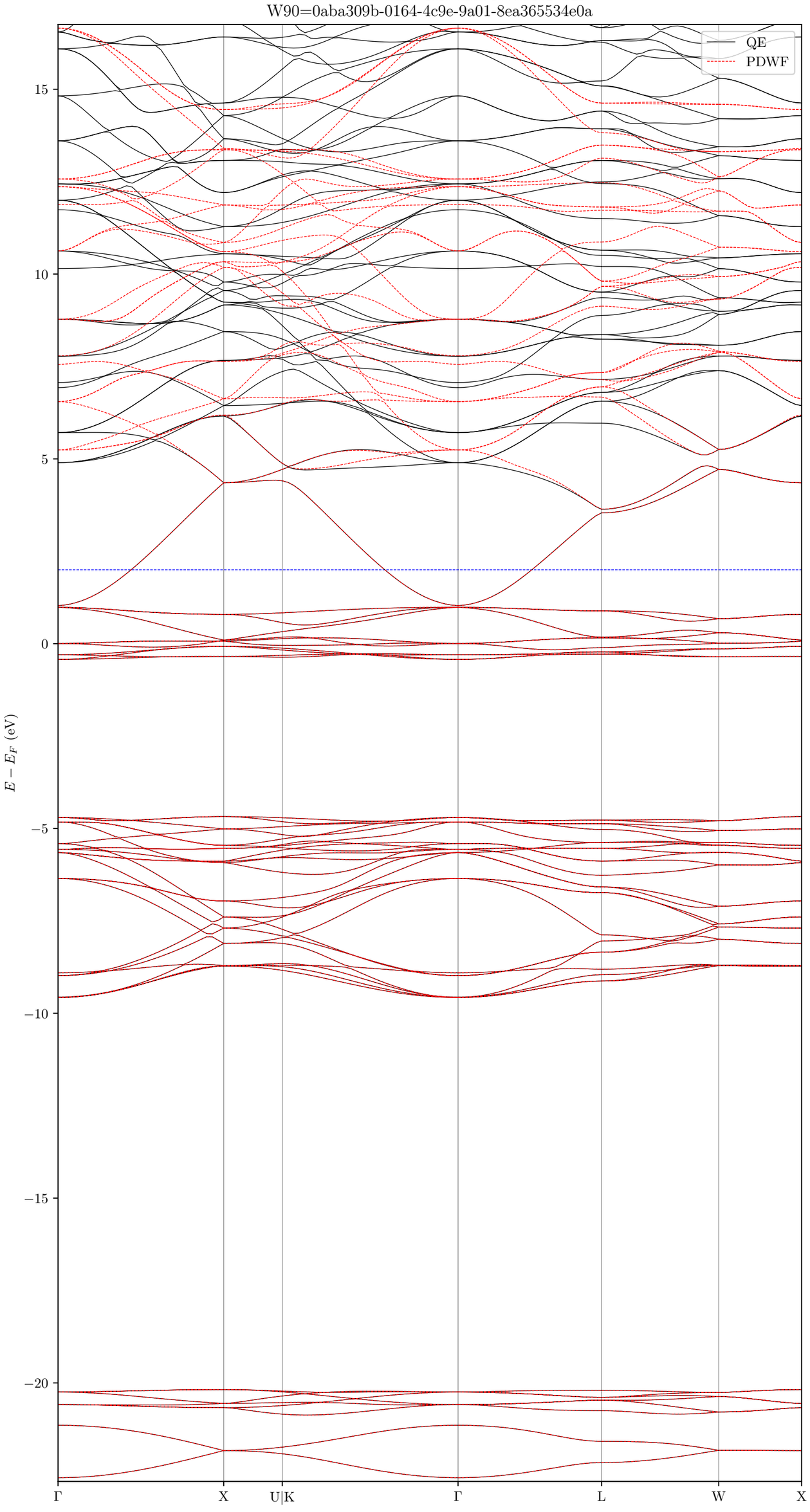



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.5 | 4.5 | 5.0 | 15.0 | 15.0 | 32.8 | 2.782 |

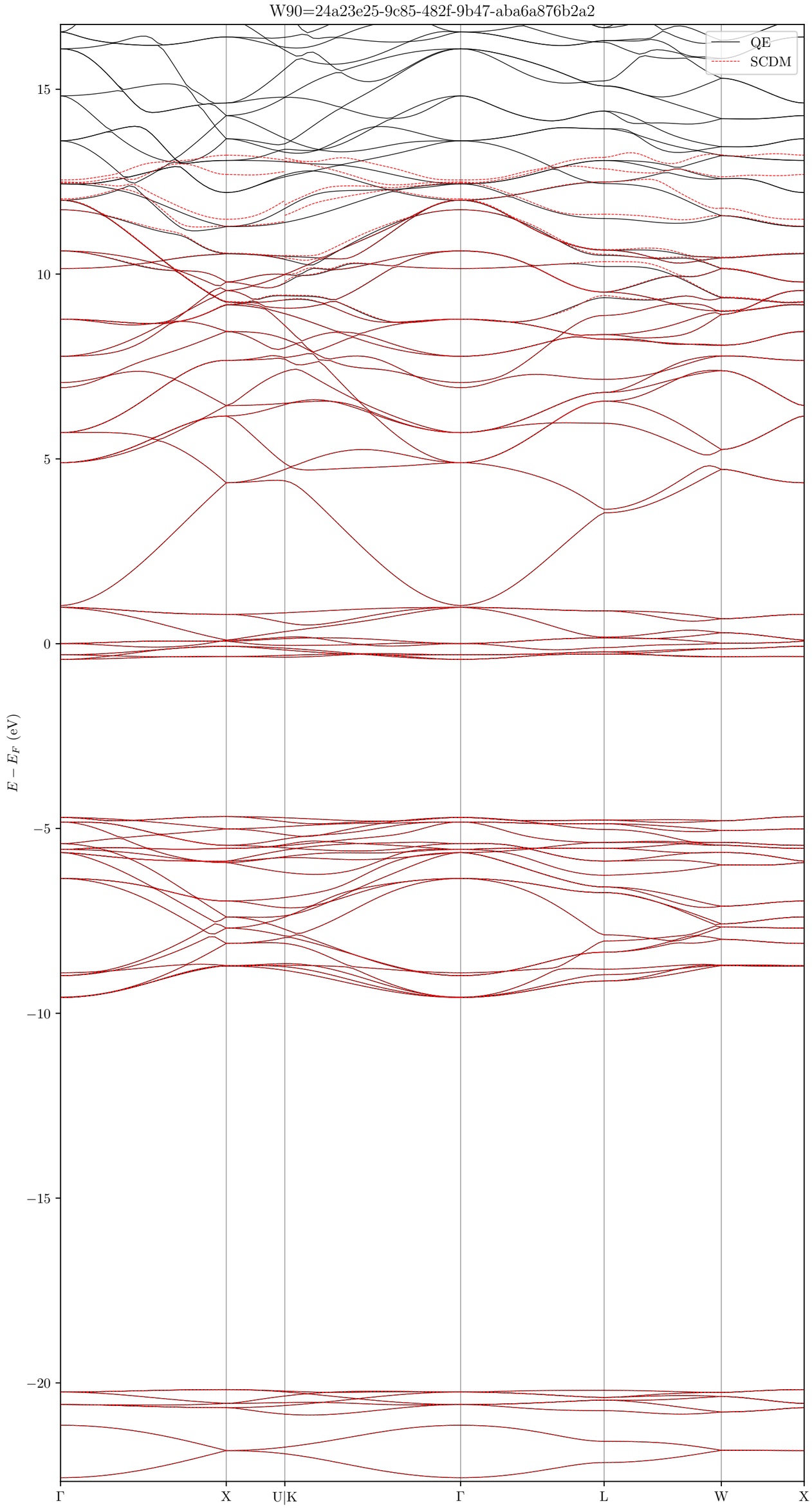
Hamiltonian decay





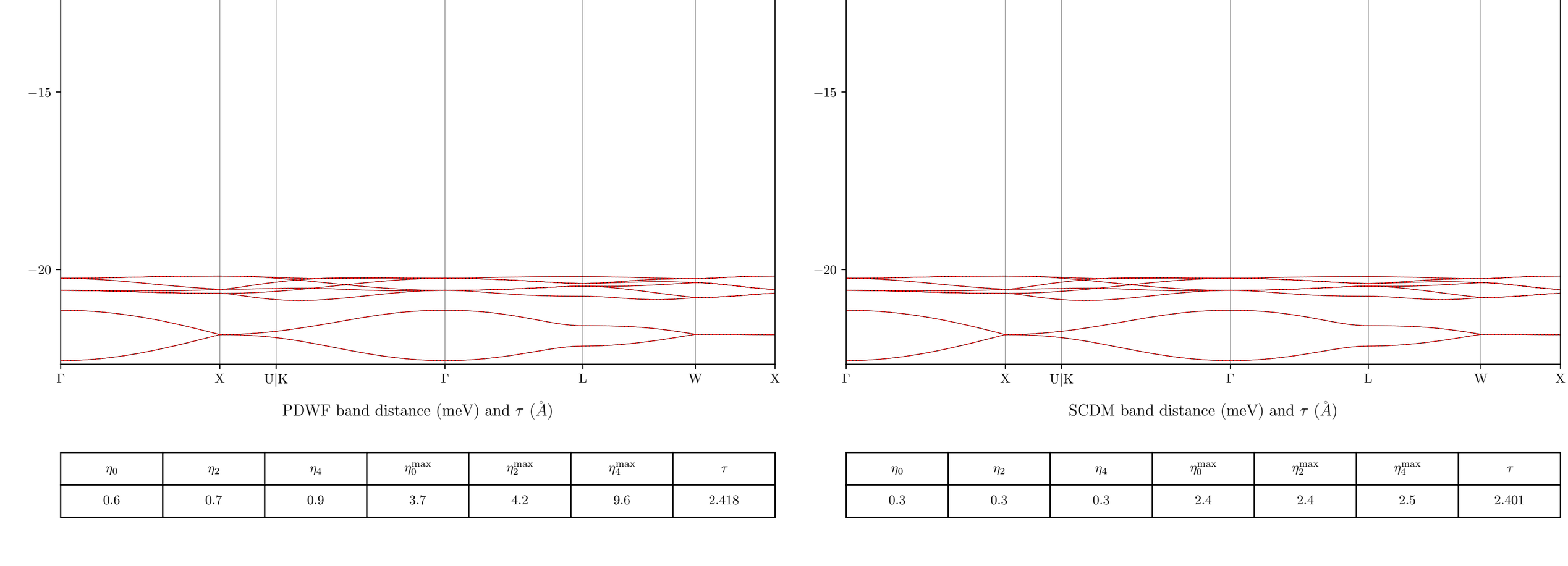

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.7 | 0.9 | 3.7 | 4.2 | 9.6 | 2.418 |

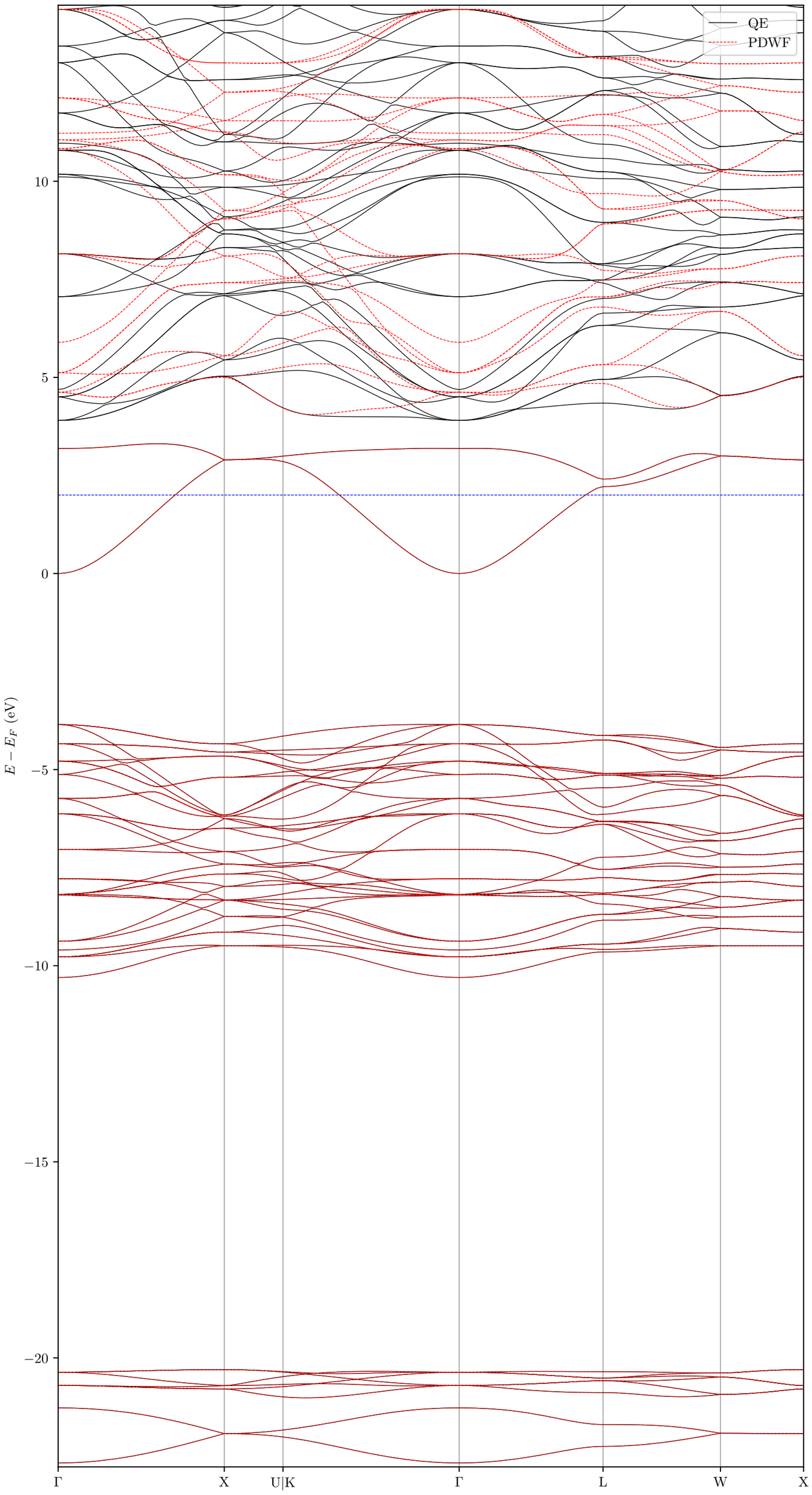



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 0.3 | 2.4 | 2.4 | 2.5 | 2.401 |



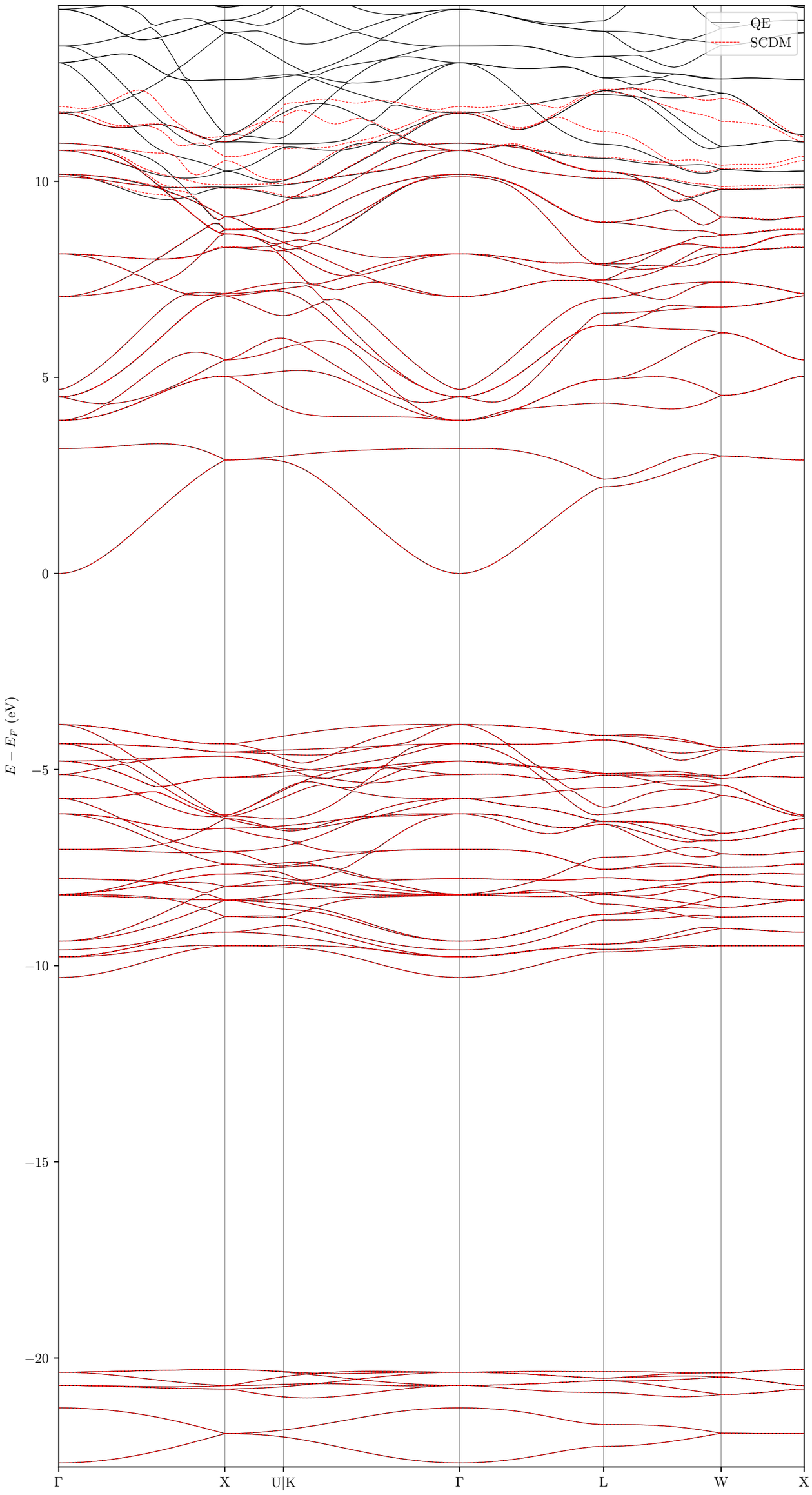
Al4O8Zn2 exclude semicore
PW=3ca34558-07bf-4386-9c1c-1c2ab1fcd024
W90=2057abb0-d27d-4e88-b46c-ff99adb7155a




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 0.6 | 5.5 | 5.5 | 5.5 | 2.392 |

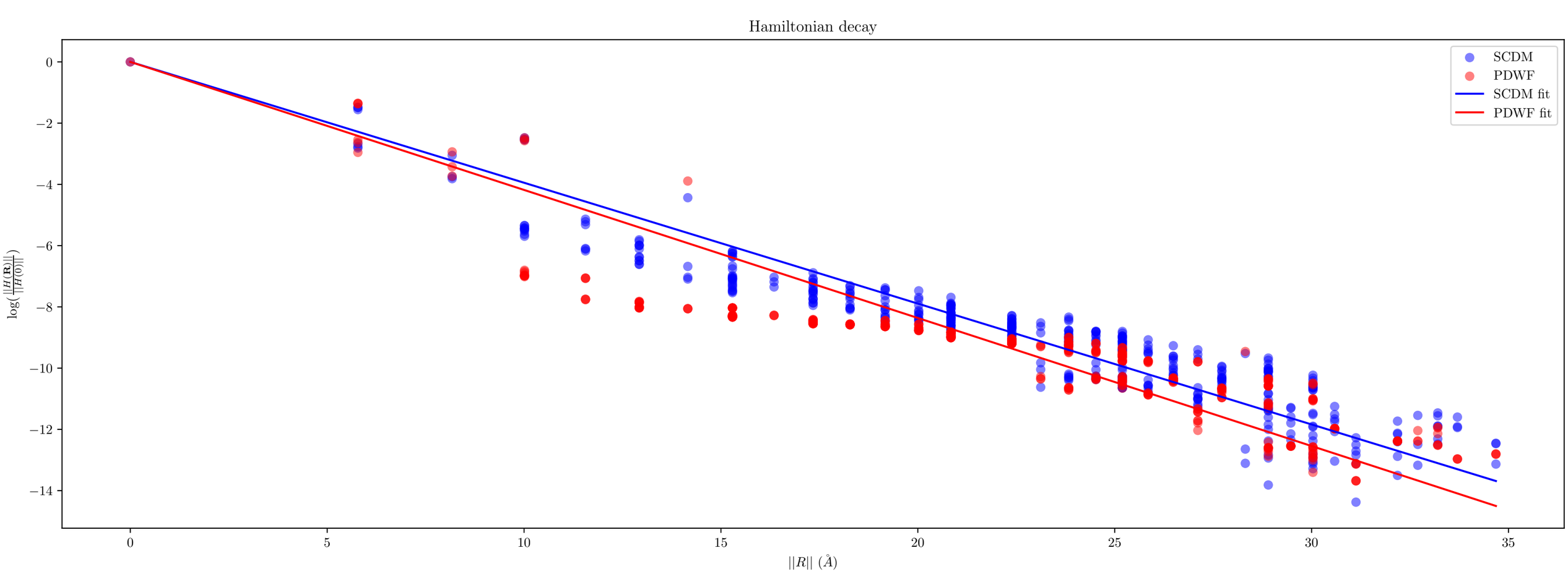
Al4O8Zn2 exclude semicore
PW=3ca34558-07bf-4386-9c1c-1c2ab1fcd024
W90=445724a6-ca14-4807-8b5a-4fae72fe5fad



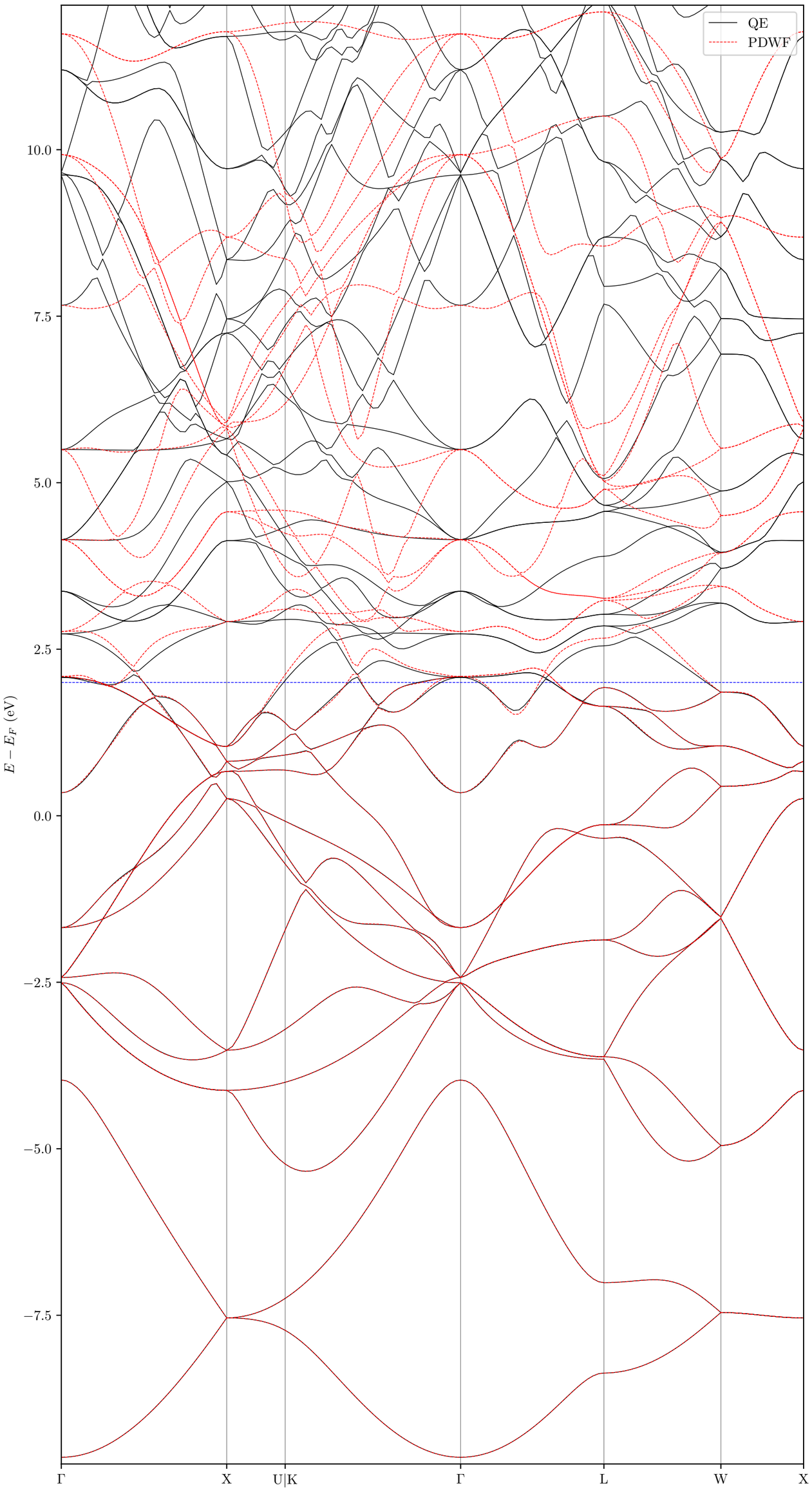

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.4 | 0.4 | 0.4 | 2.3 | 2.3 | 2.3 | 2.534 |

Hamiltonian decay



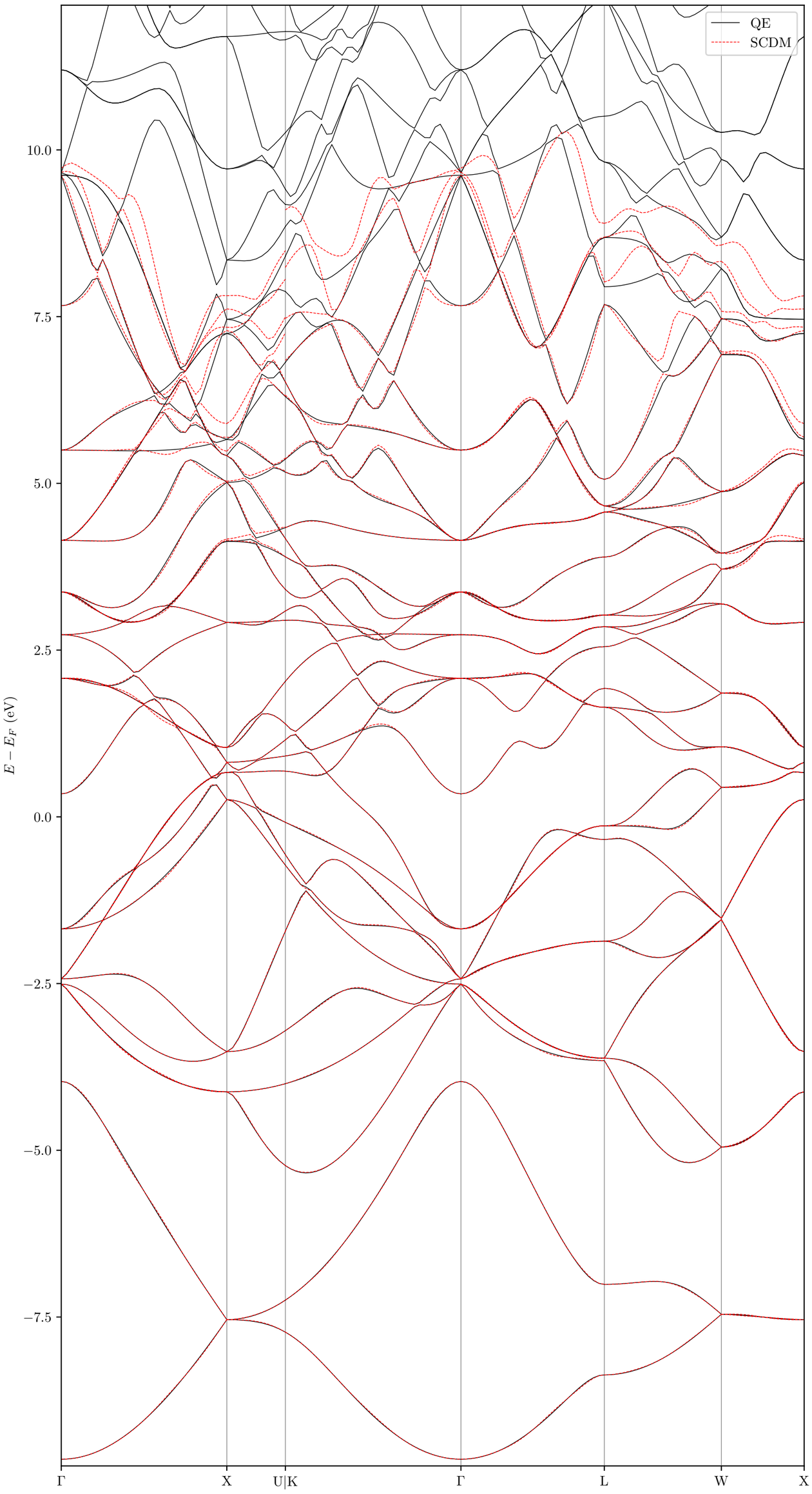
Al4Sc2 exclude semicore
PW=88813939-4a5d-4ffc-9dfe-b58271c2e7a4
W90=368dd6ee-56ac-43d1-897c-1bab79b6f8cd




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.1 | 8.4 | 177.7 | 16.0 | 62.3 | 707.7 | 2.516 |

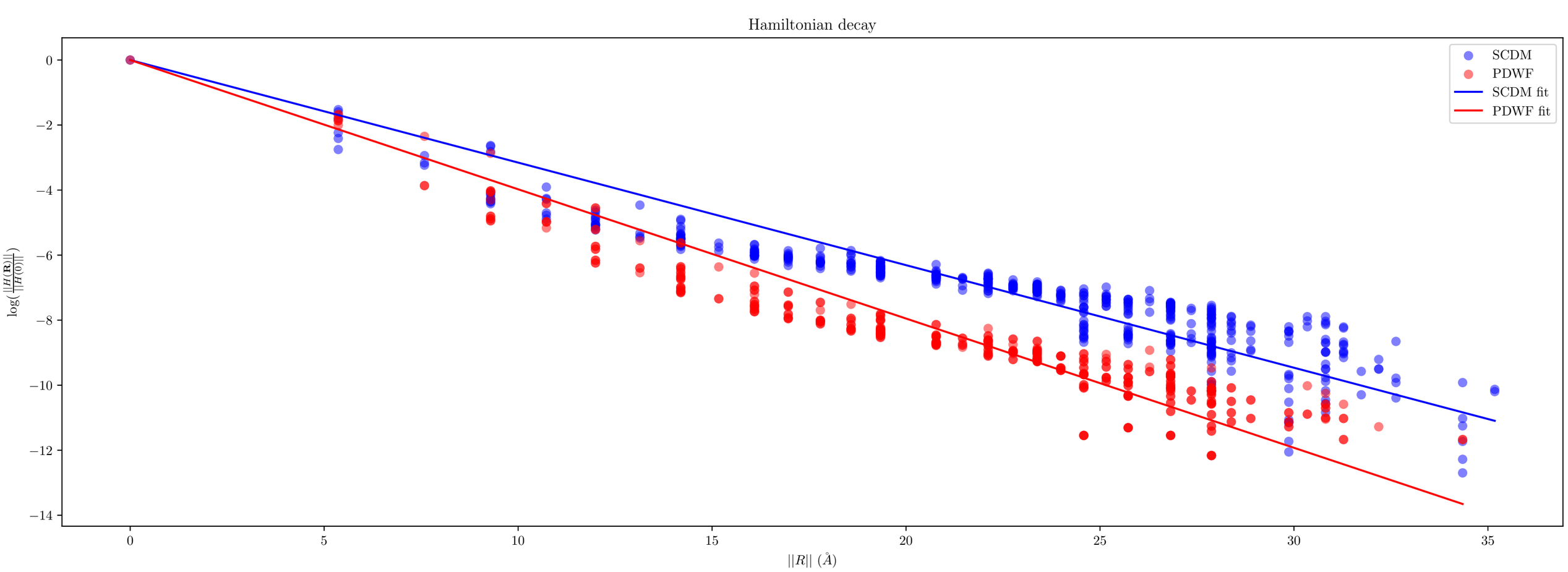
Al4Sc2 exclude semicore
PW=88813939-4a5d-4ffc-9dfe-b58271c2e7a4
W90=b8120f37-e92a-4bfa-90ab-87fd21ba4076



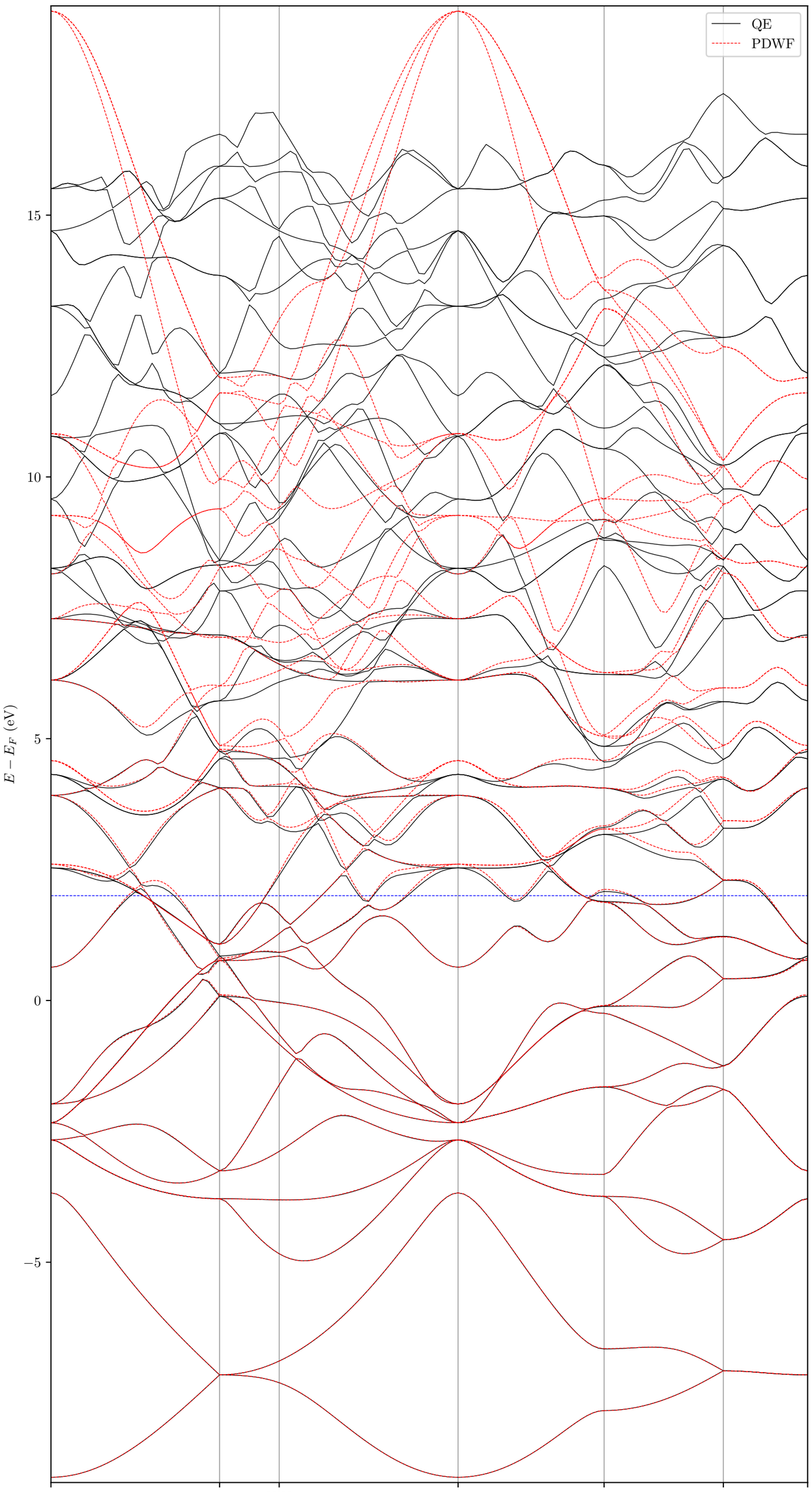

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.0 | 7.7 | 8.2 | 29.2 | 55.8 | 56.1 | 3.170 |

Hamiltonian decay



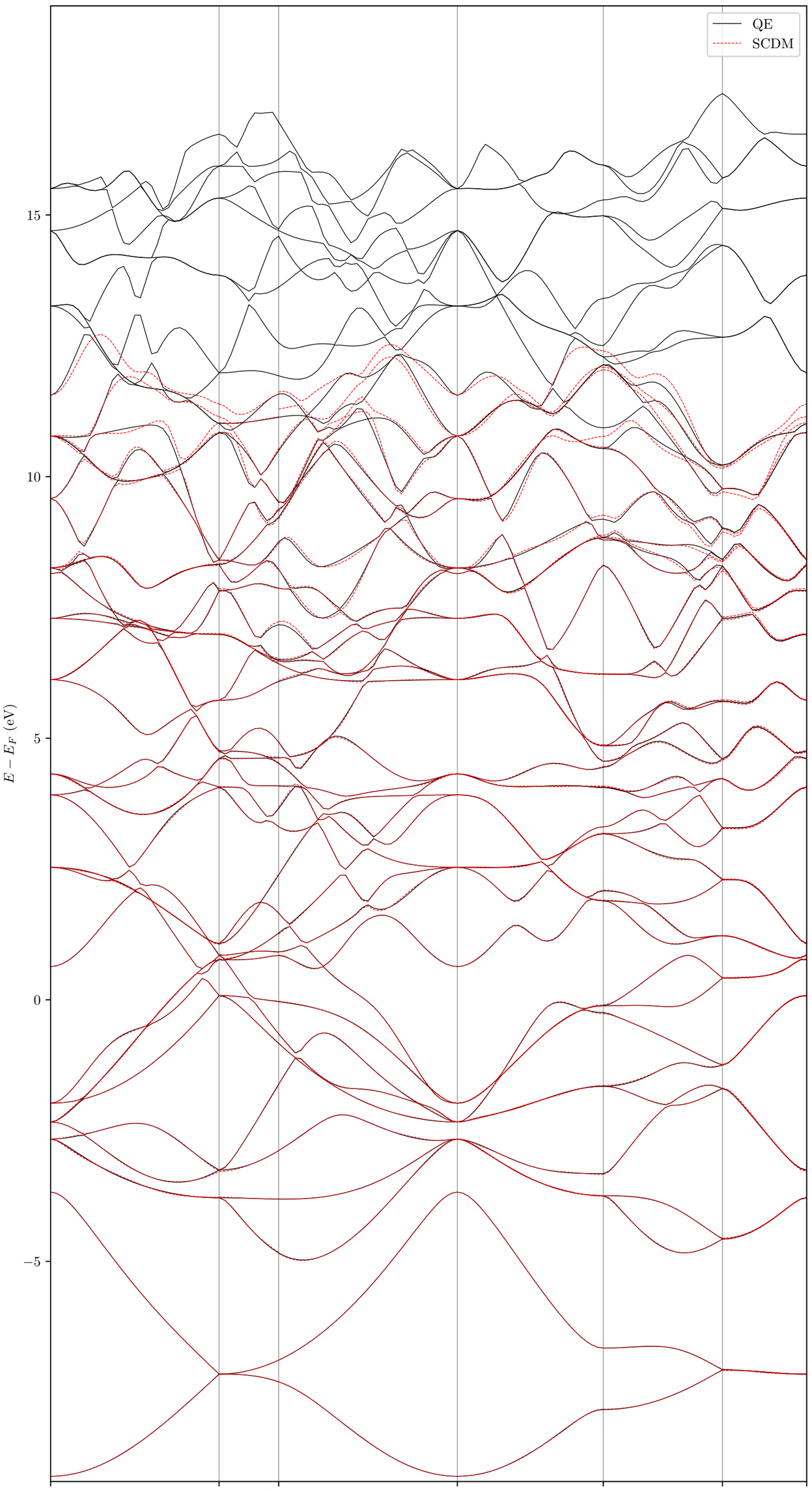
Al4Y2 exclude semicore
PW=793da2fd-5c9b-4add-b76b-a65e0ba1e2b2
W90=45c28873-2aa3-4844-ab4c-1d7c03cbf6c3




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.1 | 8.6 | 41.3 | 20.2 | 47.4 | 250.3 | 2.517 |

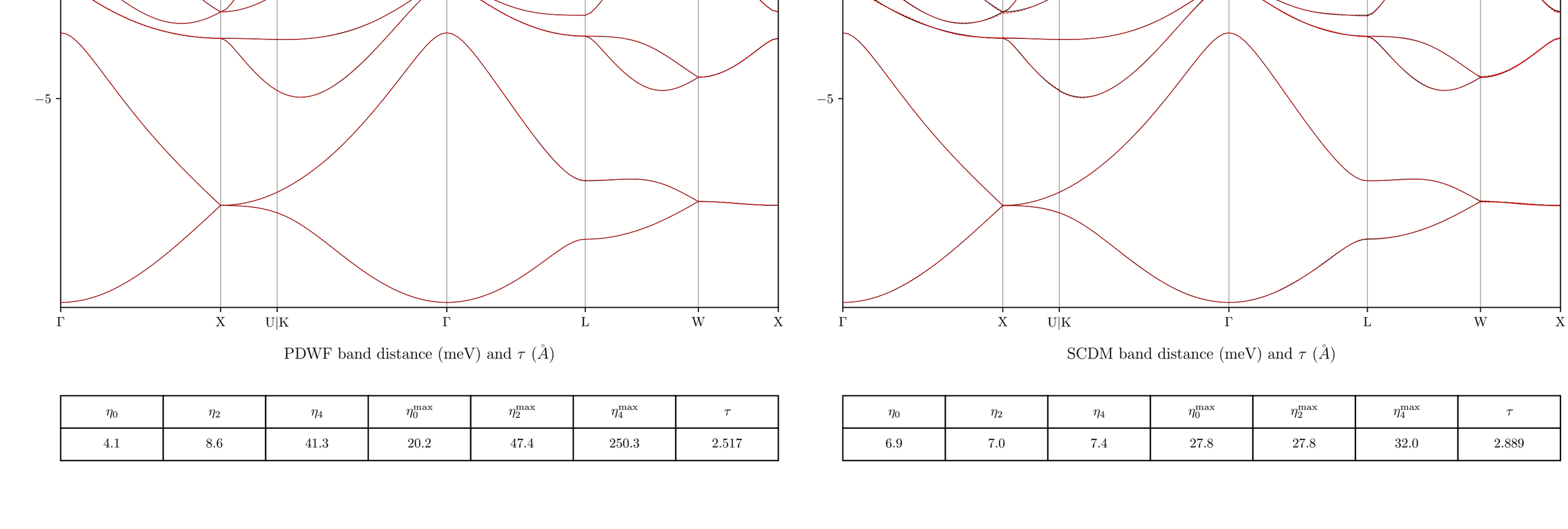
Al4Y2 exclude semicore
PW=793da2fd-5c9b-4add-b76b-a65e0ba1e2b2
W90=43c6ab8b-5c6a-4fd4-981e-ffd5dc2d5e9c

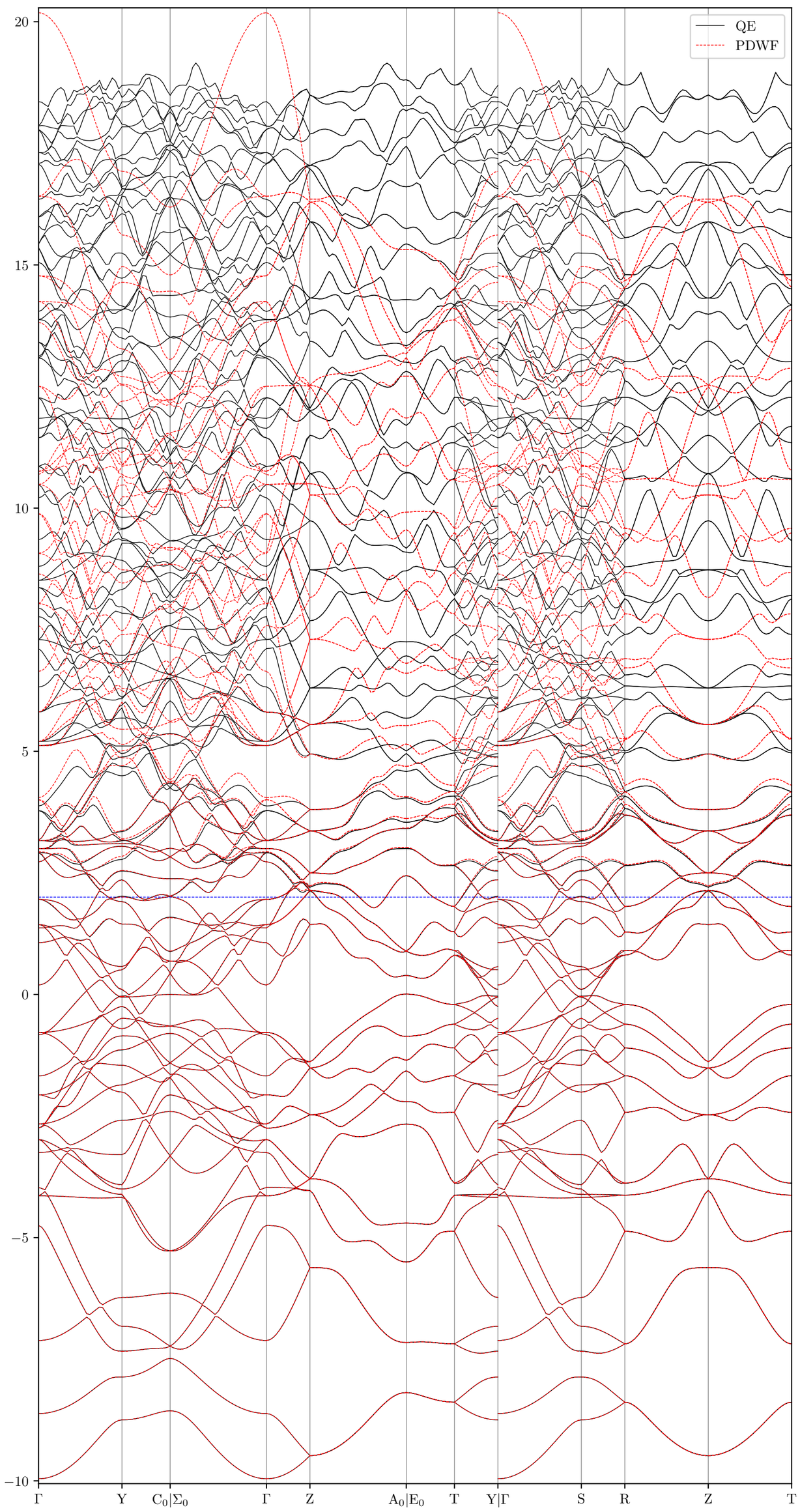



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.9 | 7.0 | 7.4 | 27.8 | 27.8 | 32.0 | 2.889 |

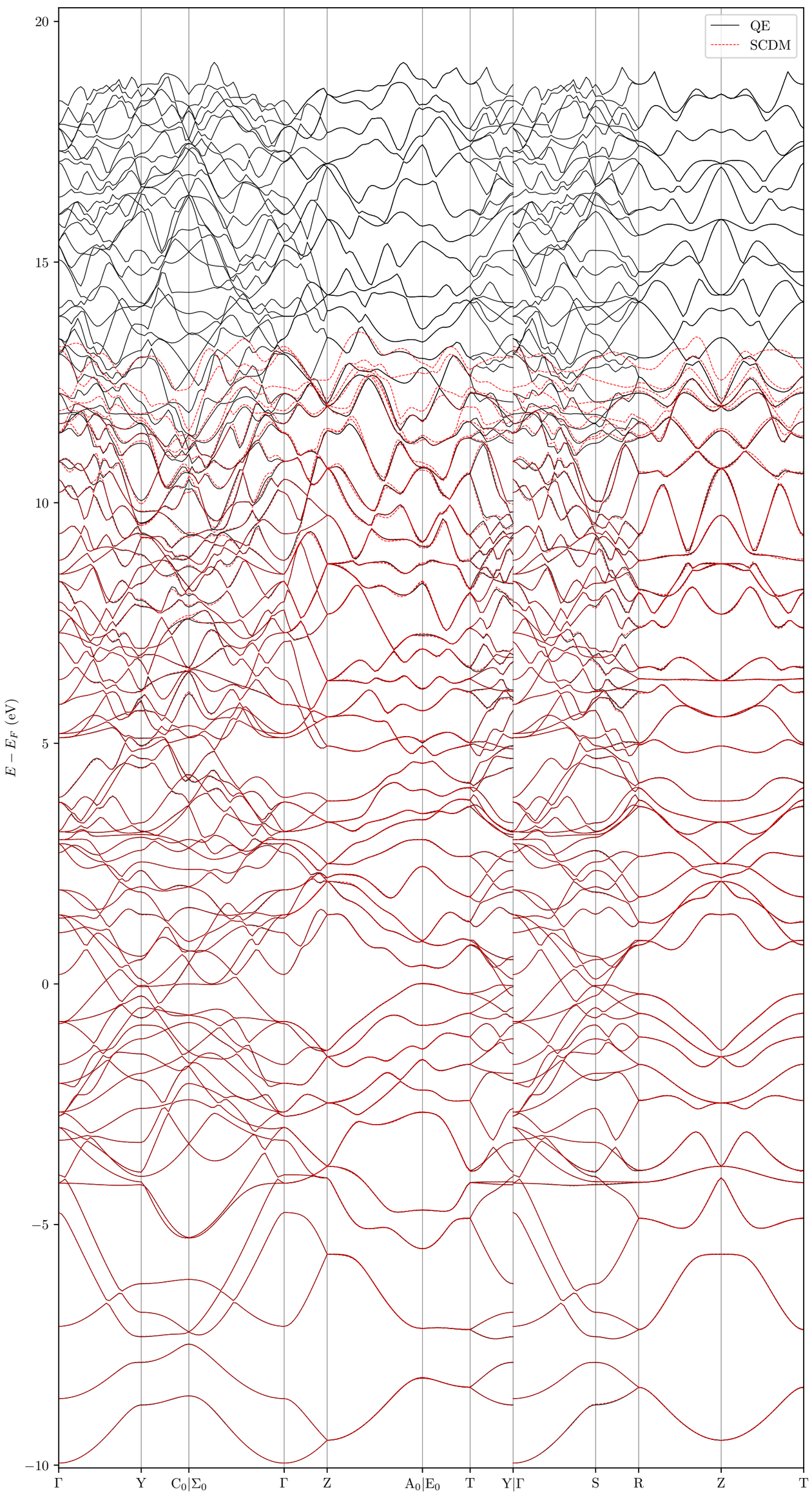
Hamiltonian decay





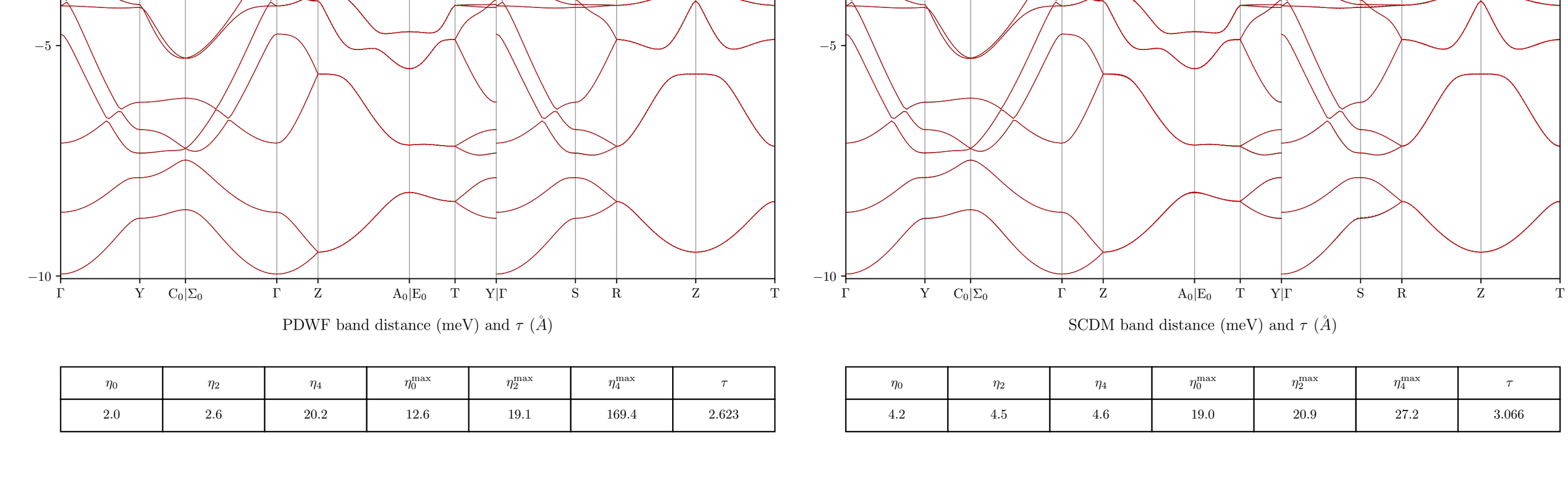

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.0 | 2.6 | 20.2 | 12.6 | 19.1 | 169.4 | 2.623 |

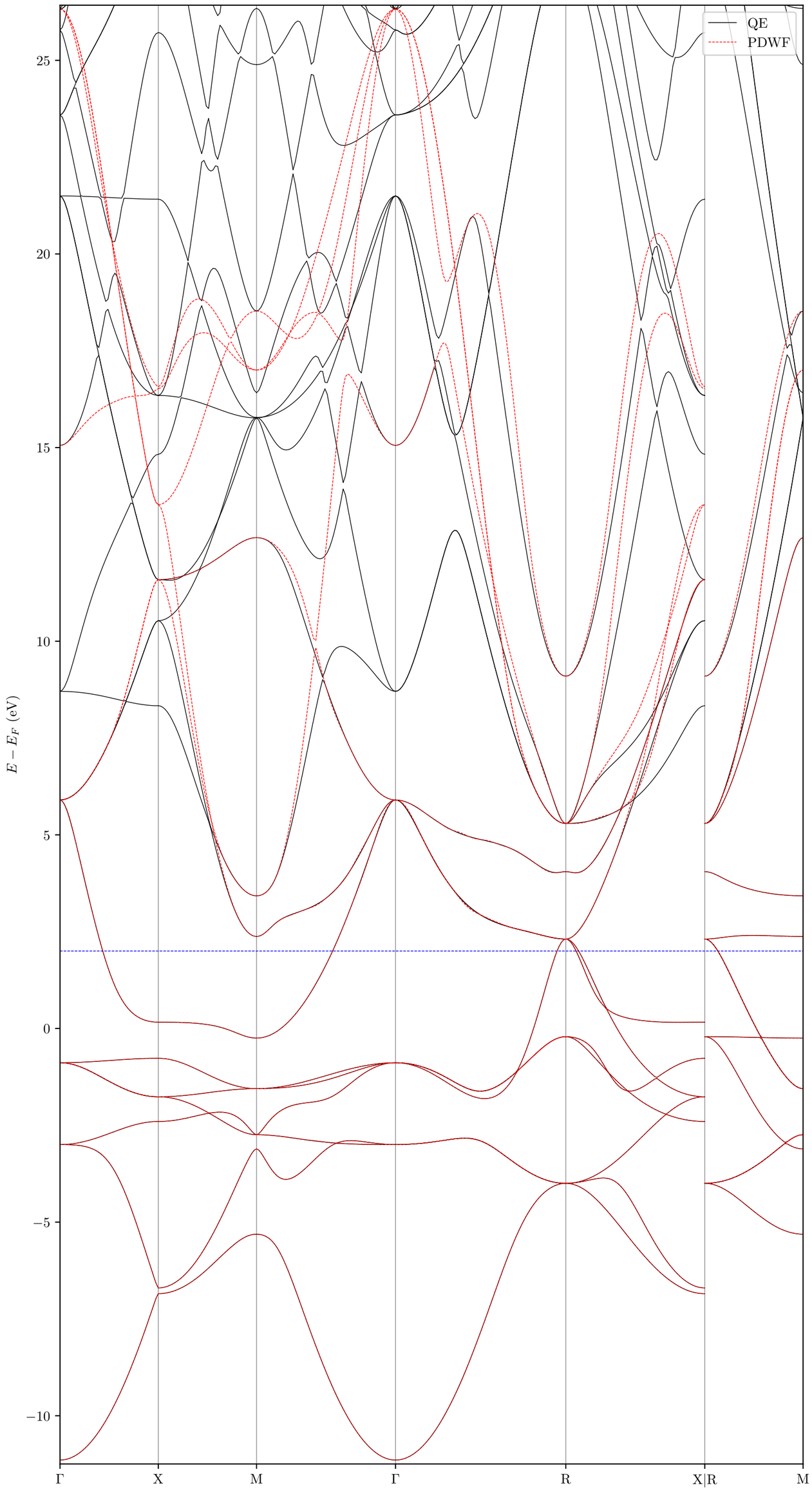



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.2 | 4.5 | 4.6 | 19.0 | 20.9 | 27.2 | 3.066 |



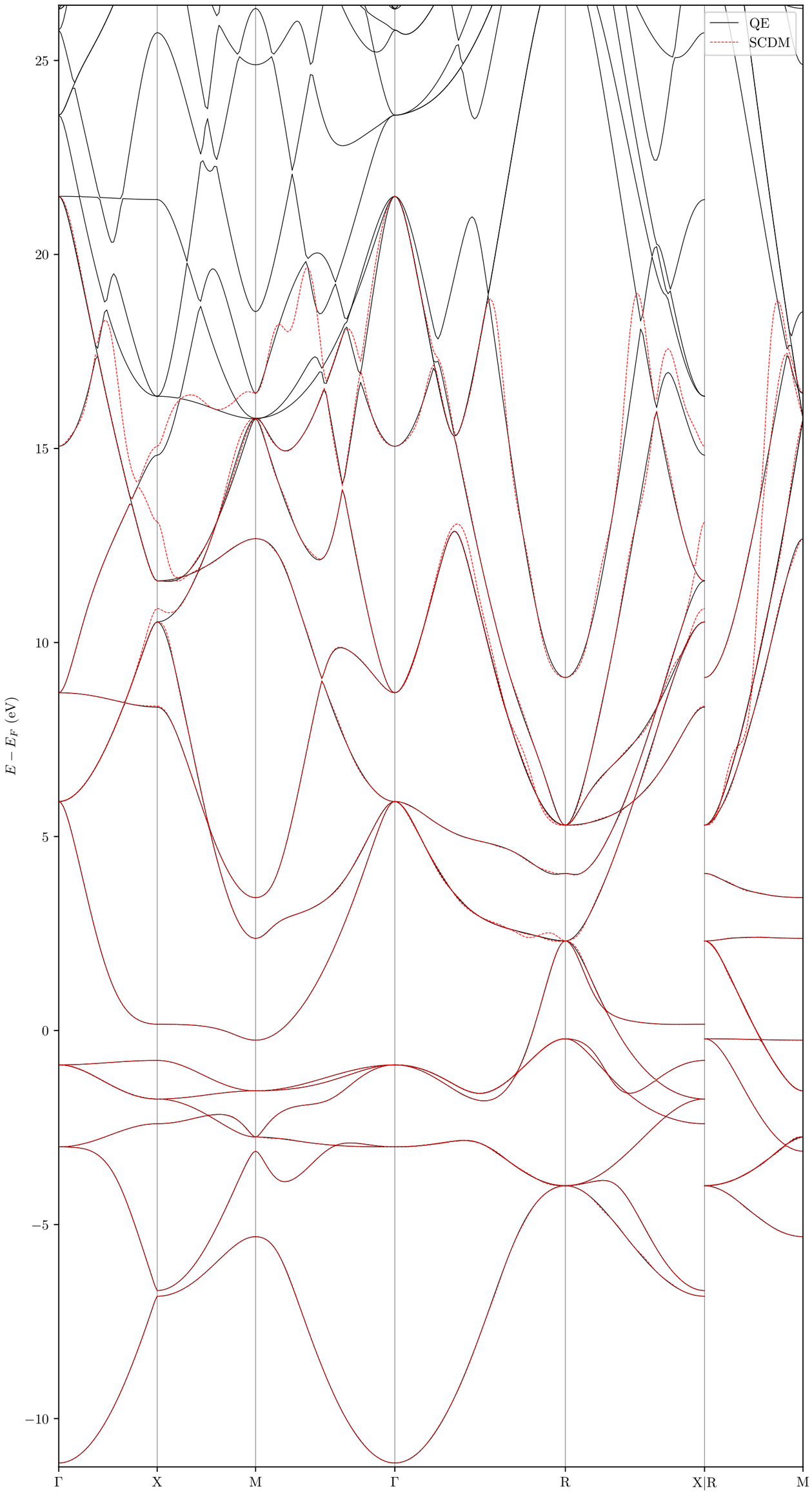
AlCo exclude semicore
PW=a4c0b3f6-224b-46b8-8ab9-3bf684e08463
W90=bce8661e-f3e1-404b-8af9-00fb5ba49ce3




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.6 | 1.9 | 4.3 | 11.1 | 13.0 | 51.0 | 1.586 |

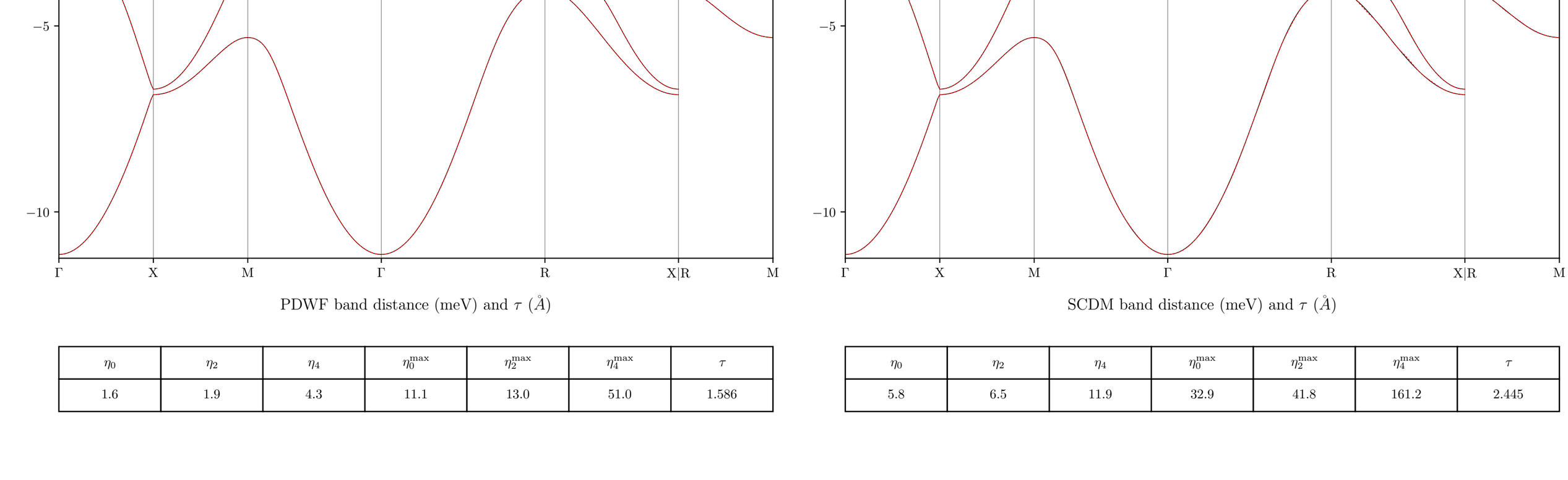
AlCo exclude semicore
PW=a4c0b3f6-224b-46b8-8ab9-3bf684e08463
W90=b63a8814-d187-4cf5-8899-007da0e5cb80



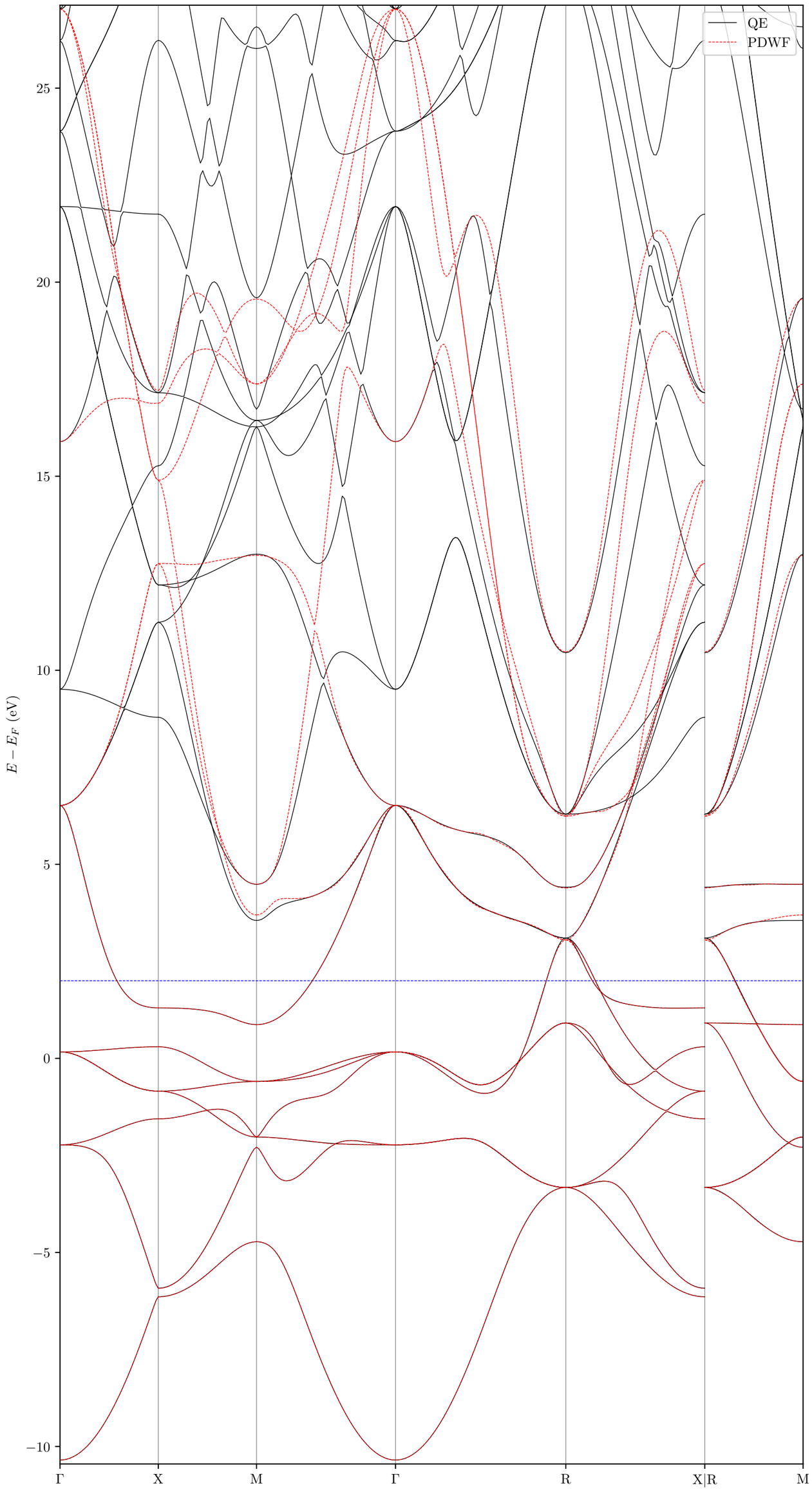

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.8 | 6.5 | 11.9 | 32.9 | 41.8 | 161.2 | 2.445 |

Hamiltonian decay



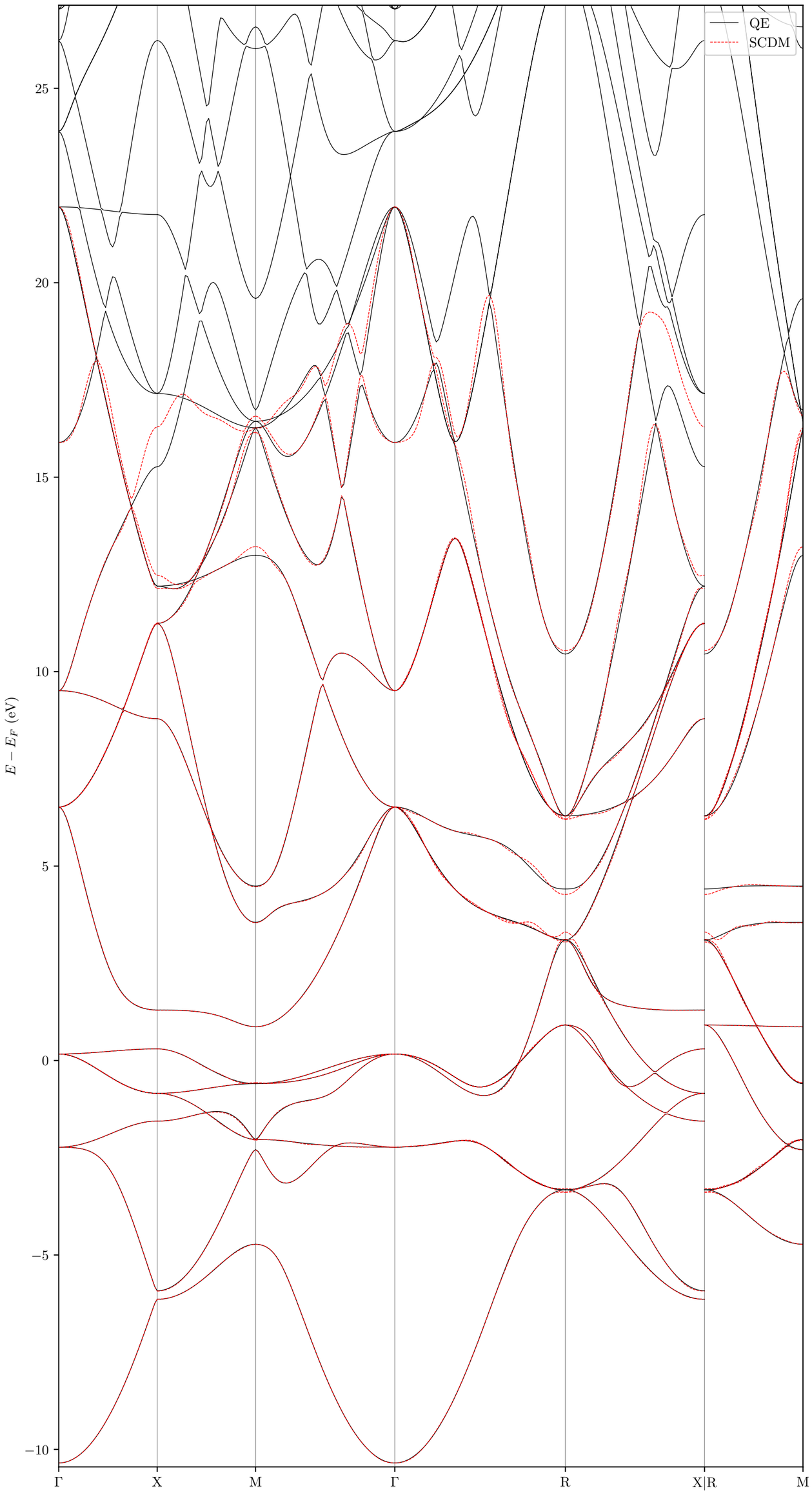
AlFe exclude semicore
PW=7f11785d-8acb-4043-be48-99a4e91dd7b3
W90=ef8b29b4-957e-4541-9e3f-8782c00cc822




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.1 | 4.0 | 17.9 | 11.9 | 28.3 | 150.9 | 1.913 |

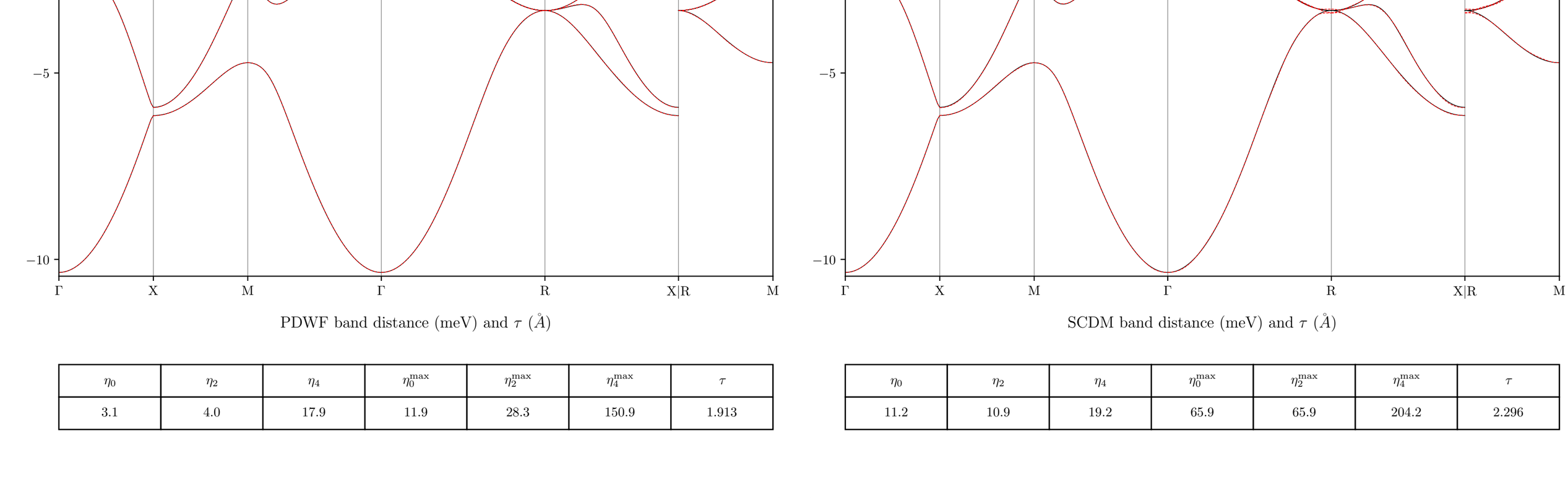
AlFe exclude semicore
PW=7f11785d-8acb-4043-be48-99a4e91dd7b3
W90=8df344ba-9f34-4b8f-99ea-fdbe06e00c2d



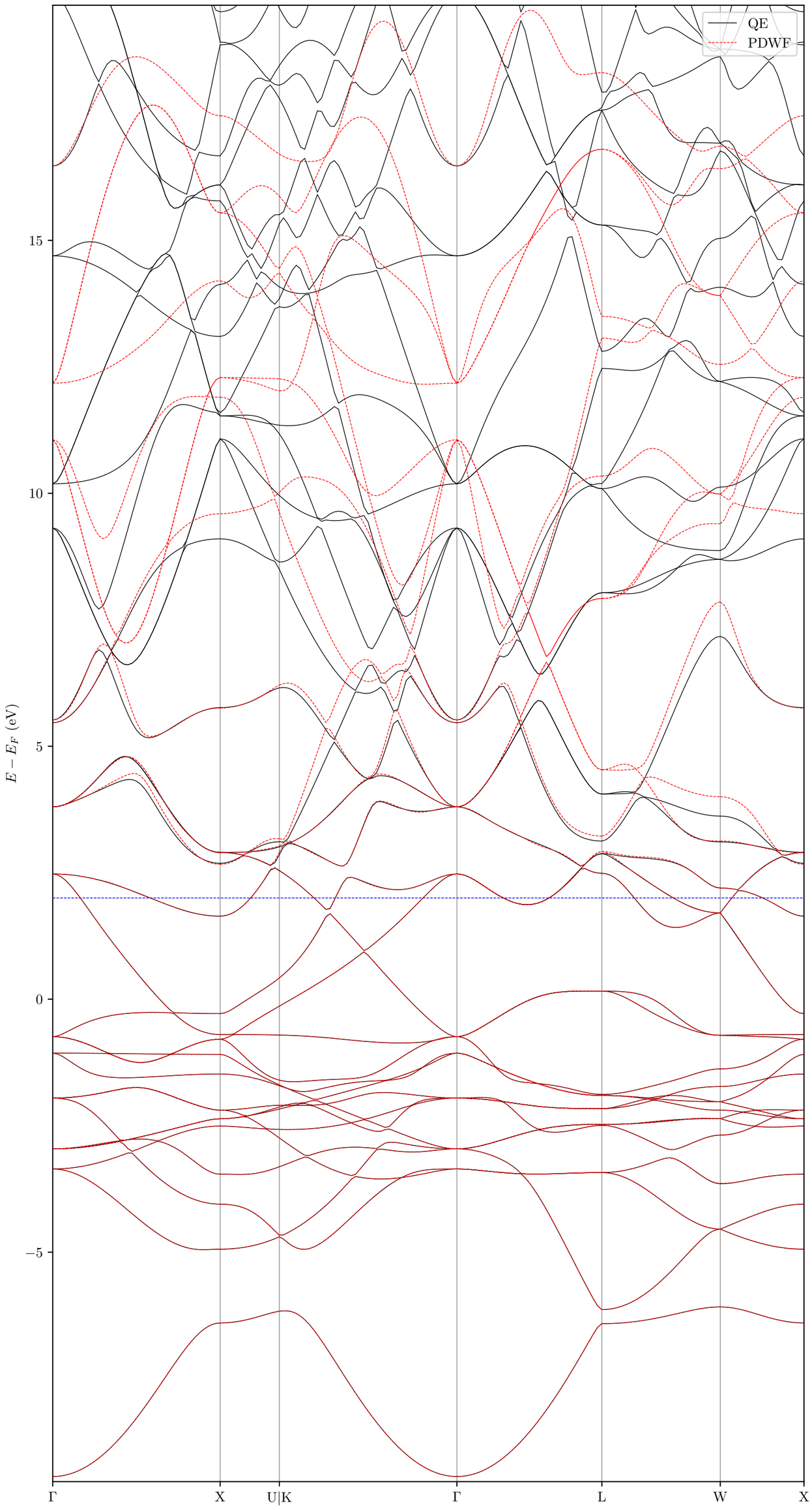

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 11.2 | 10.9 | 19.2 | 65.9 | 65.9 | 204.2 | 2.296 |

Hamiltonian decay



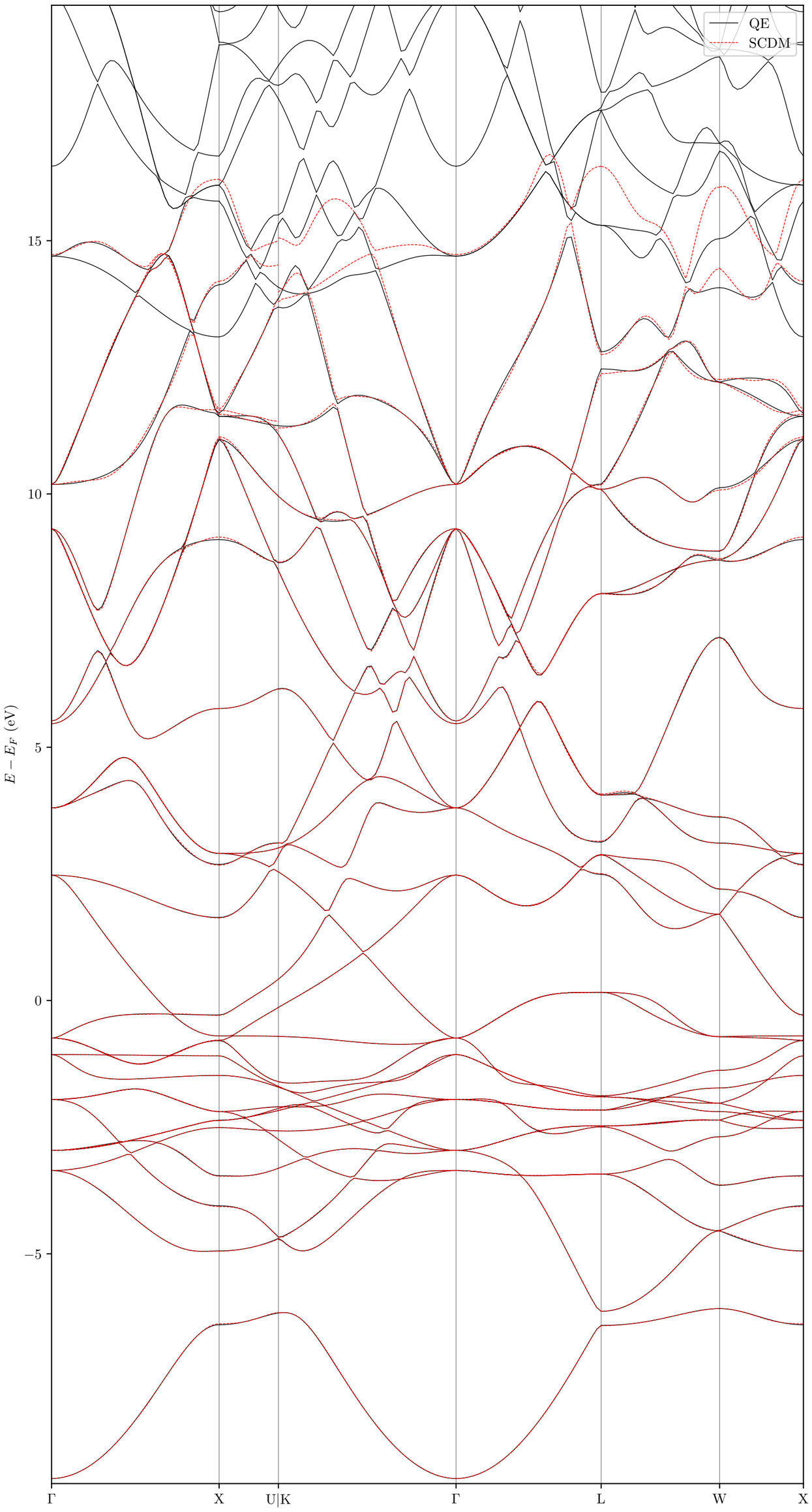
AlHfNi2 exclude semicore
PW=2eac7556-4ea4-4c33-b51e-8e5f934baea7
W90=736f06c7-dded-4eee-bcdc-fb7dcc9ae47e




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.5 | 29.8 | 7.8 | 13.3 | 305.1 | 2.174 |

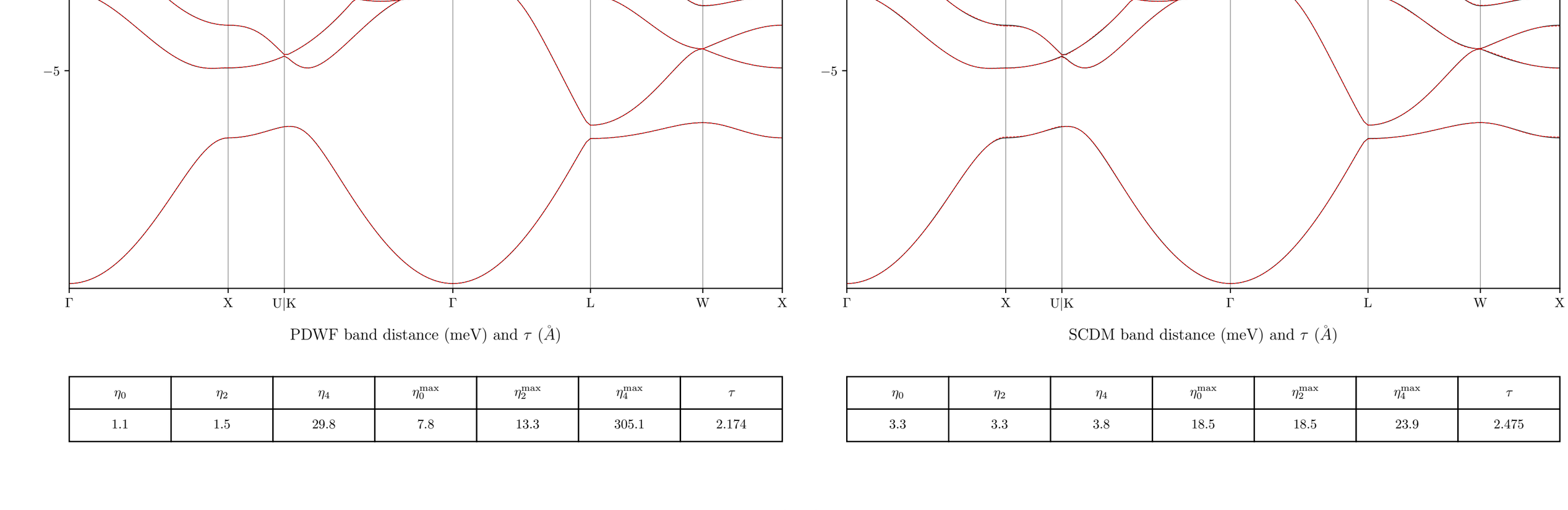
AlHfNi2 exclude semicore
PW=2eac7556-4ea4-4c33-b51e-8e5f934baea7
W90=7b53444c-5aef-41dd-b28f-a52136841b50

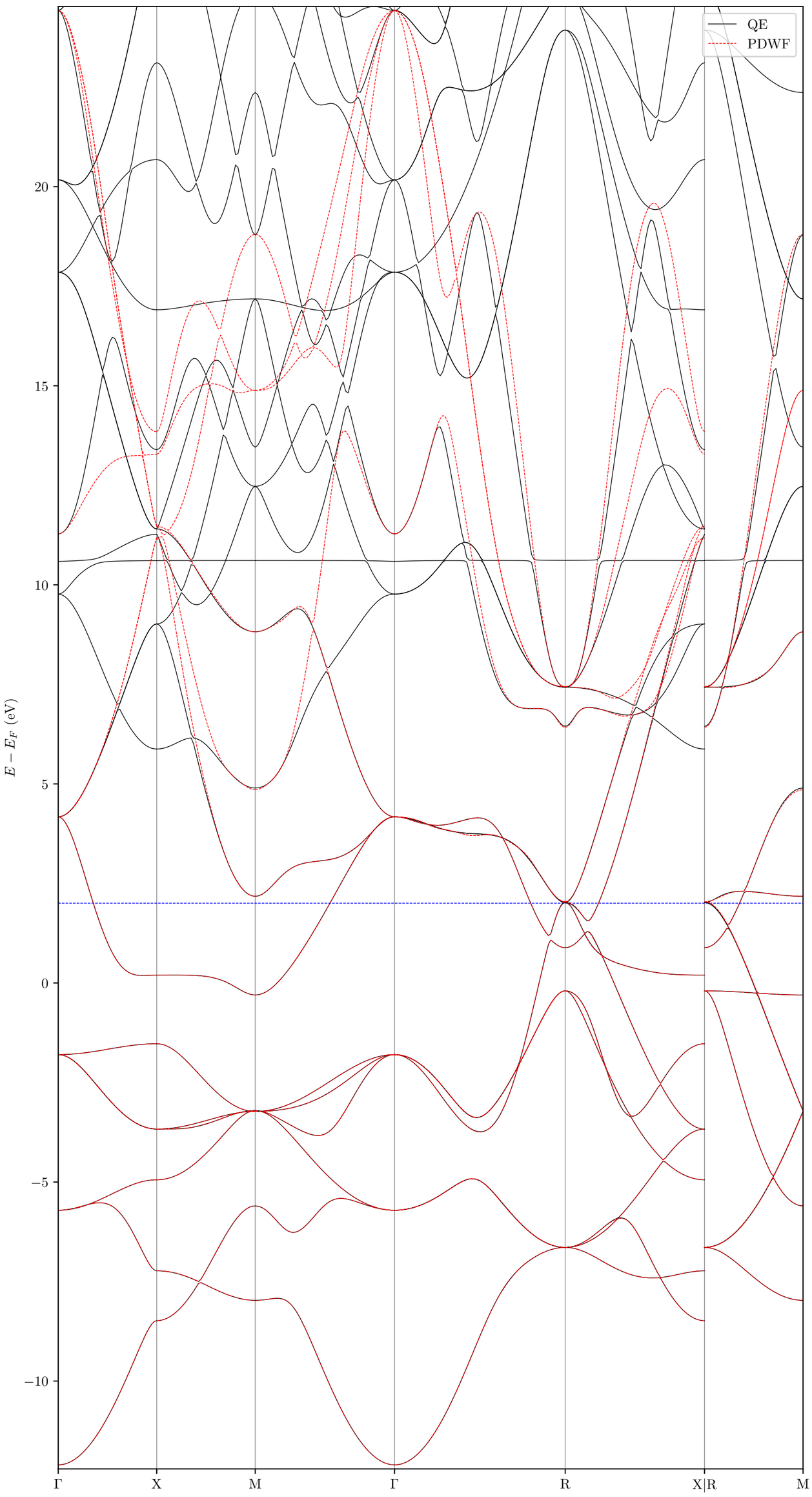



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.3 | 3.3 | 3.8 | 18.5 | 18.5 | 23.9 | 2.475 |

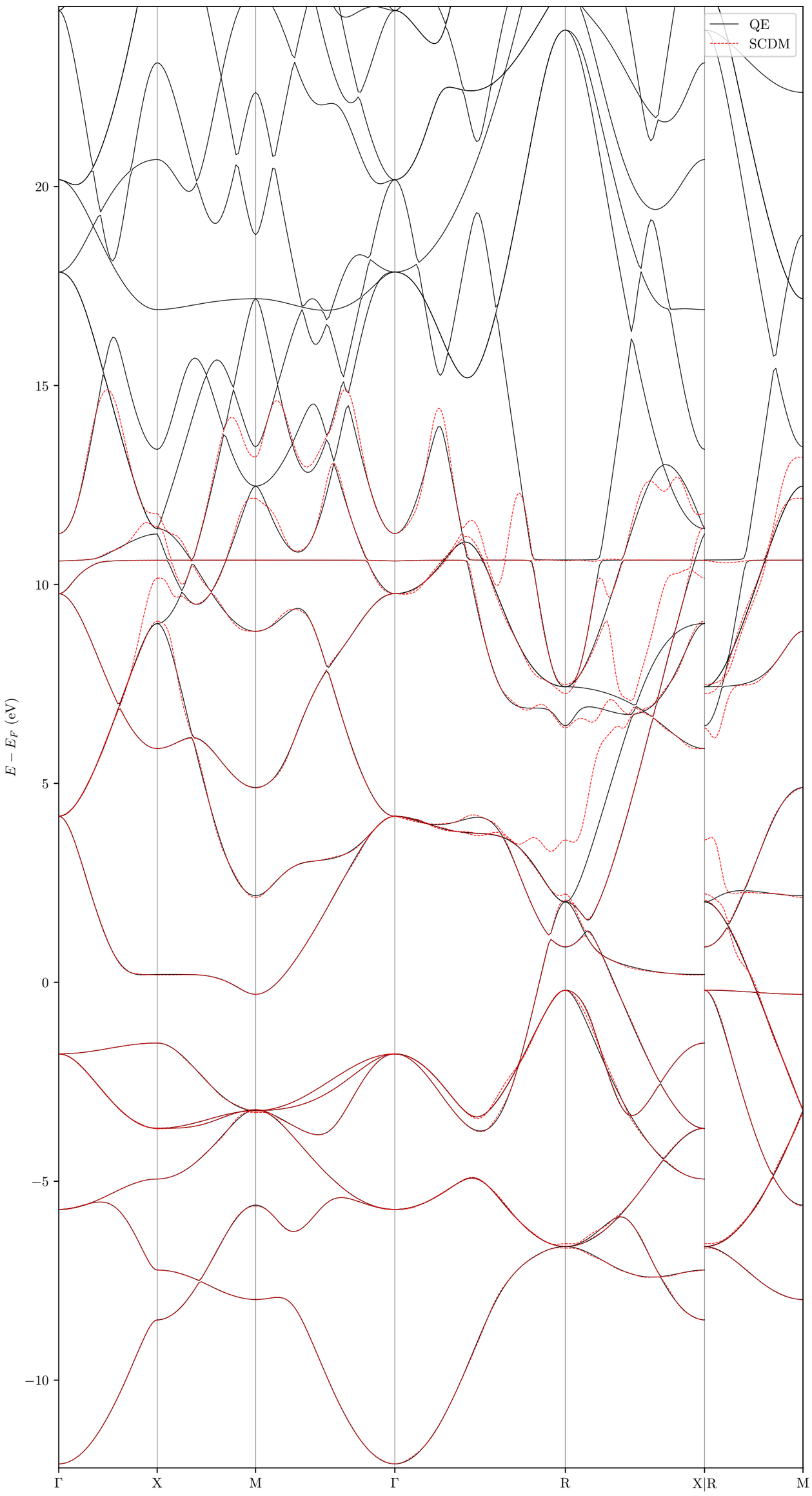
Hamiltonian decay





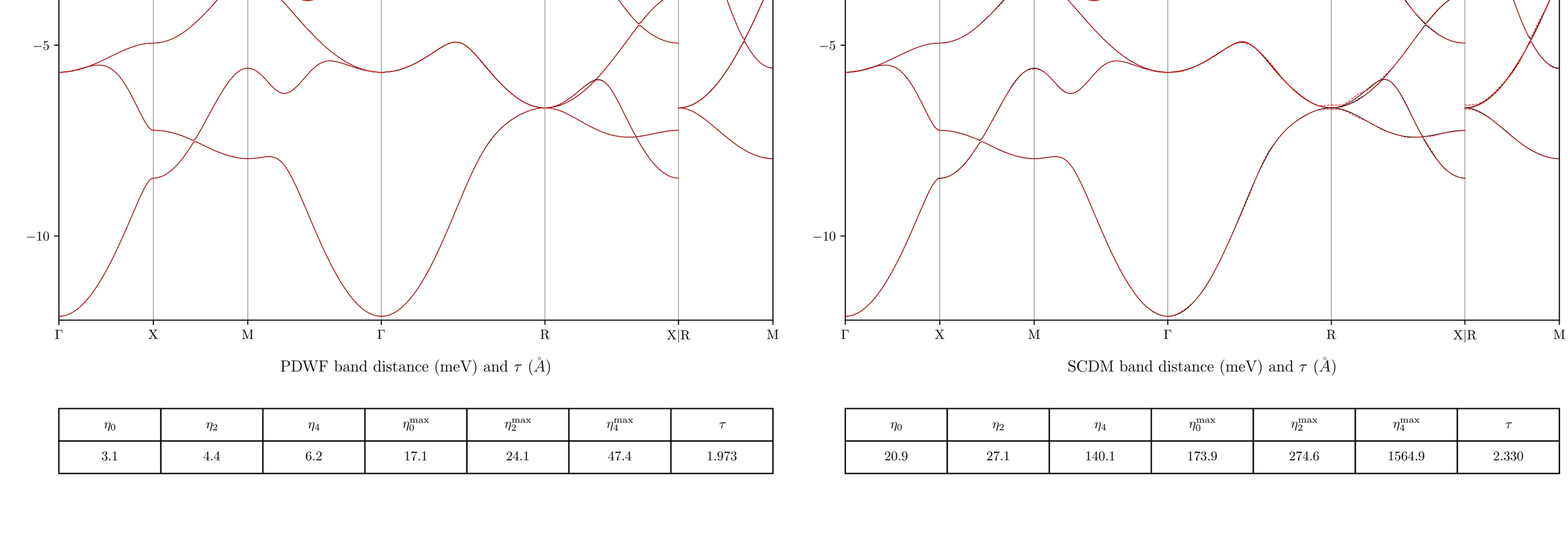

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.1 | 4.4 | 6.2 | 17.1 | 24.1 | 47.4 | 1.973 |

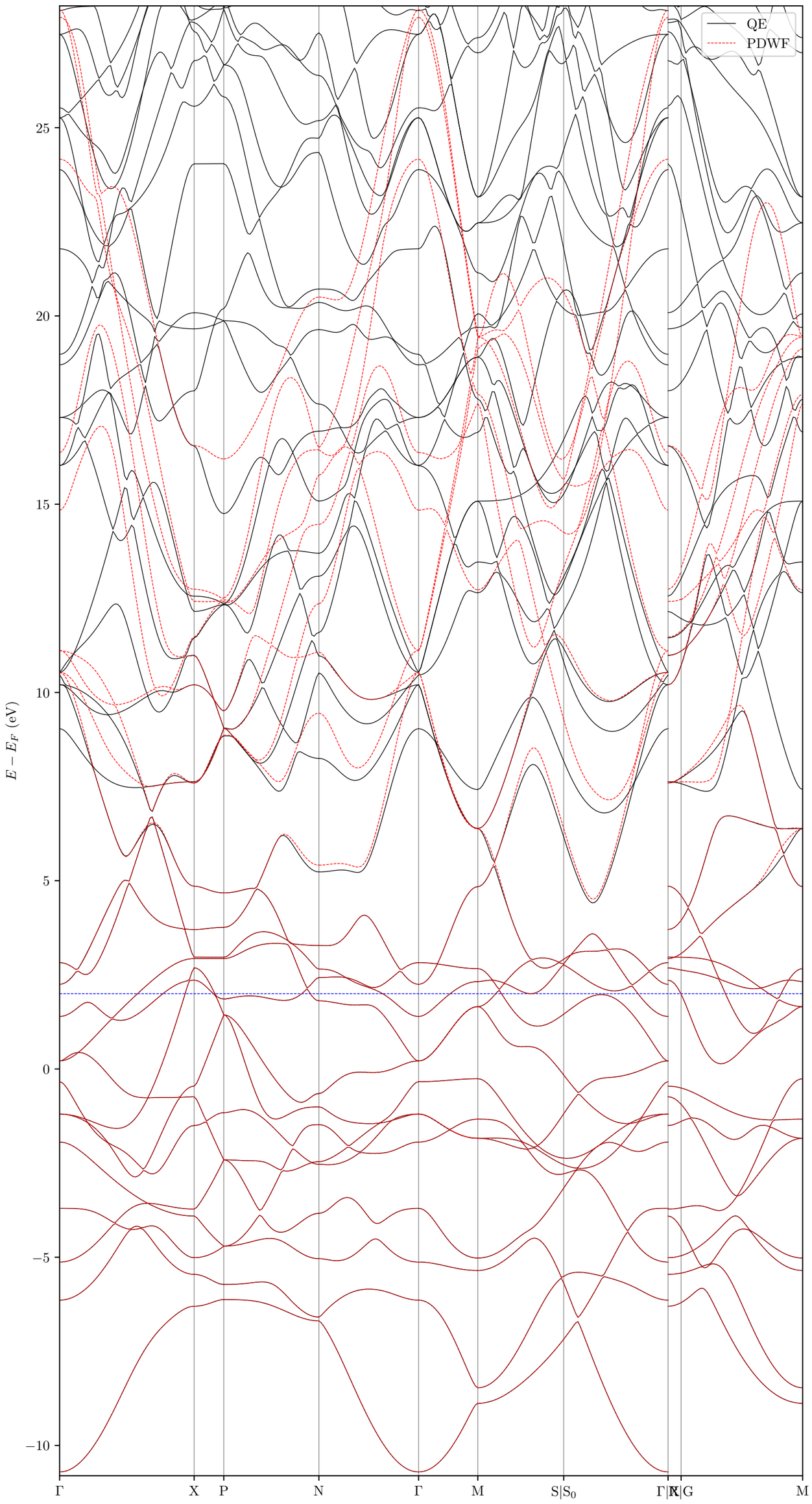



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 20.9 | 27.1 | 140.1 | 173.9 | 274.6 | 1564.9 | 2.330 |



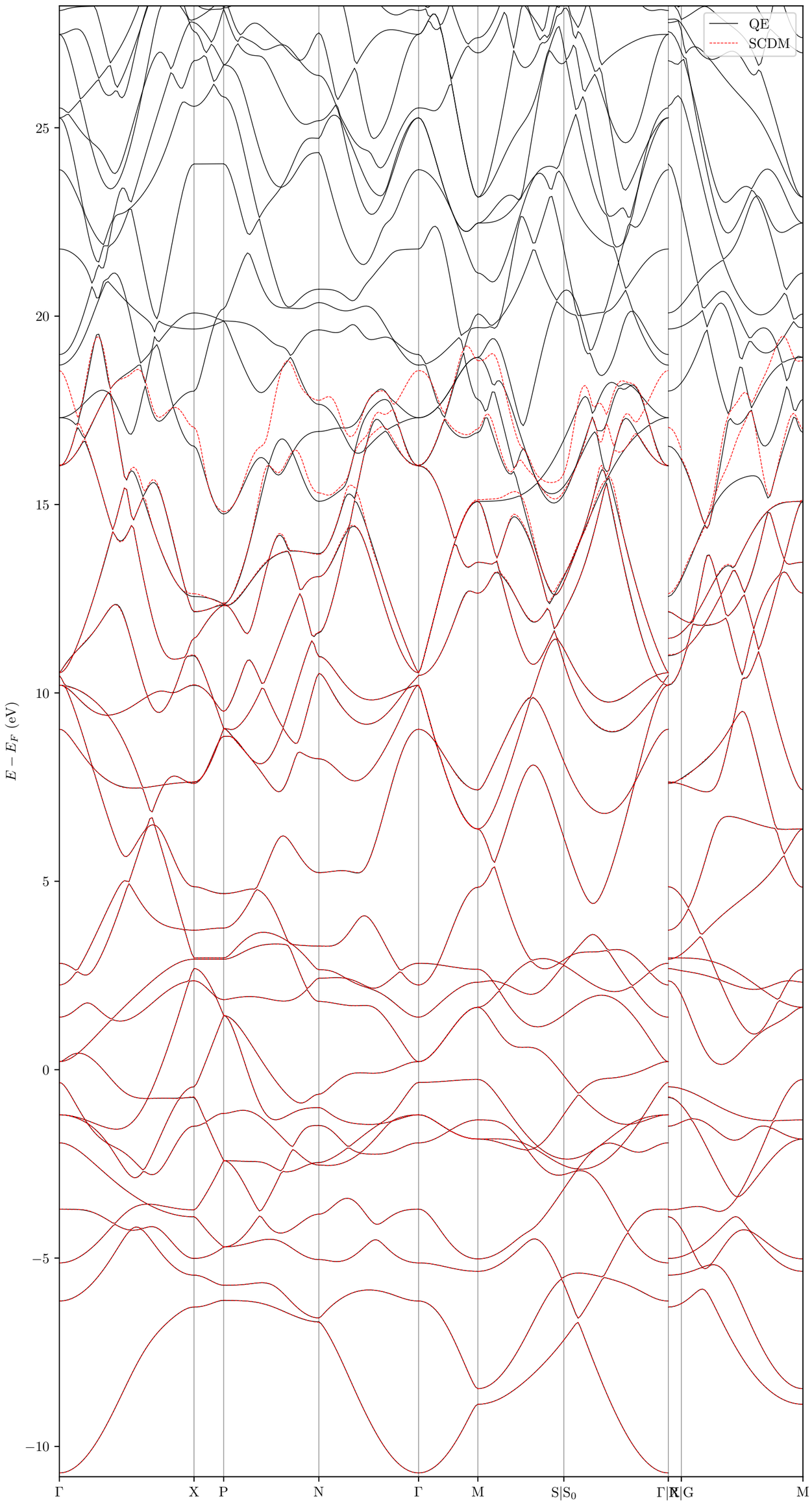
AlRe2 exclude semicore
PW=587d62e9-a5e8-4209-bd91-2c7720b5eab4
W90=d0cae88a-7f12-4367-b721-f76b9db38ff3




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.5 | 1.6 | 1.8 | 8.0 | 8.0 | 17.4 | 2.460 |

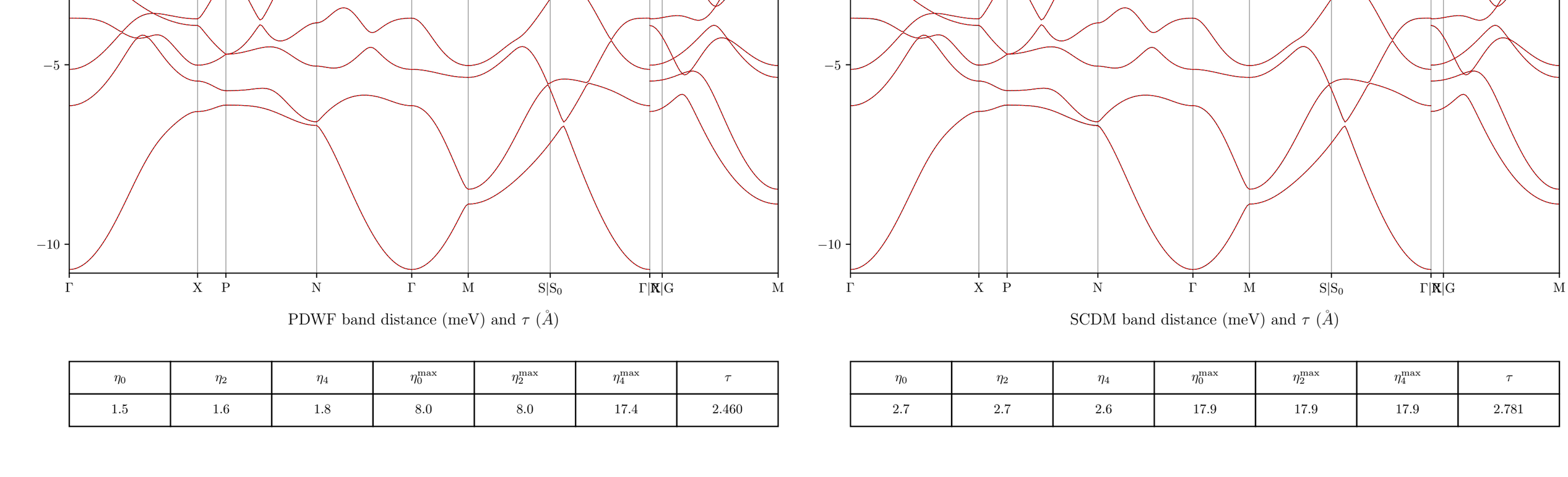
AlRe2 exclude semicore
PW=587d62e9-a5e8-4209-bd91-2c7720b5eab4
W90=c09626bf-db0d-4ab3-8dbe-f0a9063c56d1

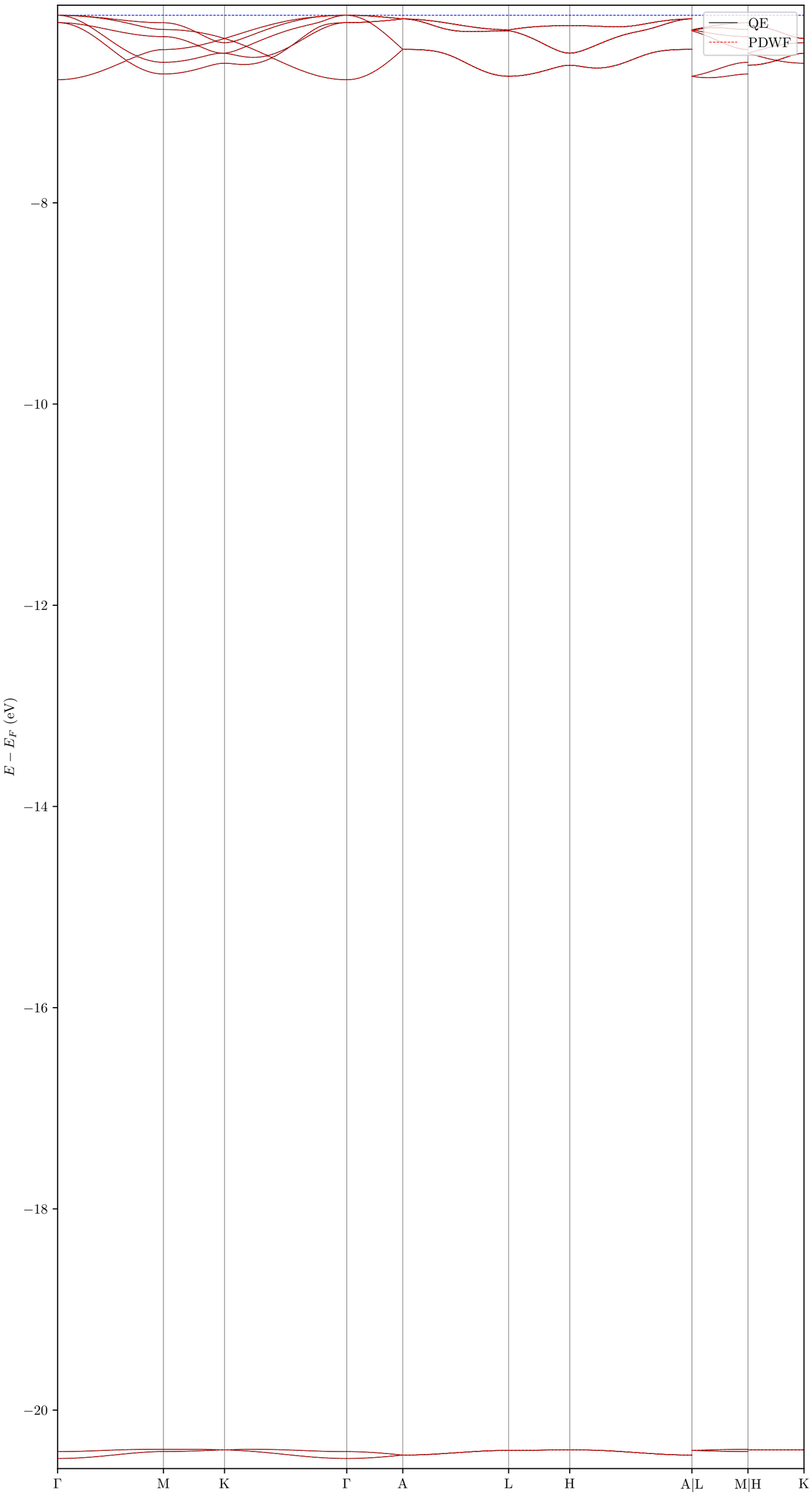



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.7 | 2.7 | 2.6 | 17.9 | 17.9 | 17.9 | 2.781 |

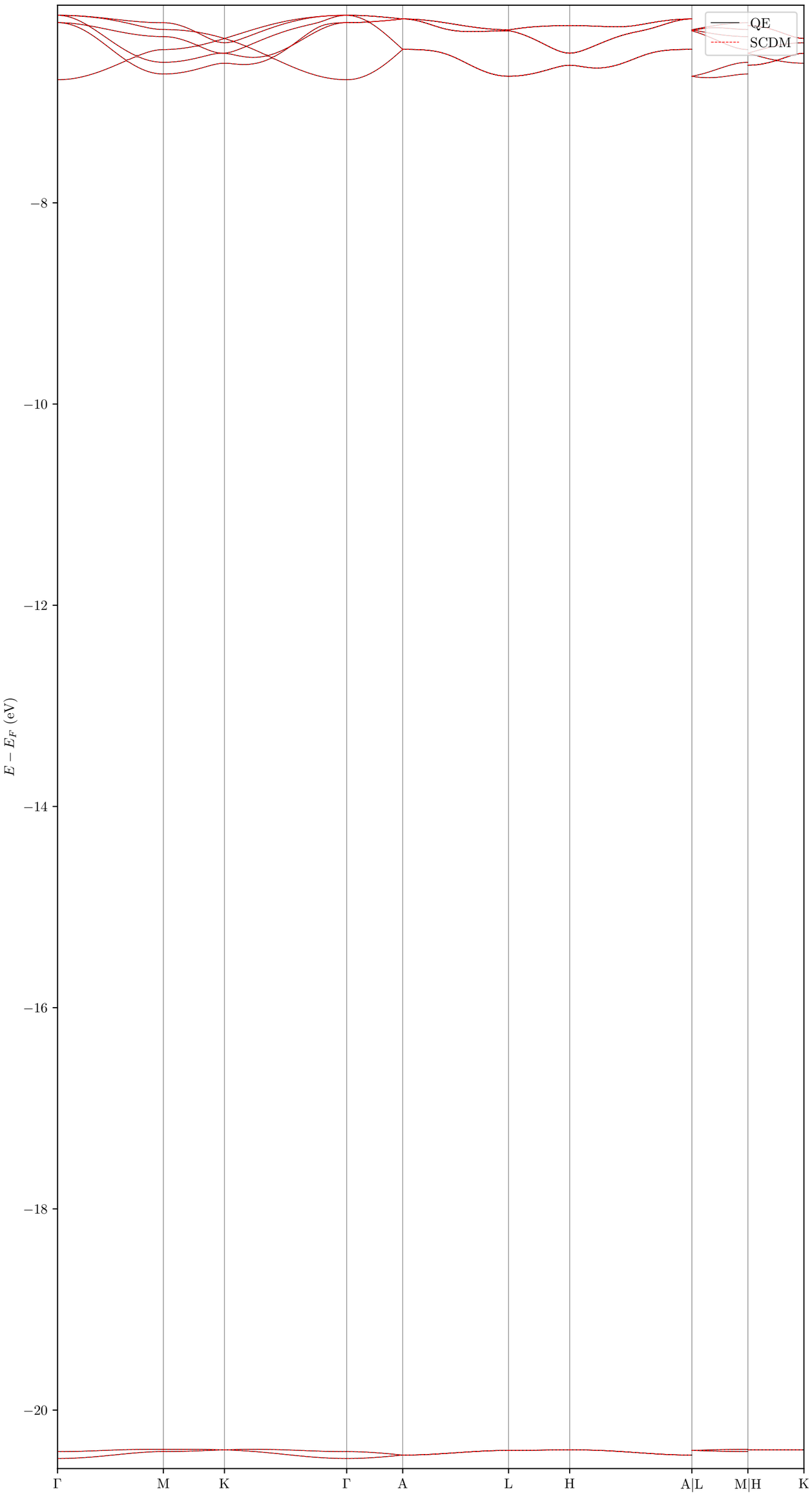
Hamiltonian decay





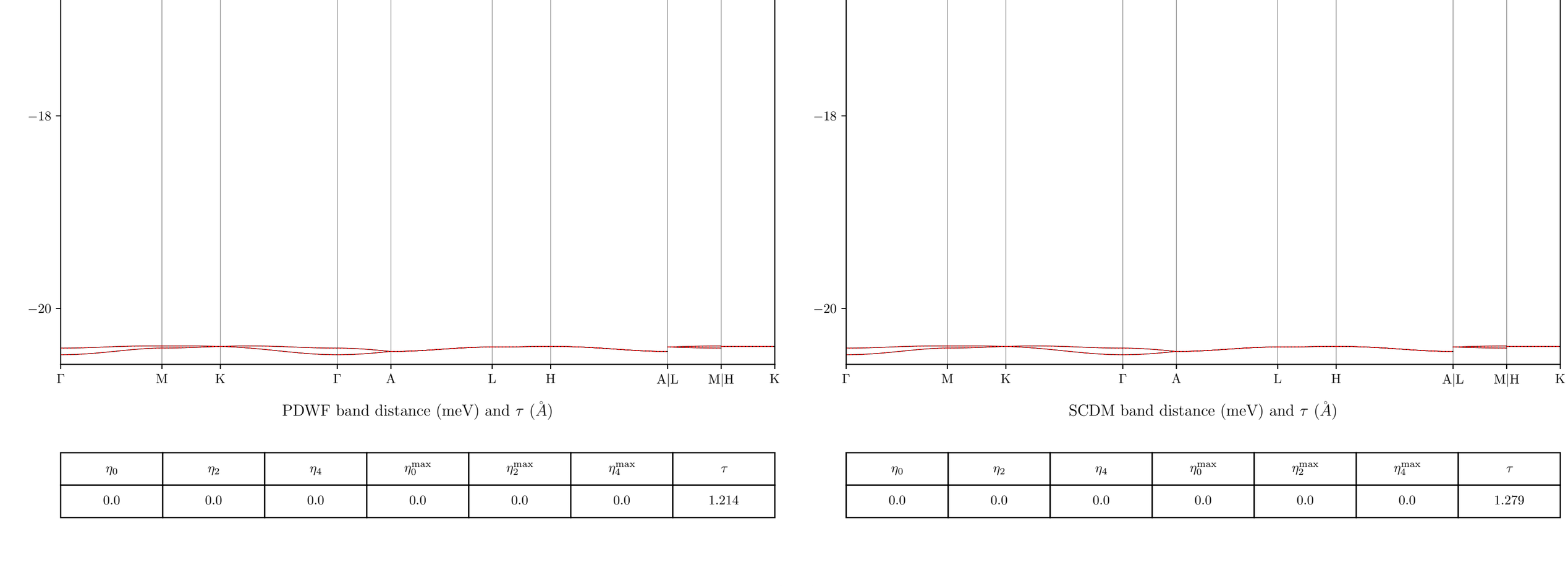

PDWF band distance (meV) and $\tau$ ($\AA$)

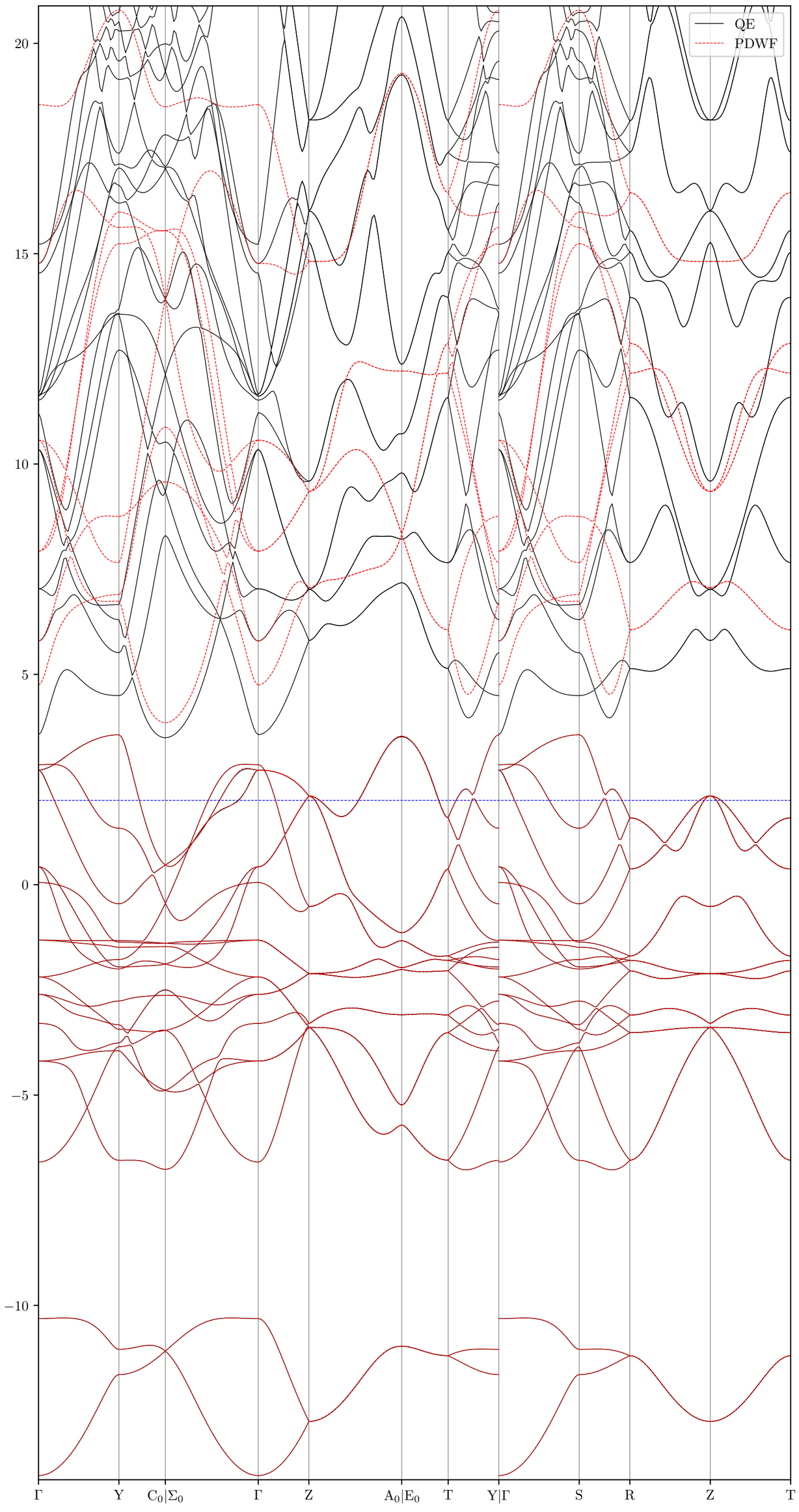
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 1.214 |




SCDM band distance (meV) and $\tau$ ($\AA$)

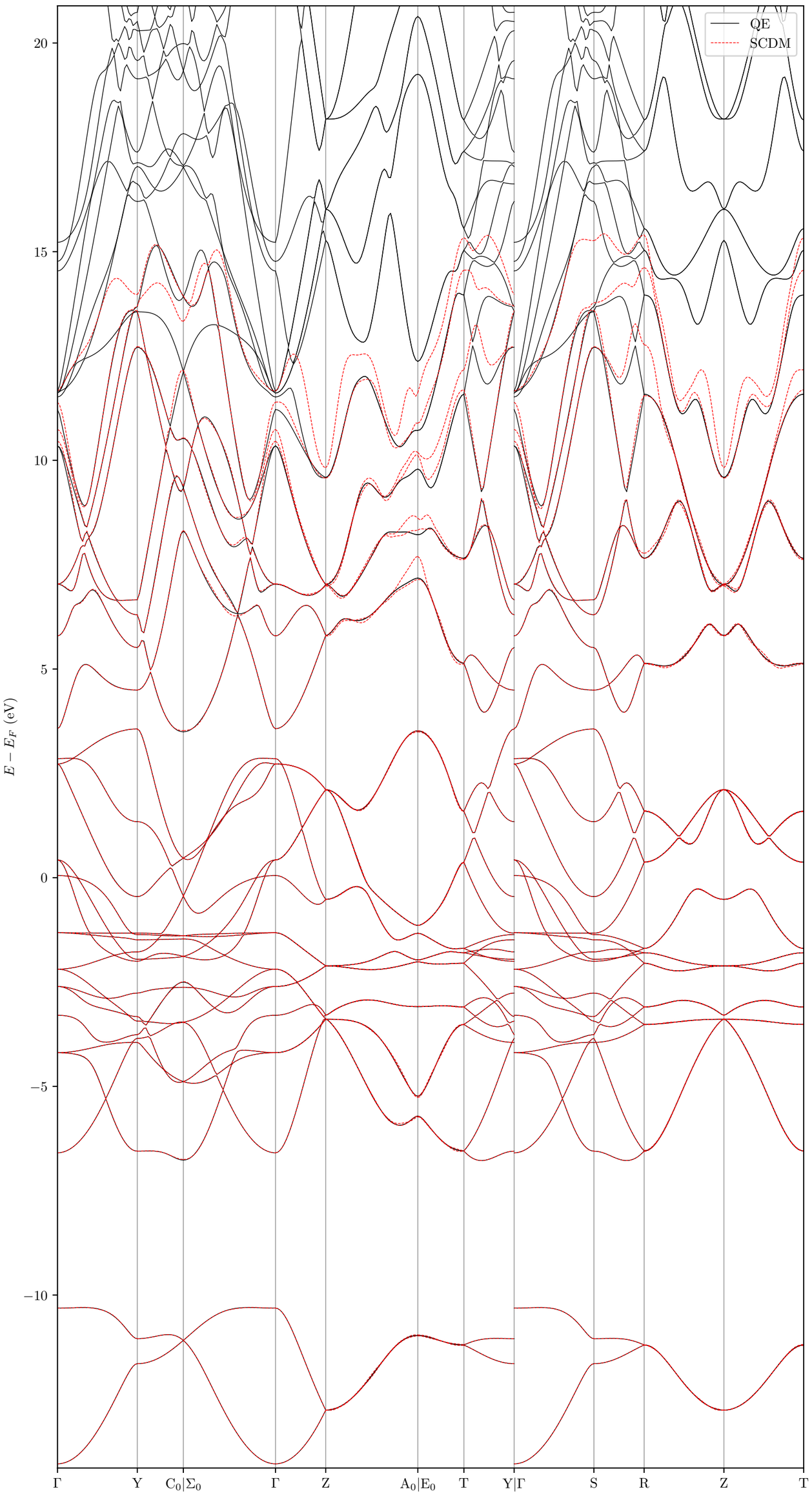
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 1.279 |





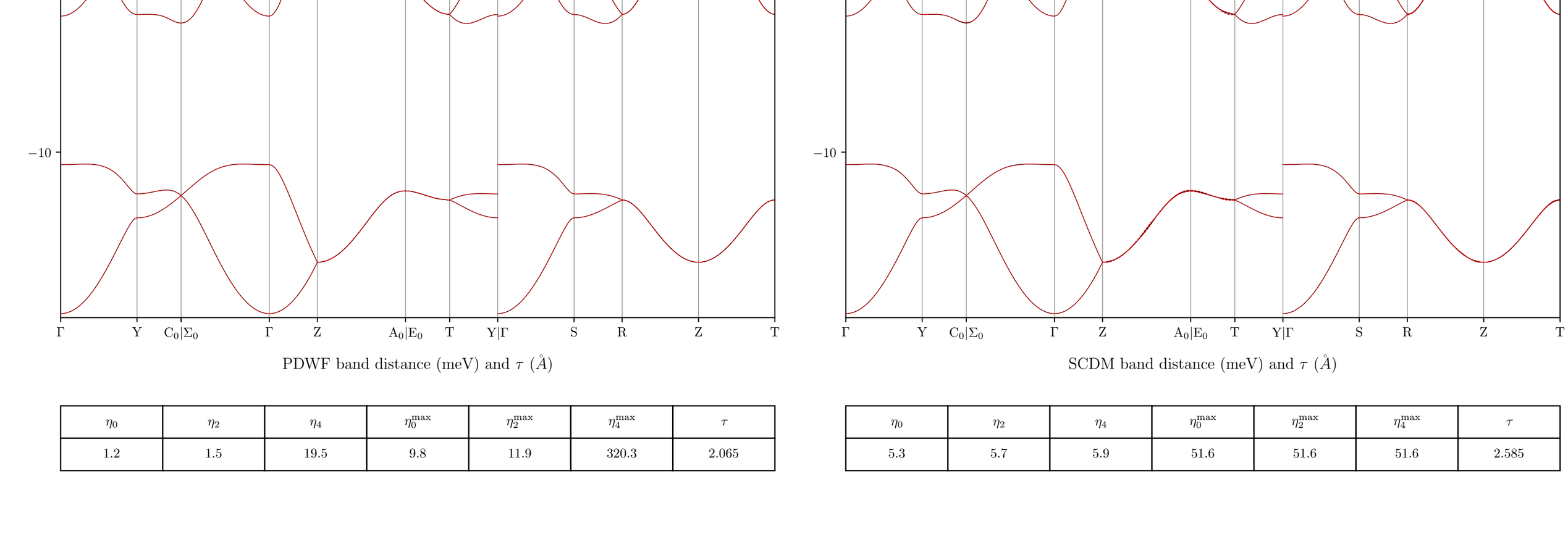

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.5 | 19.5 | 9.8 | 11.9 | 320.3 | 2.065 |

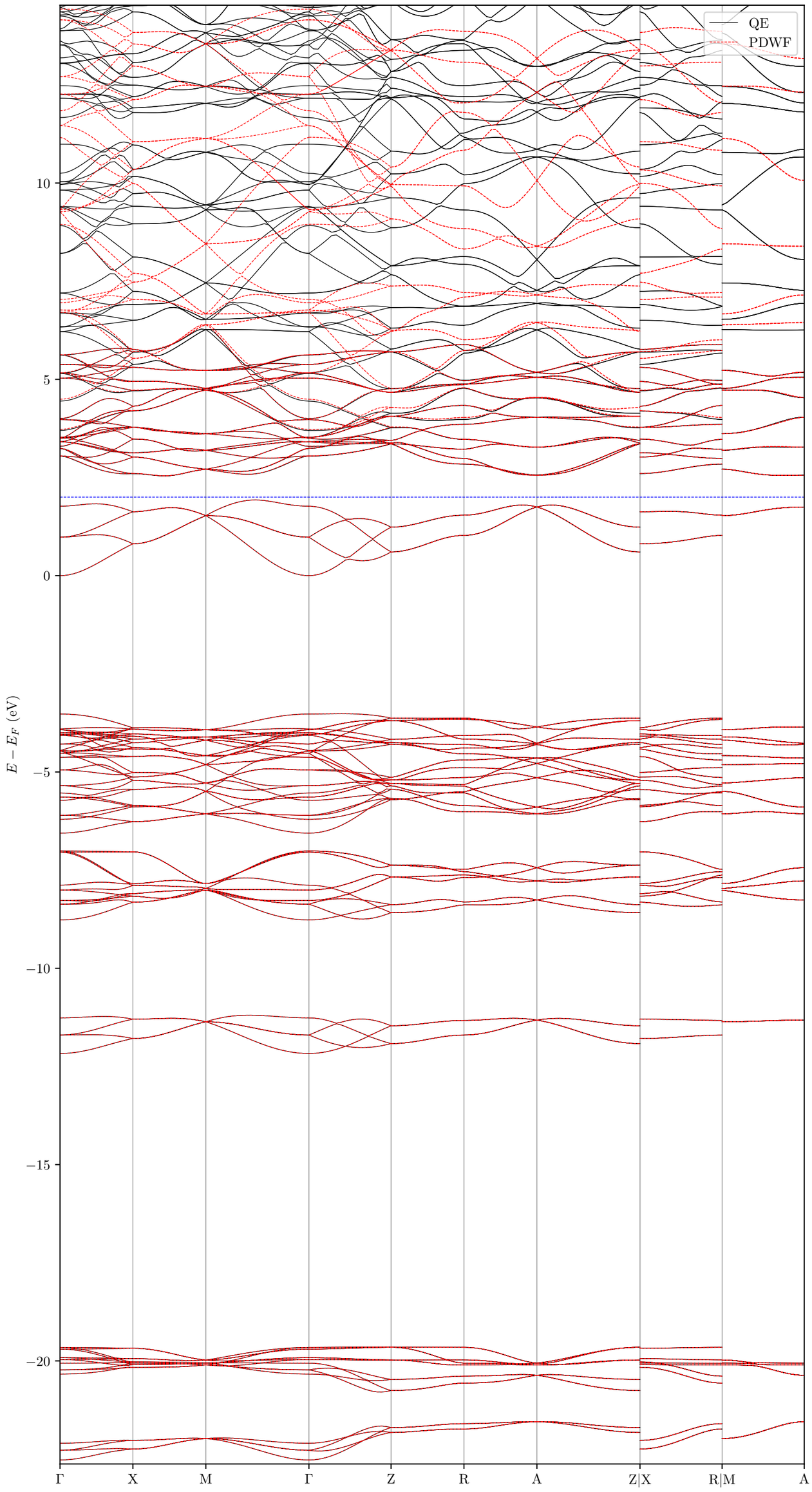



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.3 | 5.7 | 5.9 | 51.6 | 51.6 | 51.6 | 2.585 |



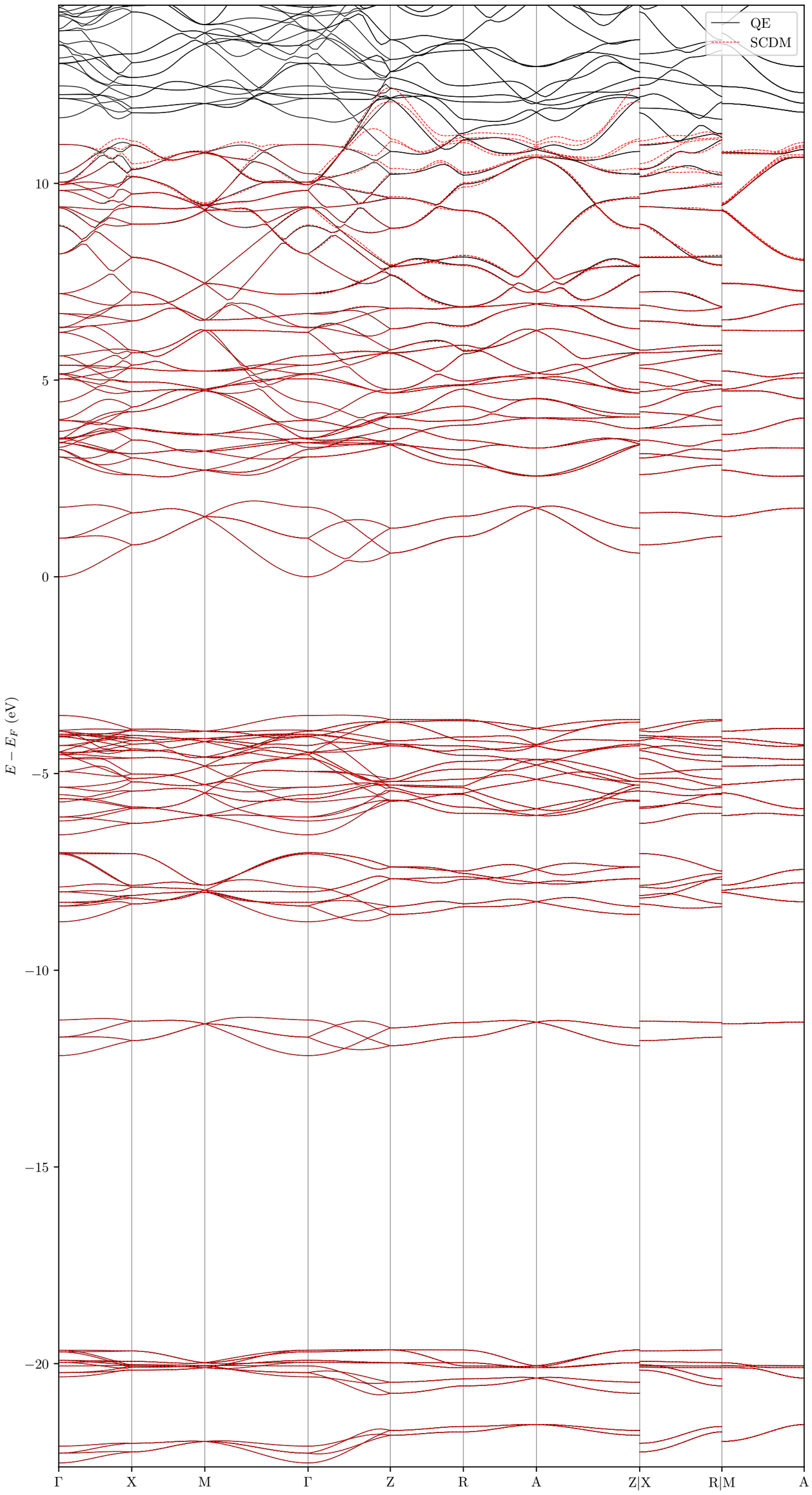
As4O16Y4 exclude semicore
PW=22bdd6e4-7a55-4a93-9e0f-5d3b954b3904
W90=96bc9f2f-af71-4d1b-99c3-af3f6486e365




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.5 | 0.9 | 4.7 | 4.7 | 9.9 | 2.726 |

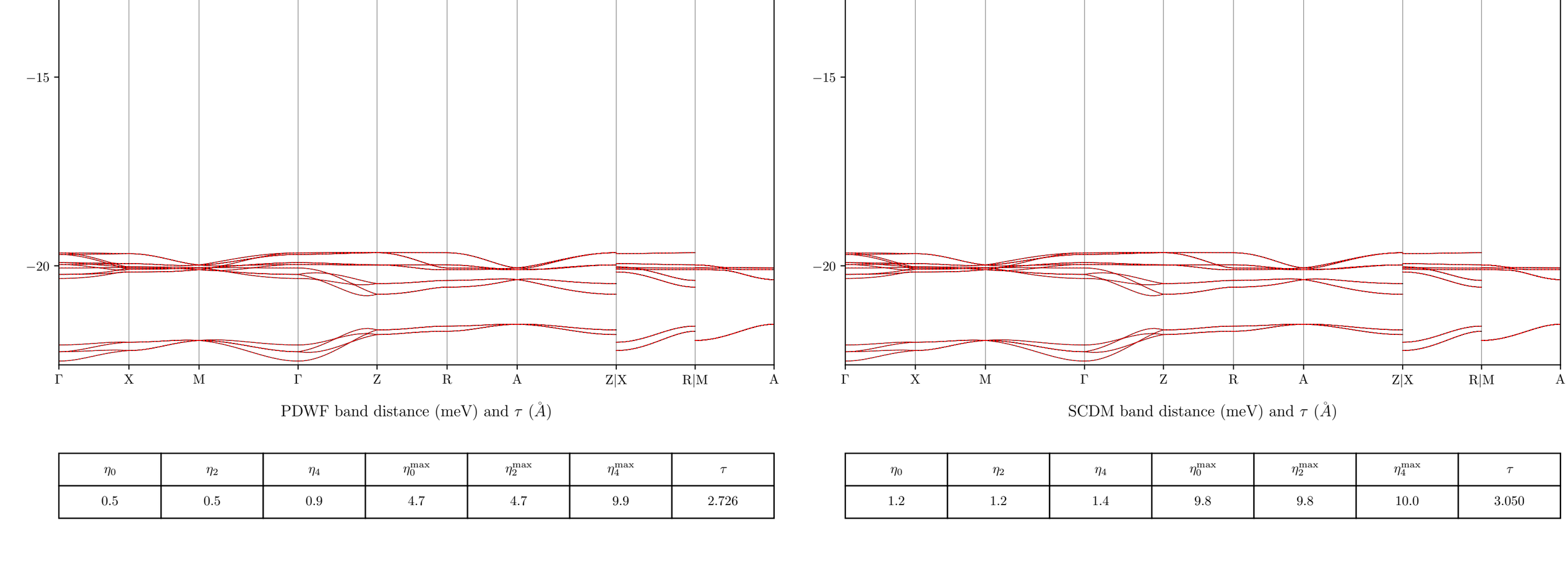
As4O16Y4 exclude semicore
PW=22bdd6e4-7a55-4a93-9e0f-5d3b954b3904
W90=c21953a5-59e8-4036-8596-755fefed7c76



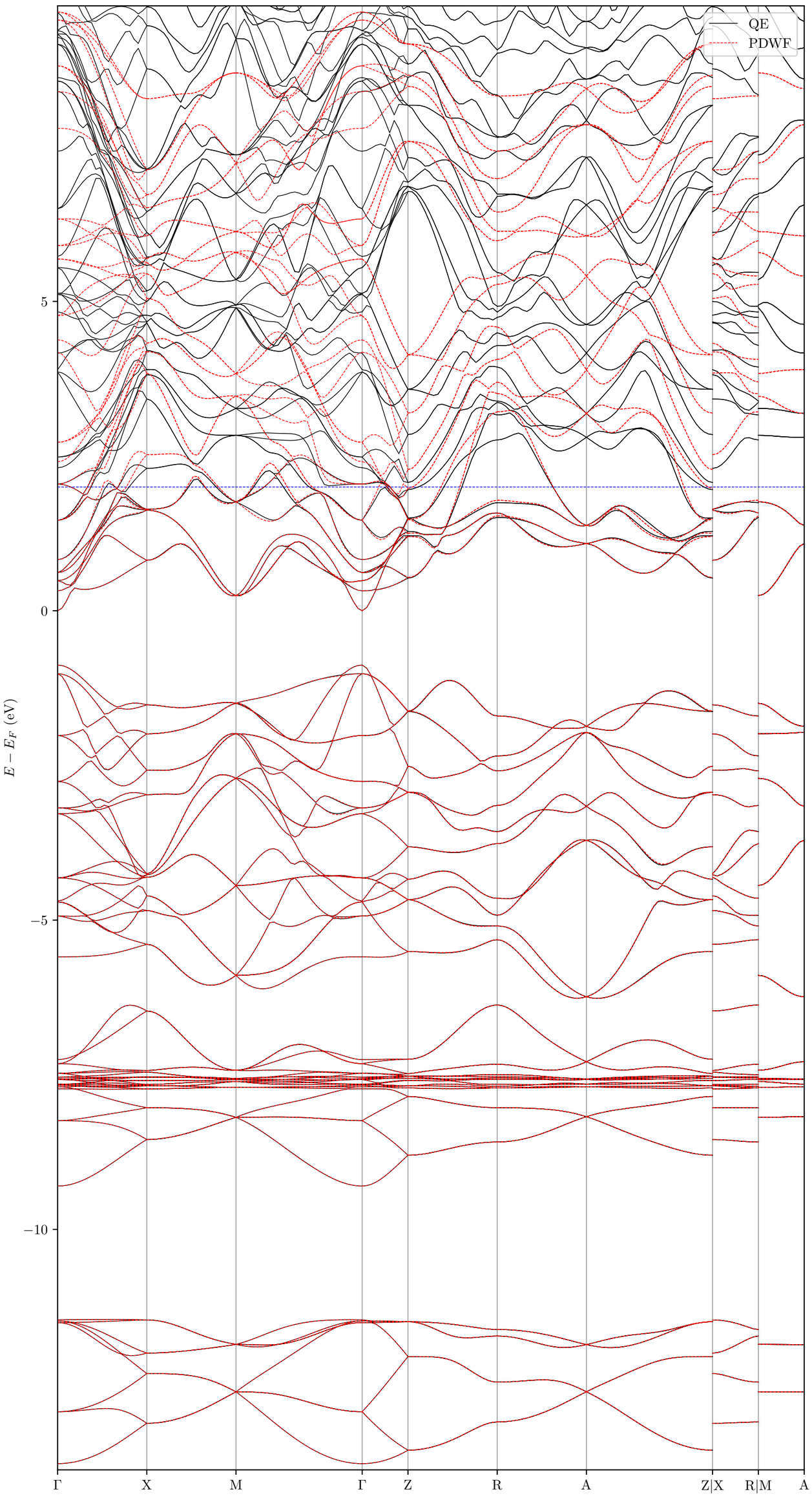

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.2 | 1.4 | 9.8 | 9.8 | 10.0 | 3.050 |

Hamiltonian decay



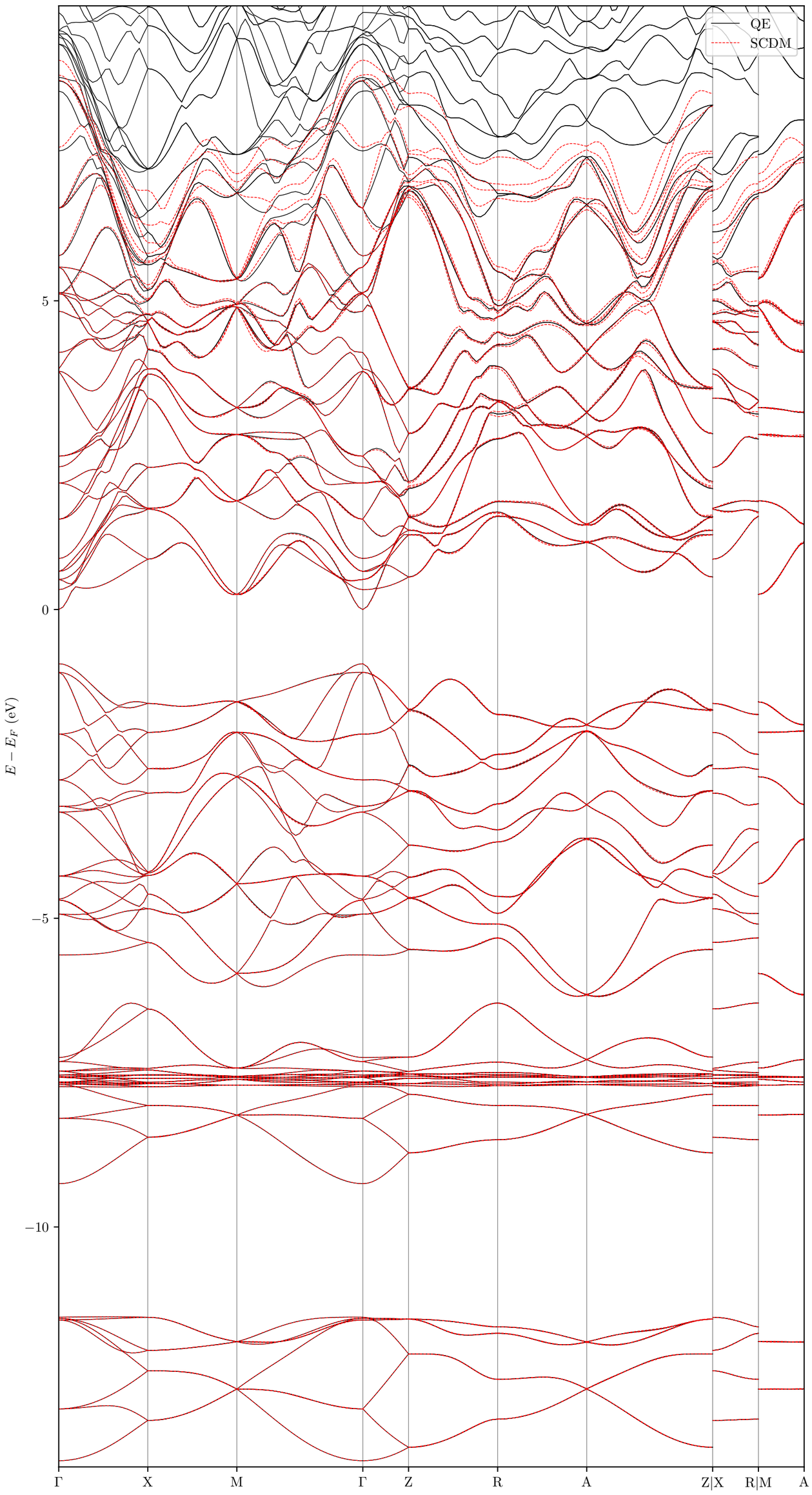
As8Si4Zn4 exclude semicore
PW=322b5976-49af-4131-af2d-2940602d7137
W90=46b37832-98cb-4c7d-b886-5e37d23614e9




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.8 | 4.8 | 105.6 | 18.8 | 54.5 | 591.3 | 3.046 |

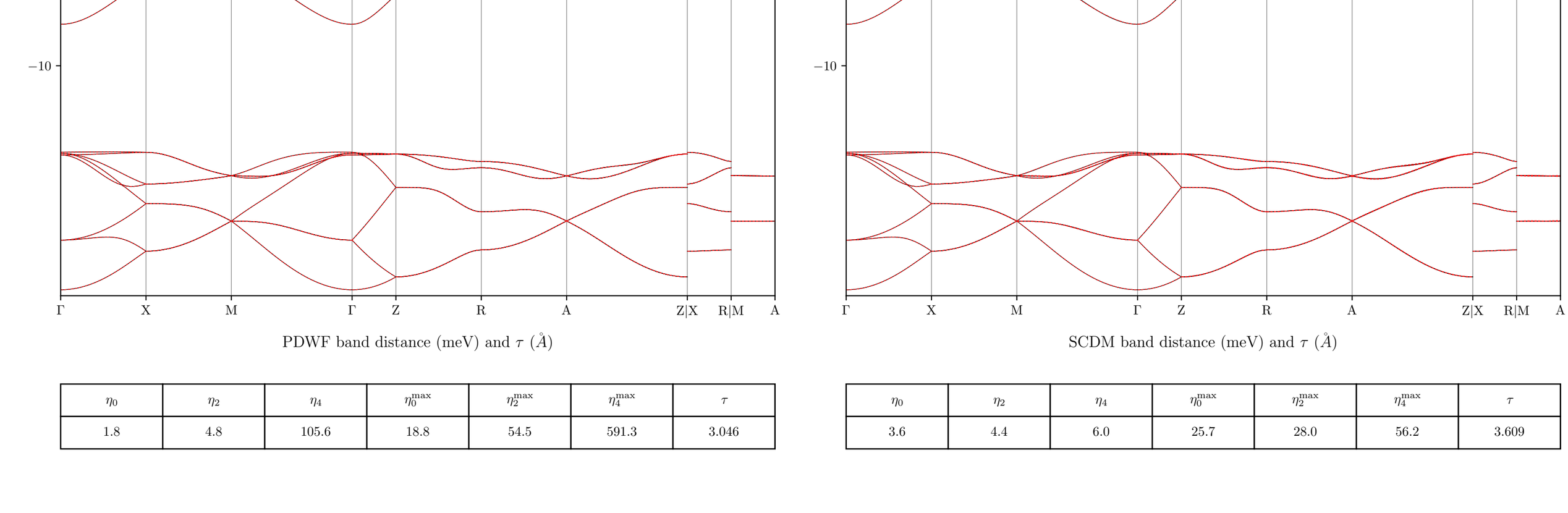
As8Si4Zn4 exclude semicore
PW=322b5976-49af-4131-af2d-2940602d7137
W90=d1043d26-7b2a-4ccb-8c58-3a8bb9be64f0

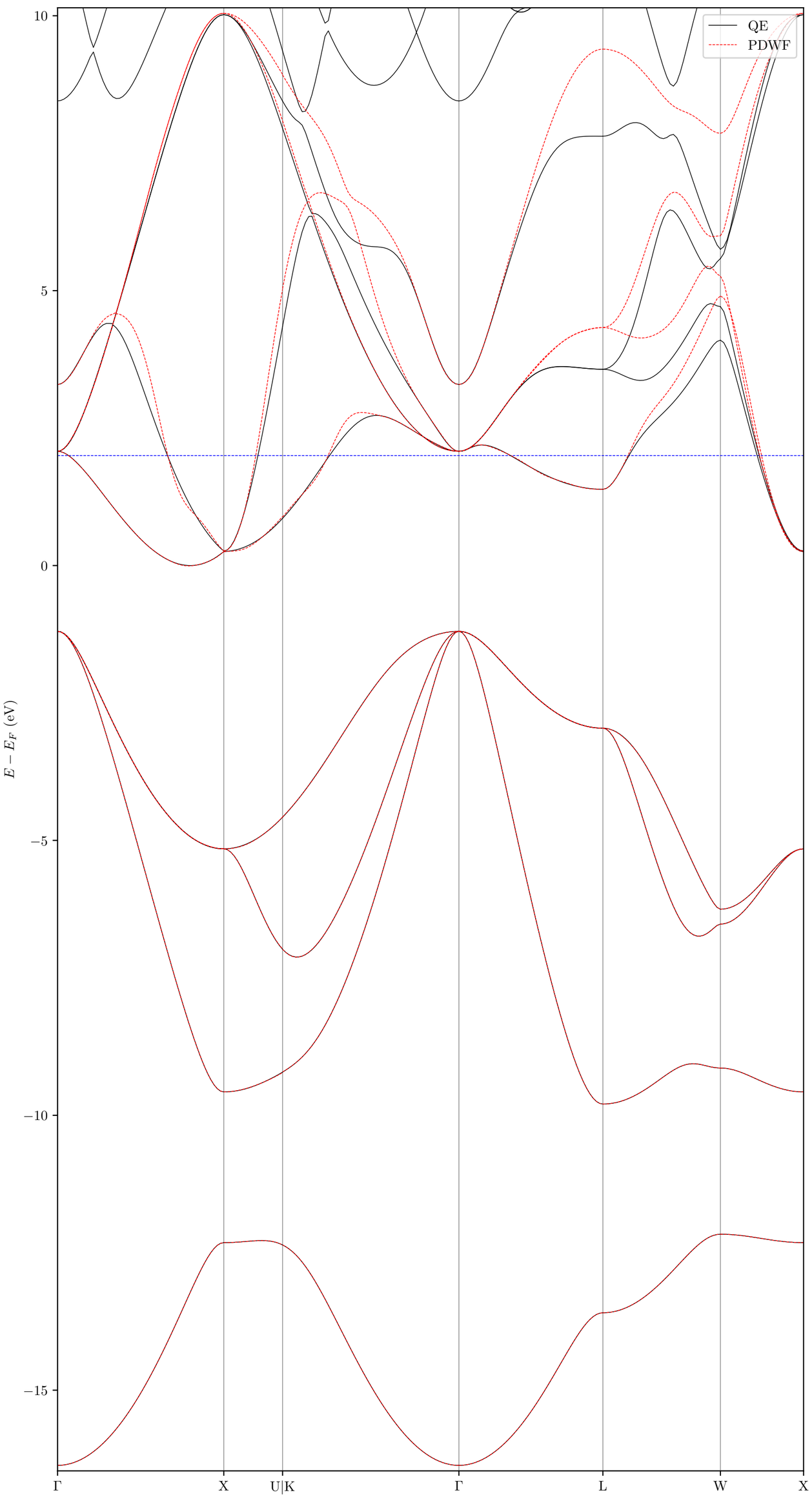



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.6 | 4.4 | 6.0 | 25.7 | 28.0 | 56.2 | 3.609 |

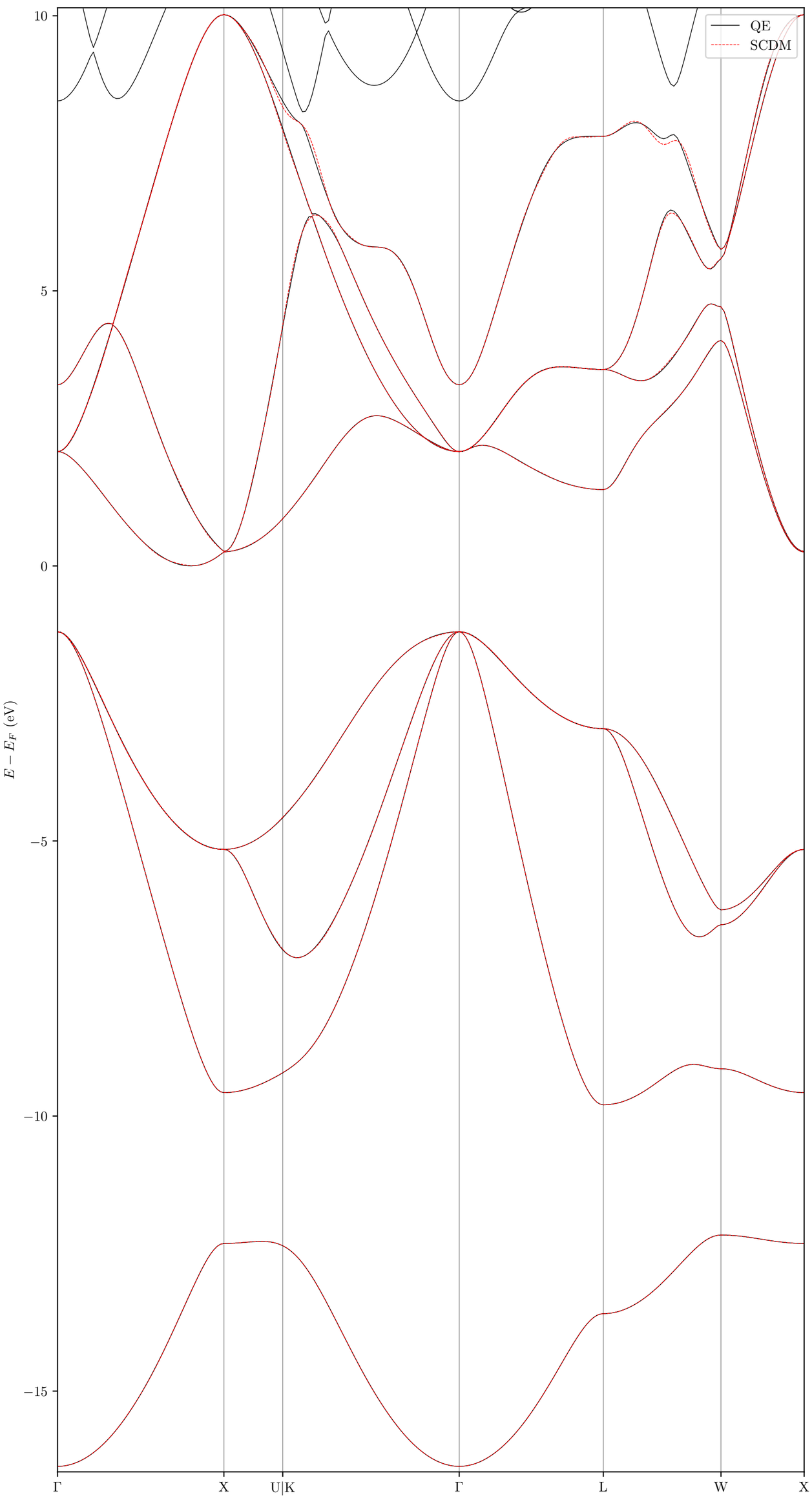
Hamiltonian decay





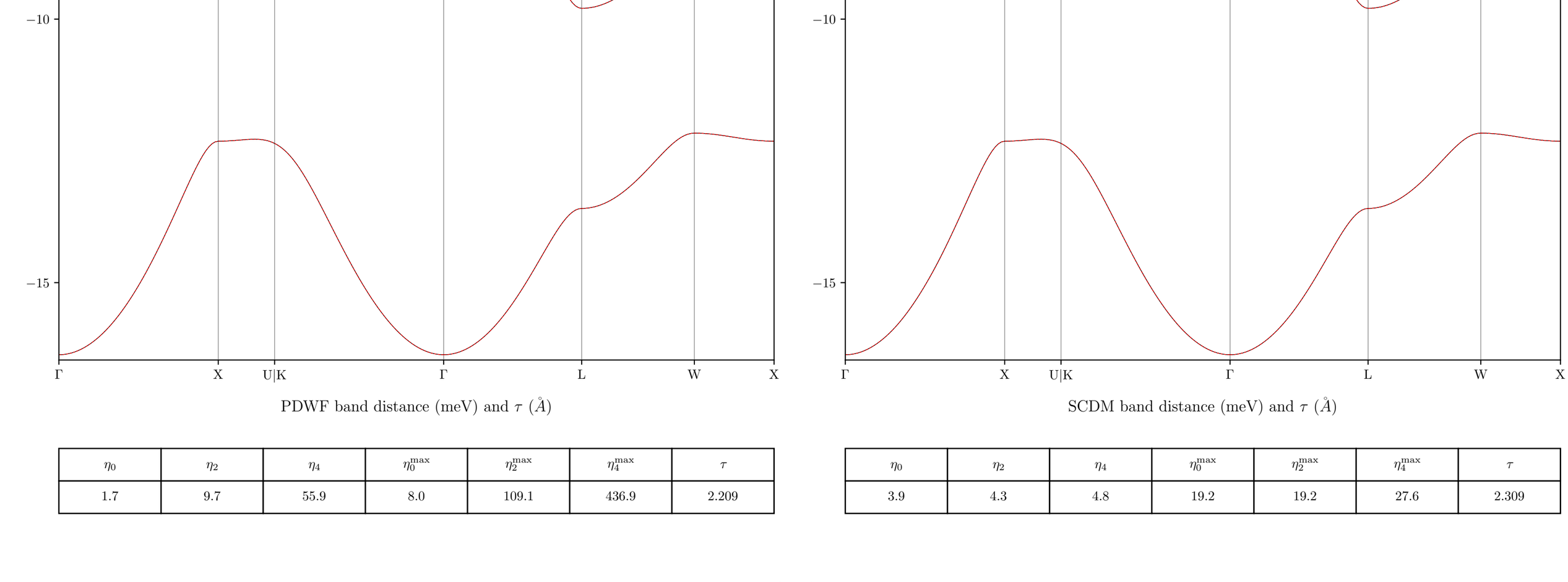

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.7 | 9.7 | 55.9 | 8.0 | 109.1 | 436.9 | 2.209 |

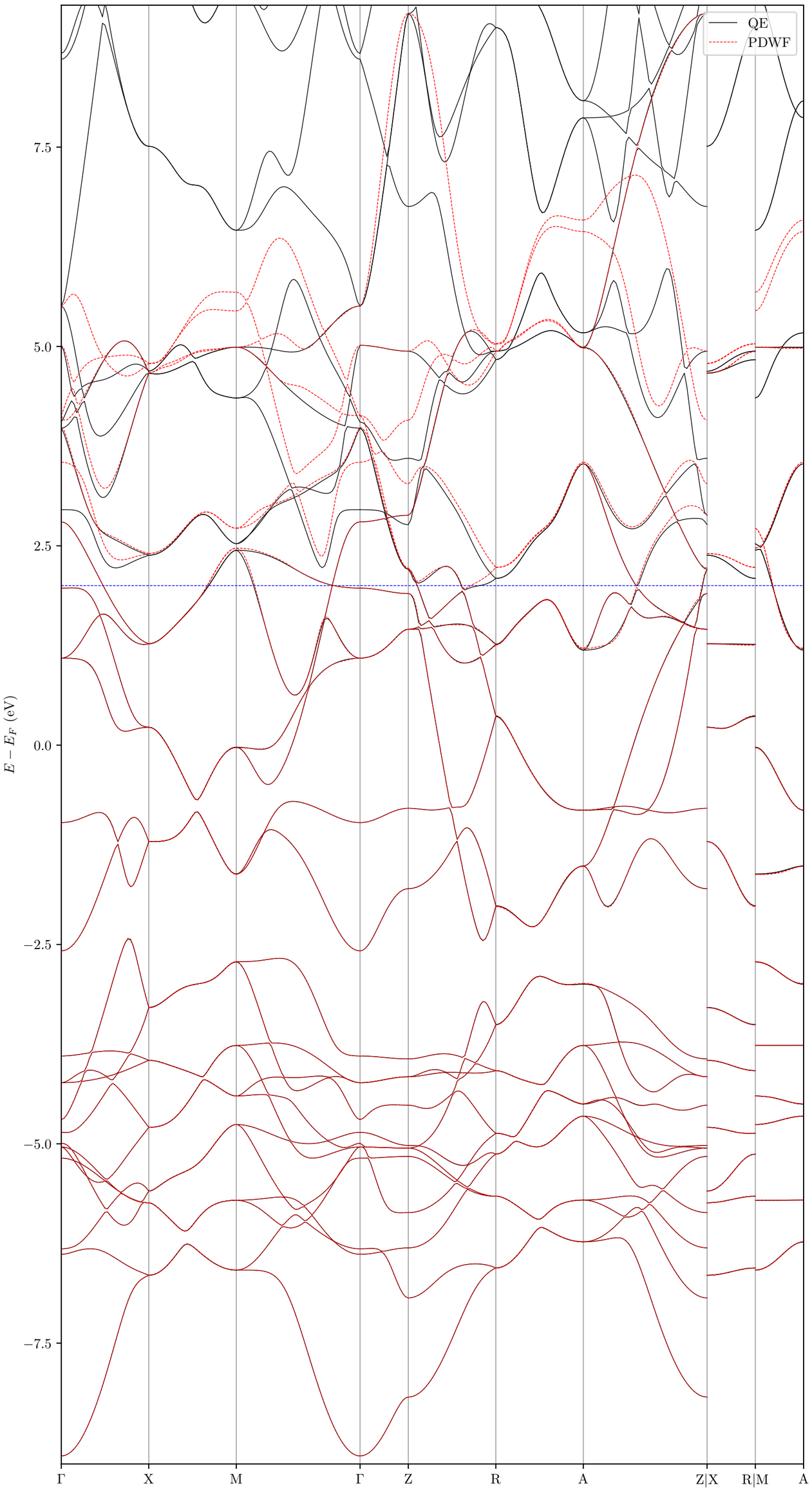



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.9 | 4.3 | 4.8 | 19.2 | 19.2 | 27.6 | 2.309 |



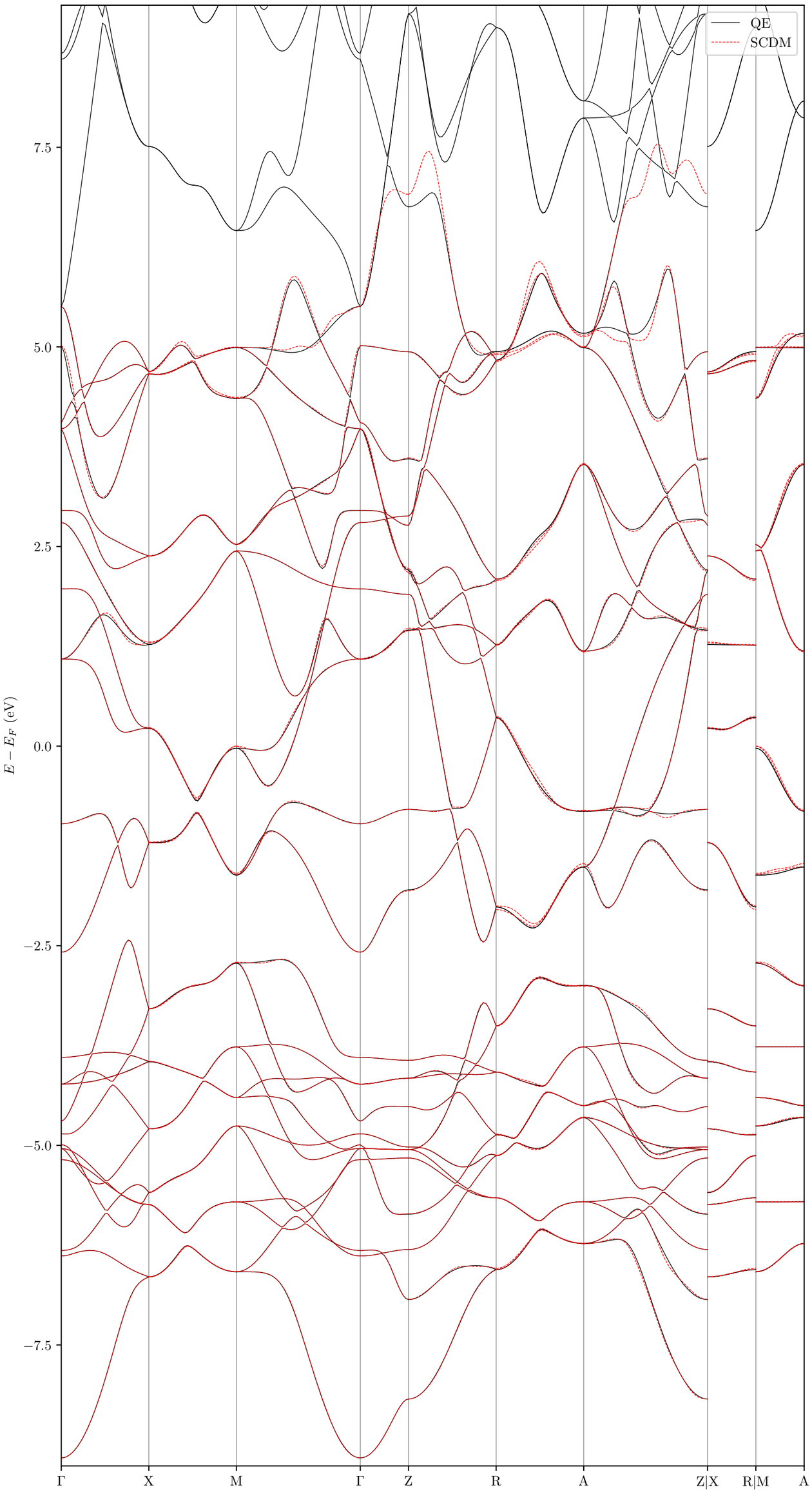
Au2Hf2 exclude semicore
PW=2128aafd-7350-43dd-b7d5-b39d2f96ae94
W90=521eeba9-29fe-420a-9977-02fdac8f2302




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.1 | 6.3 | 62.5 | 13.2 | 42.0 | 705.6 | 2.075 |

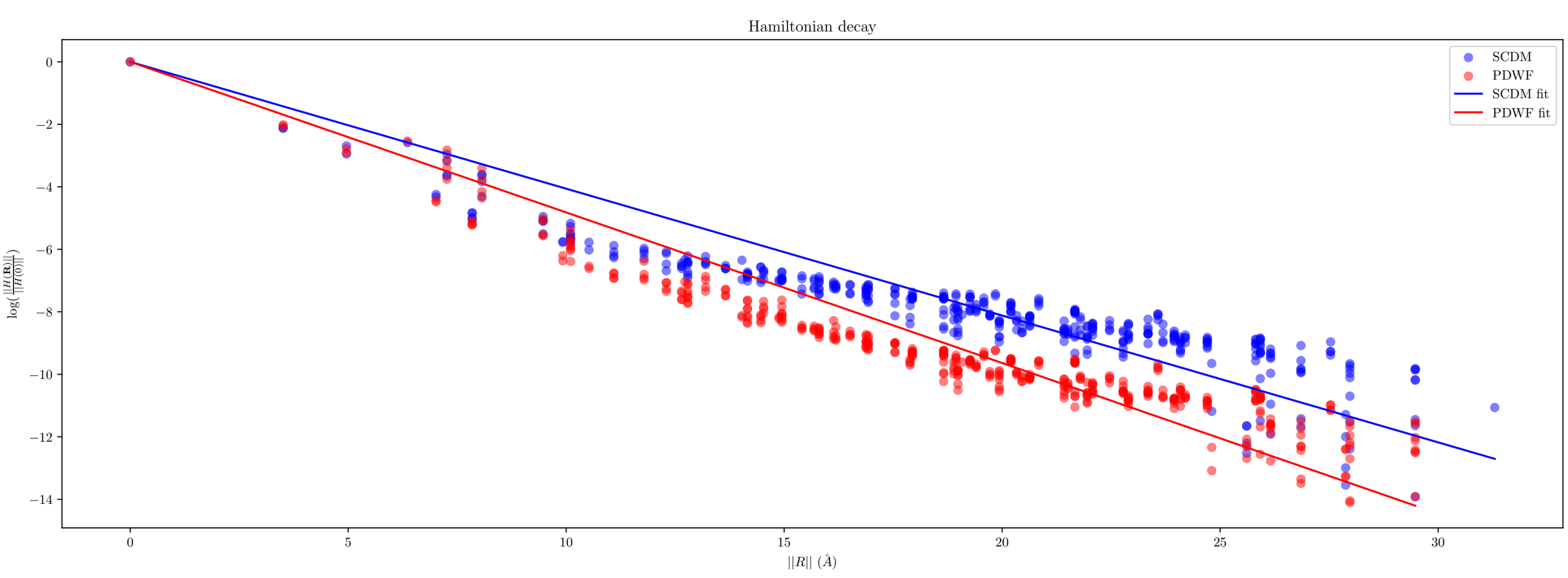
Au2Hf2 exclude semicore
PW=2128aafd-7350-43dd-b7d5-b39d2f96ae94
W90=7cf5e47c-d996-475c-9f19-93fdb6e62e85



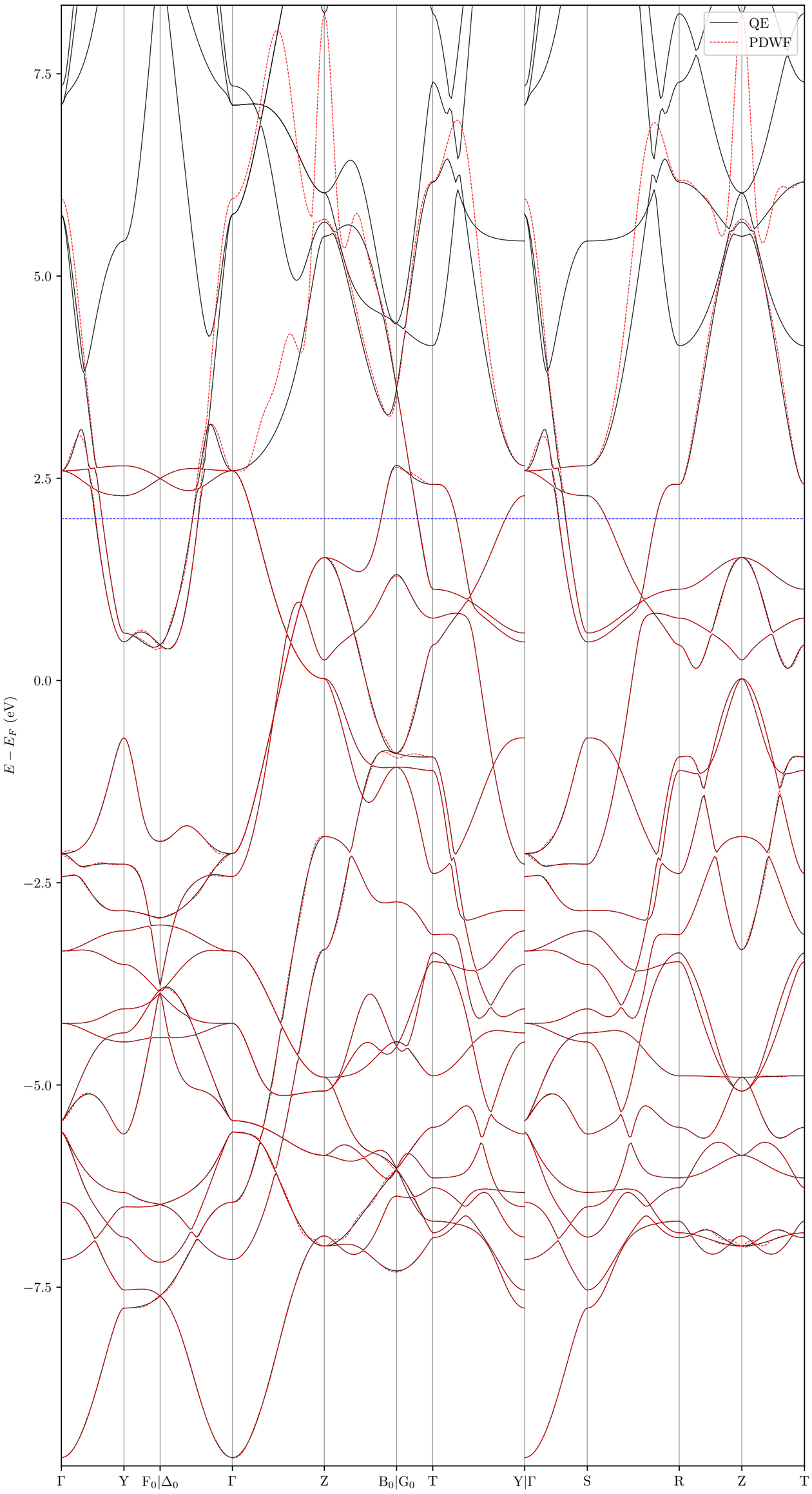

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 9.4 | 9.9 | 11.0 | 72.1 | 72.1 | 81.8 | 2.463 |

Hamiltonian decay



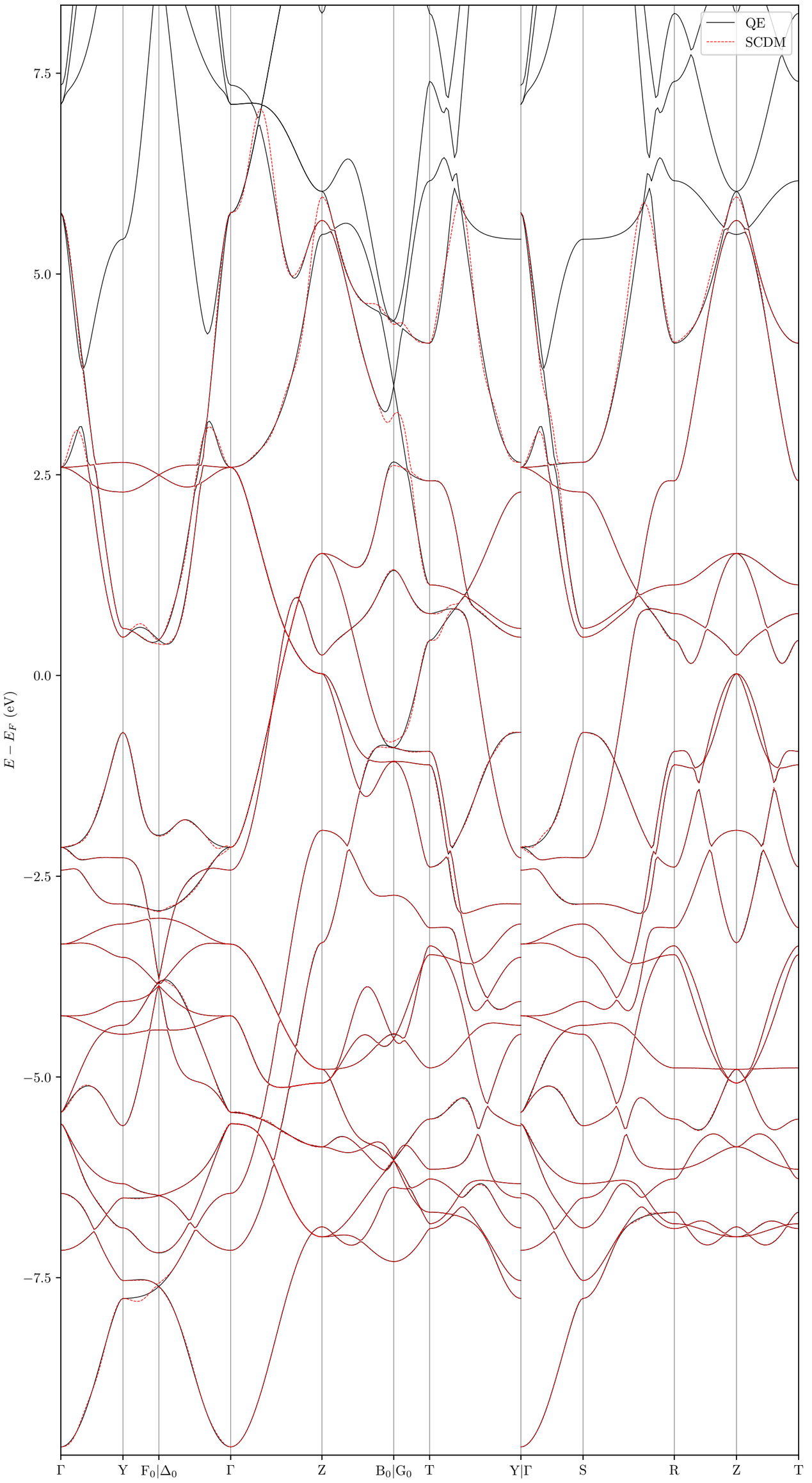
Au2Nb exclude semicore
PW=38c5069c-1b94-4ec1-909e-24fc7924f790
W90=839a3dad-2aec-4ad9-8083-afb97457e237




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.3 | 8.7 | 32.7 | 76.8 | 77.6 | 597.8 | 2.186 |

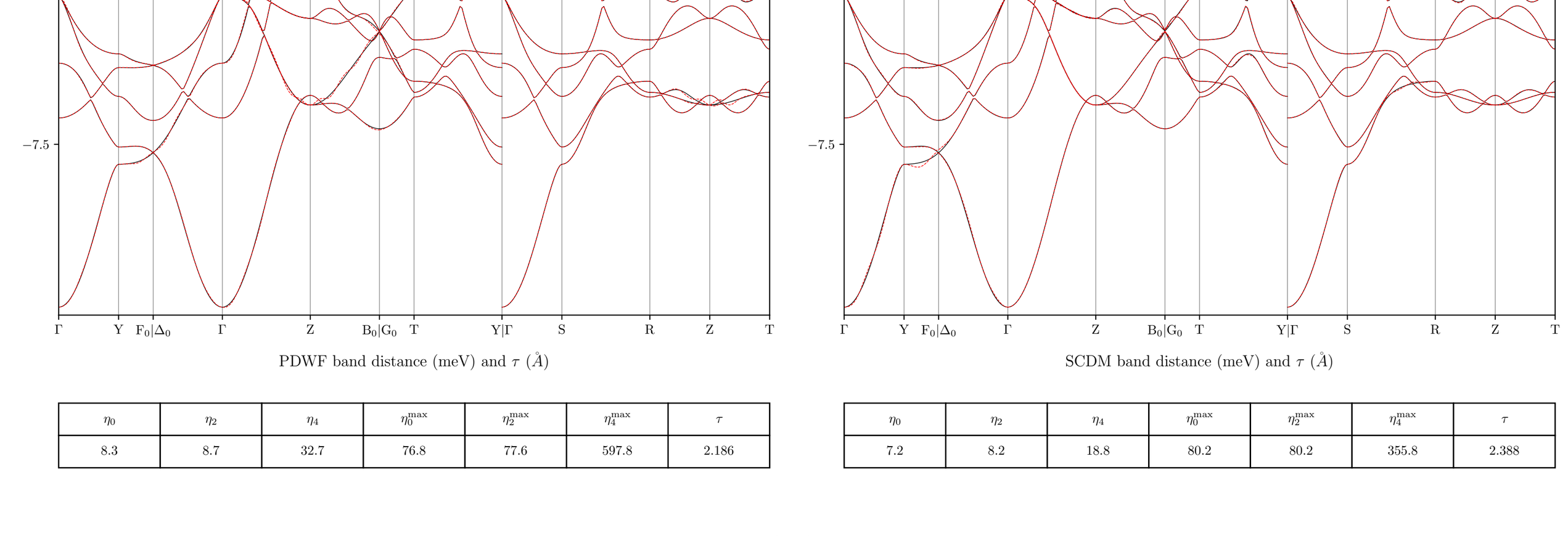
Au2Nb exclude semicore
PW=38c5069c-1b94-4ec1-909e-24fc7924f790
W90=47b82446-6272-4d6b-857c-a9cbb2c60aae

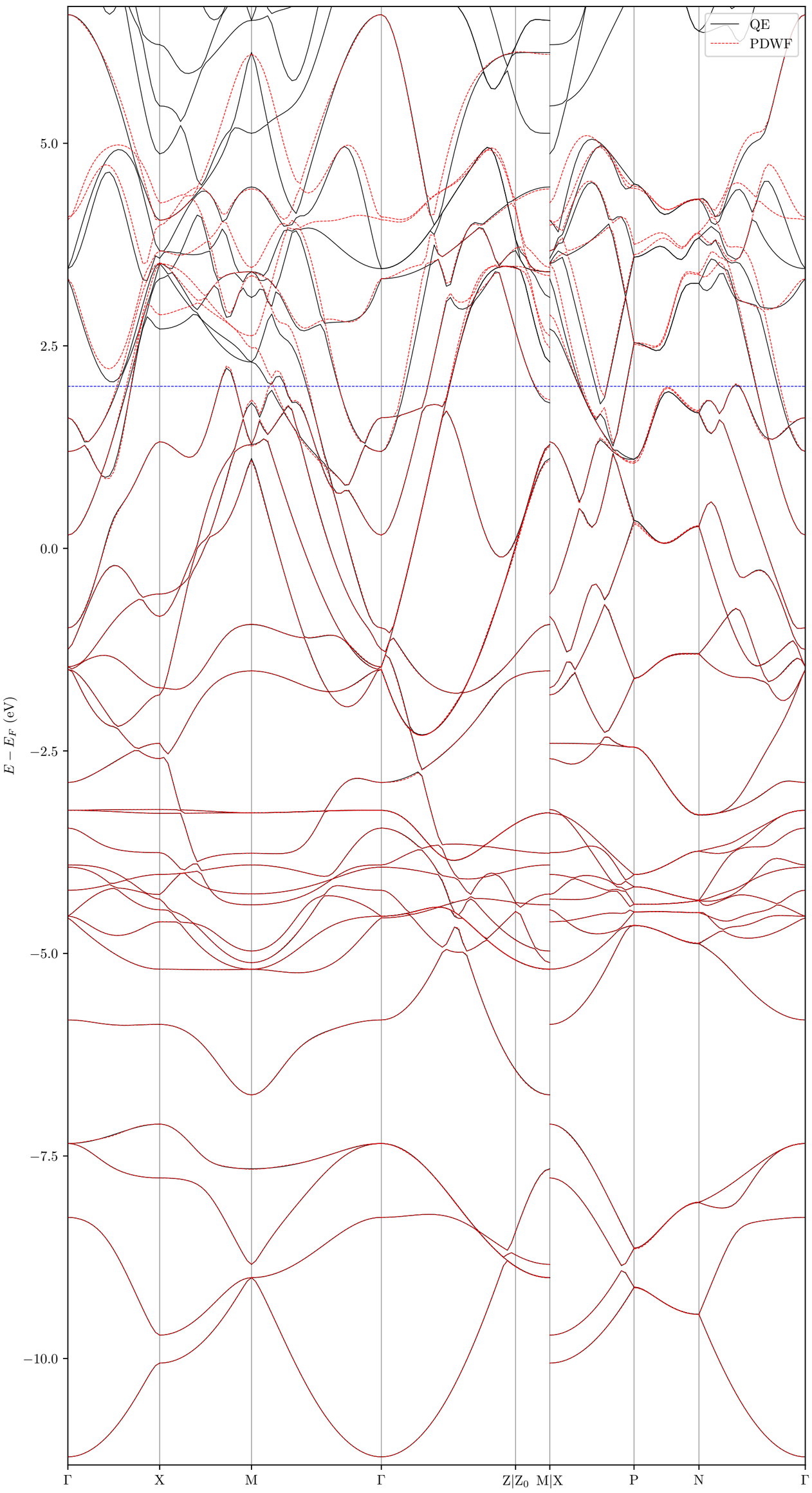



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.2 | 8.2 | 18.8 | 80.2 | 80.2 | 355.8 | 2.388 |

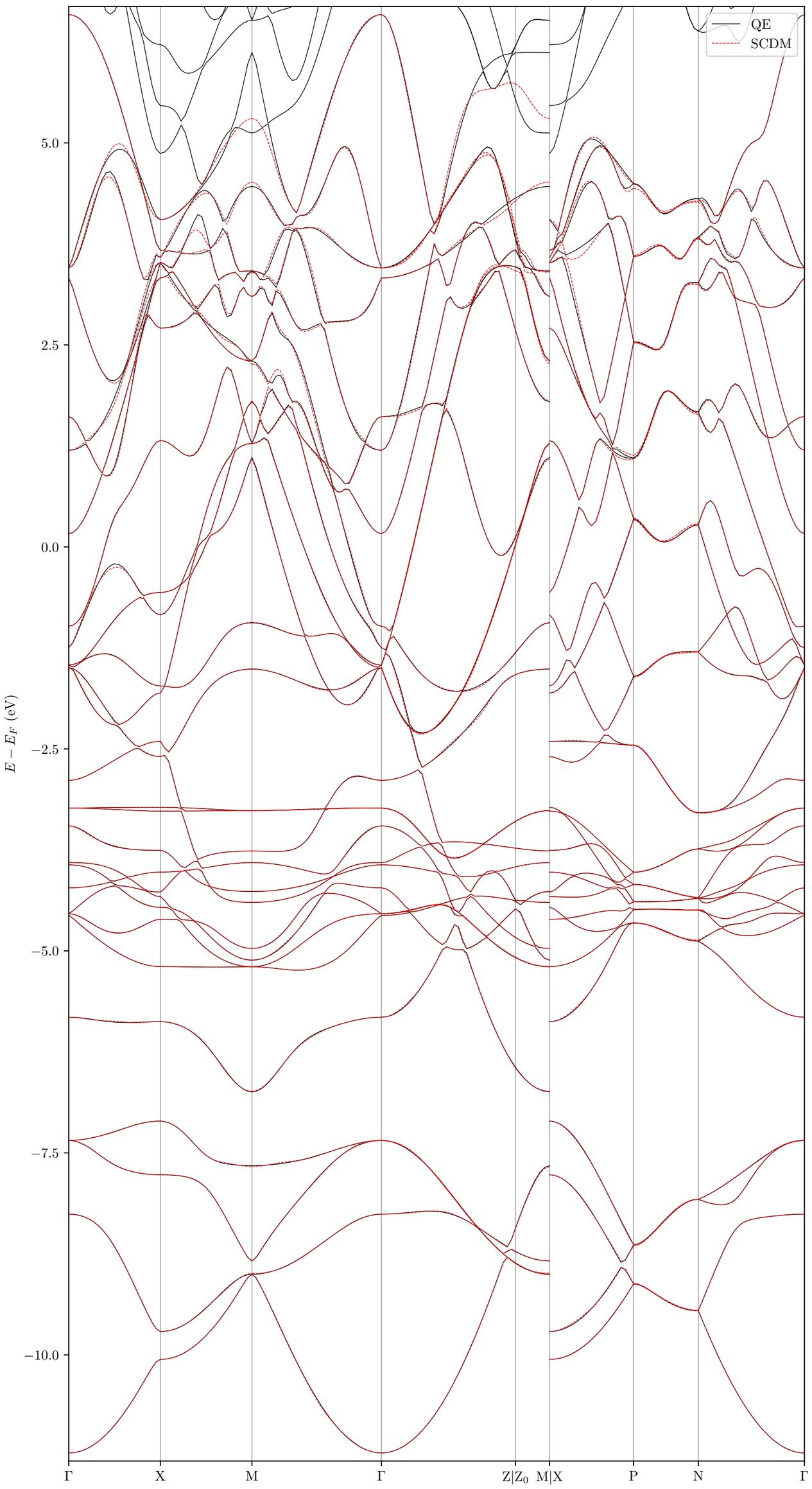
Hamiltonian decay





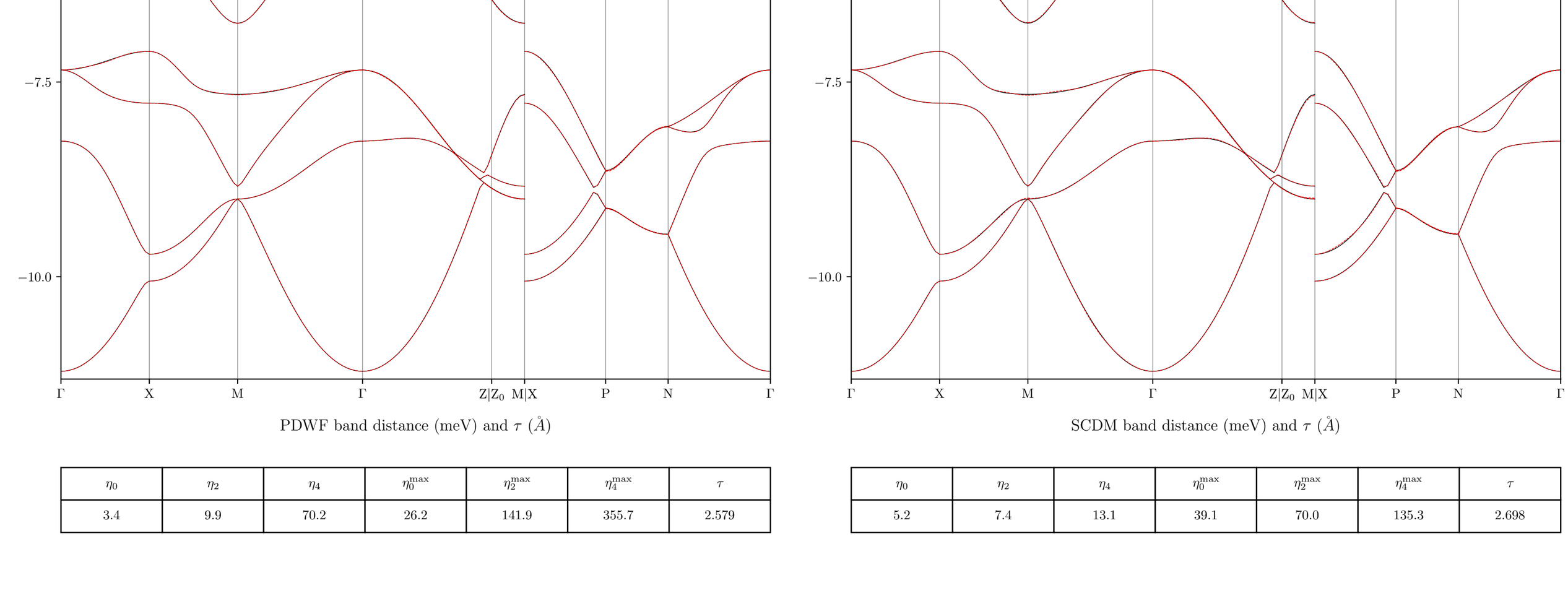

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

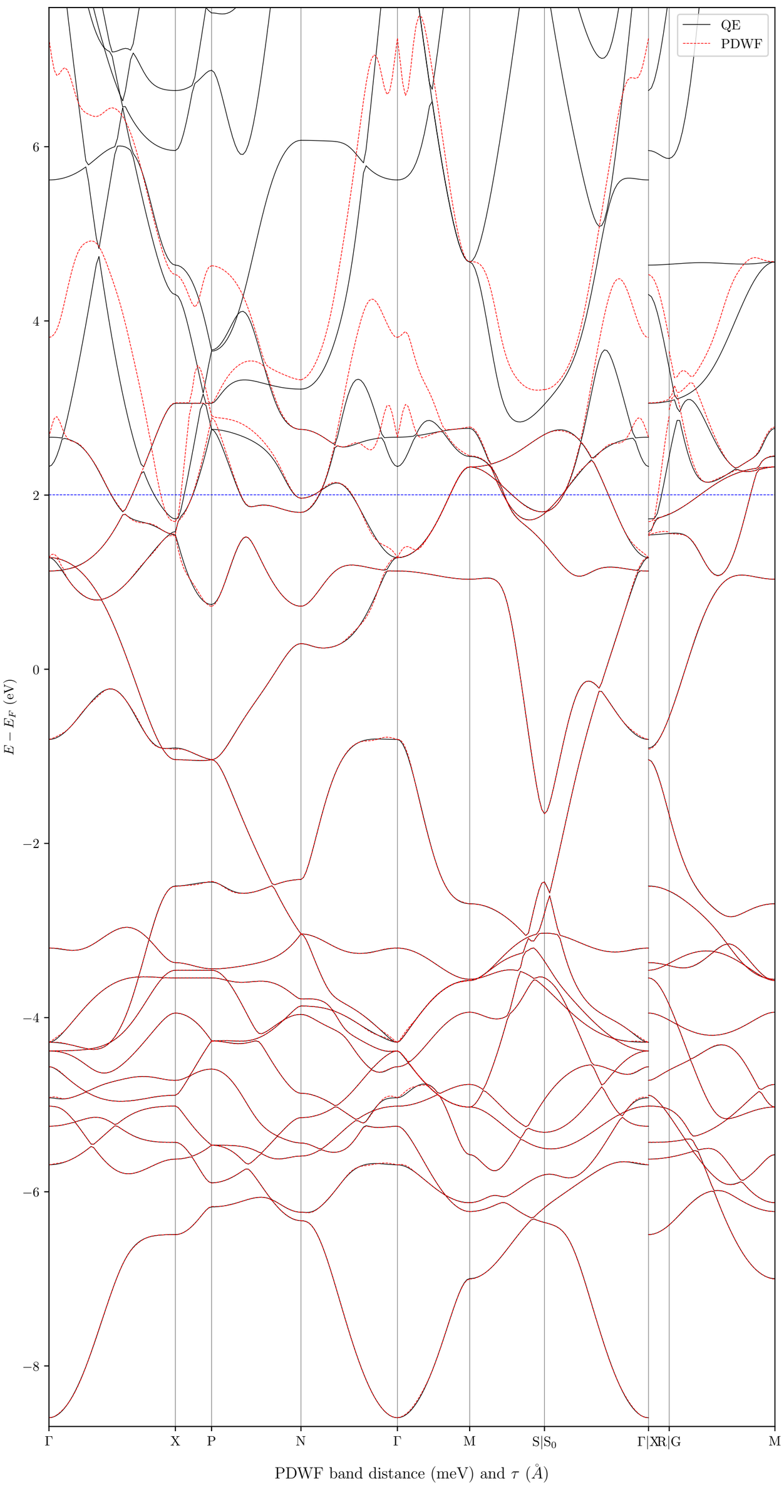
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.4 | 9.9 | 70.2 | 26.2 | 141.9 | 355.7 | 2.579 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

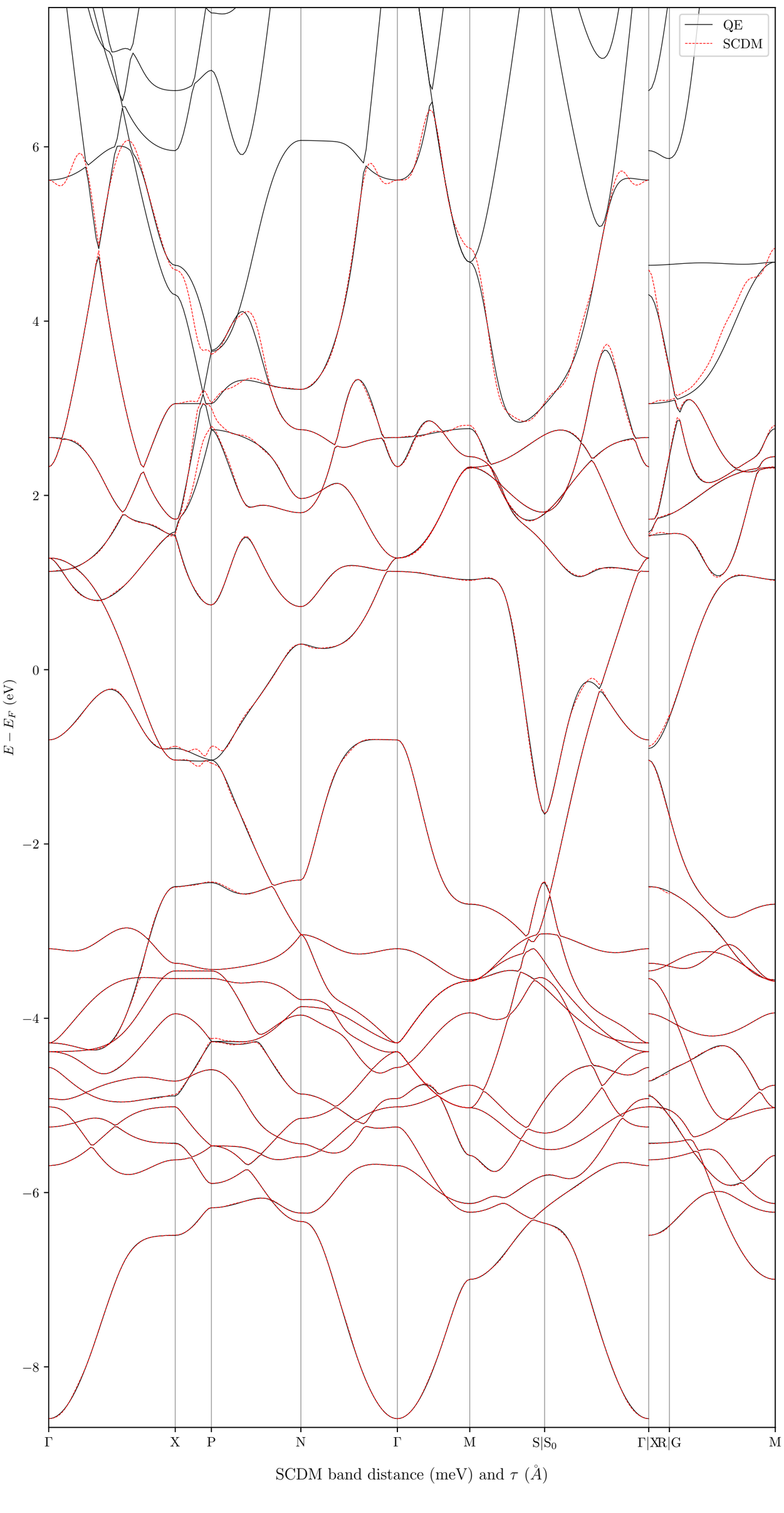
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.2 | 7.4 | 13.1 | 39.1 | 70.0 | 135.3 | 2.698 |





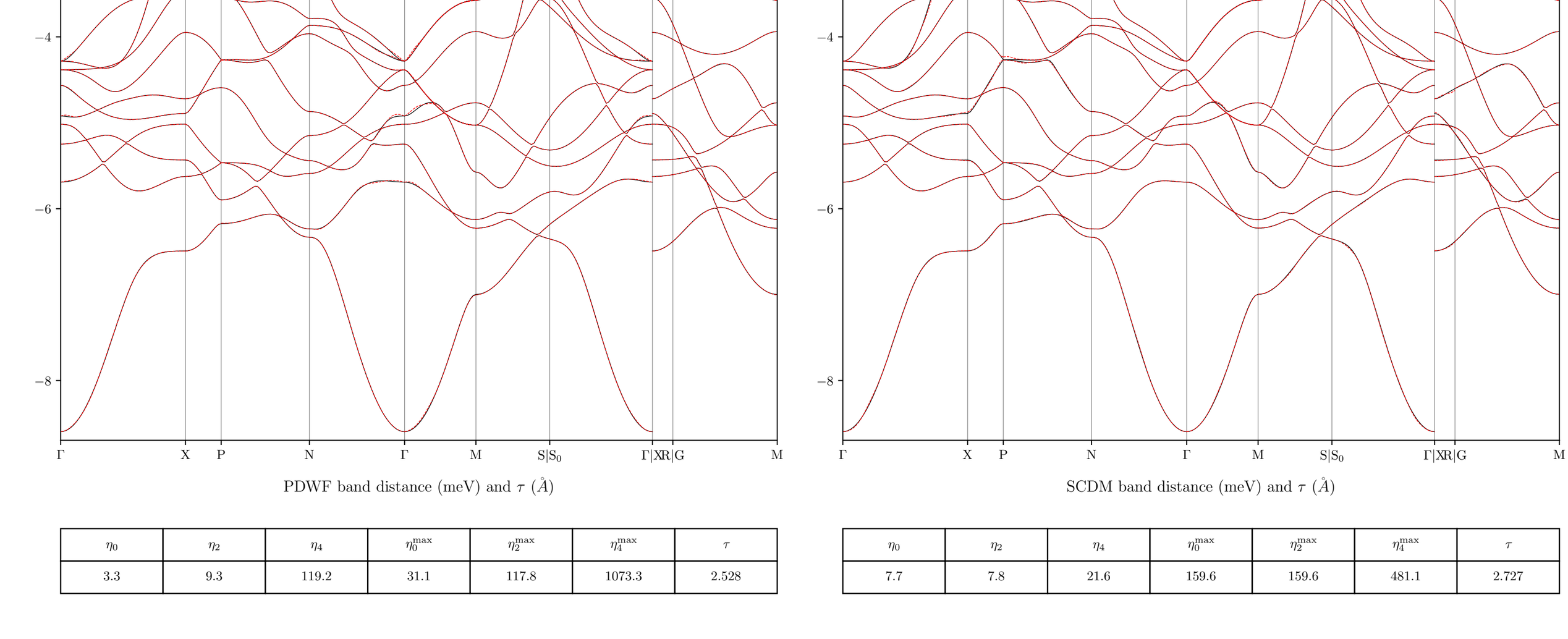

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.3 | 9.3 | 119.2 | 31.1 | 117.8 | 1073.3 | 2.528 |

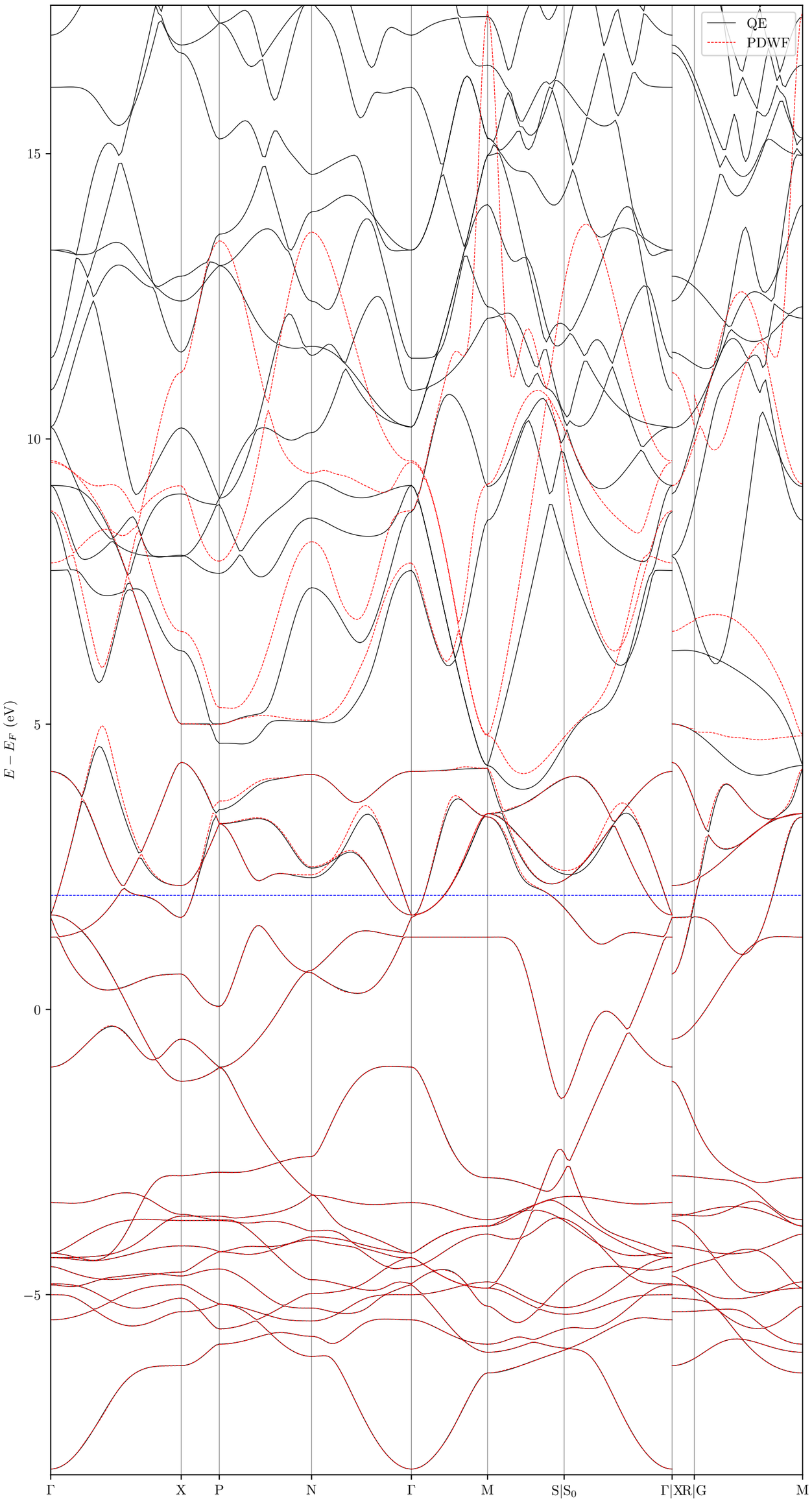



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.7 | 7.8 | 21.6 | 159.6 | 159.6 | 481.1 | 2.727 |



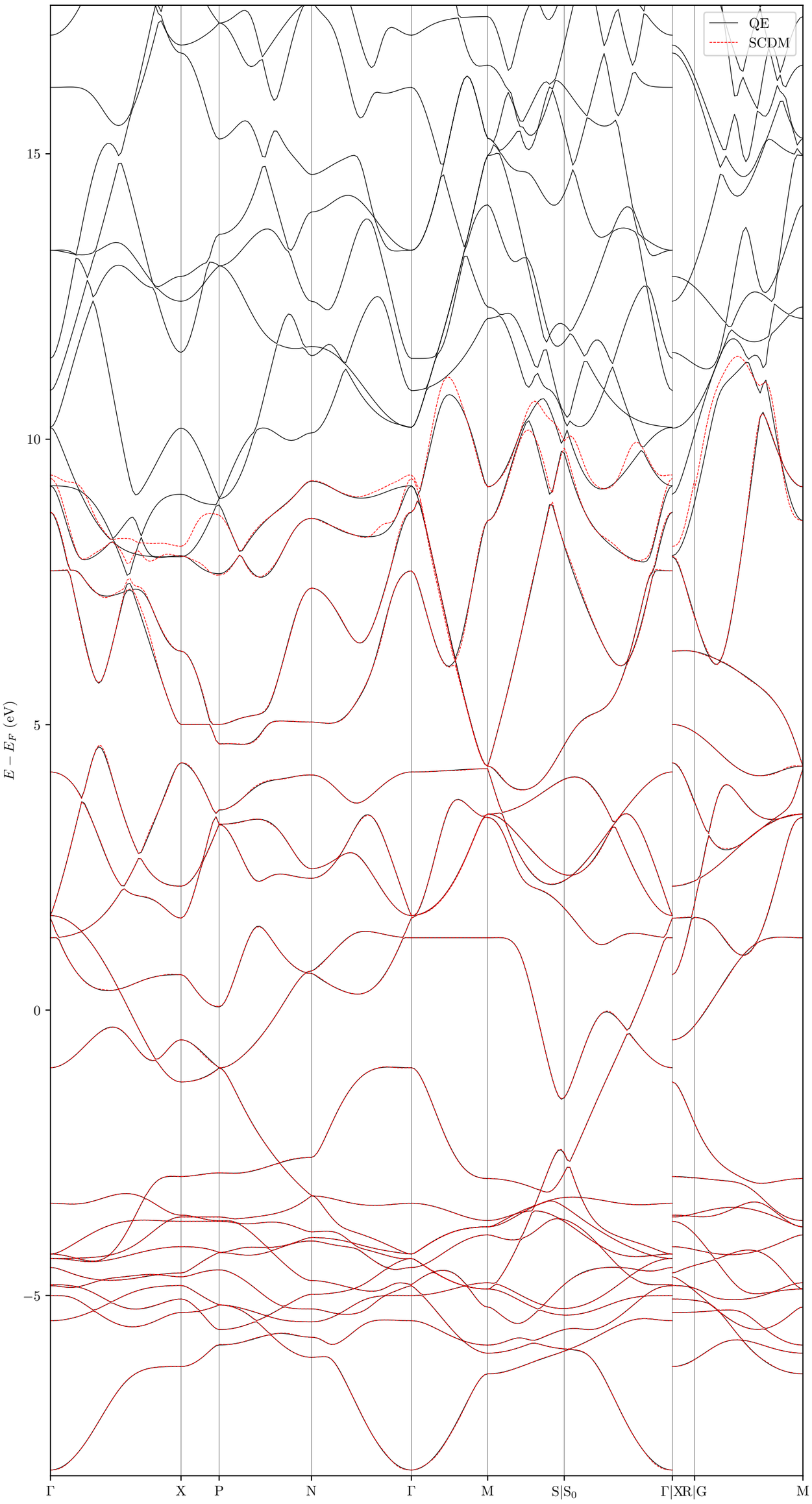
Au2Y exclude semicore
PW=60dc0f77-918a-4cca-a398-07a643cf8394
W90=06058a35-2811-4ce6-aae1-2af2b0c238dc




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.1 | 3.0 | 23.7 | 18.4 | 51.0 | 255.8 | 2.614 |

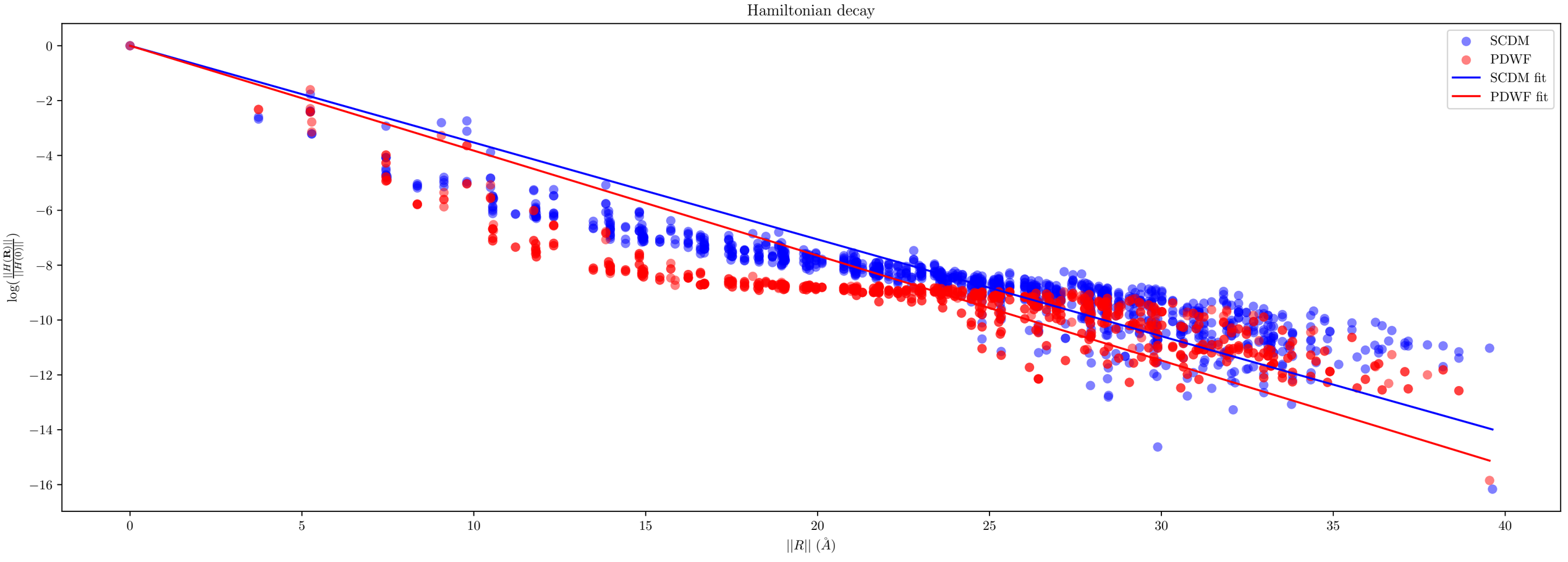
Au2Y exclude semicore
PW=60dc0f77-918a-4cca-a398-07a643cf8394
W90=db1a39f0-9436-4b75-b894-0d0bbfa40e1f



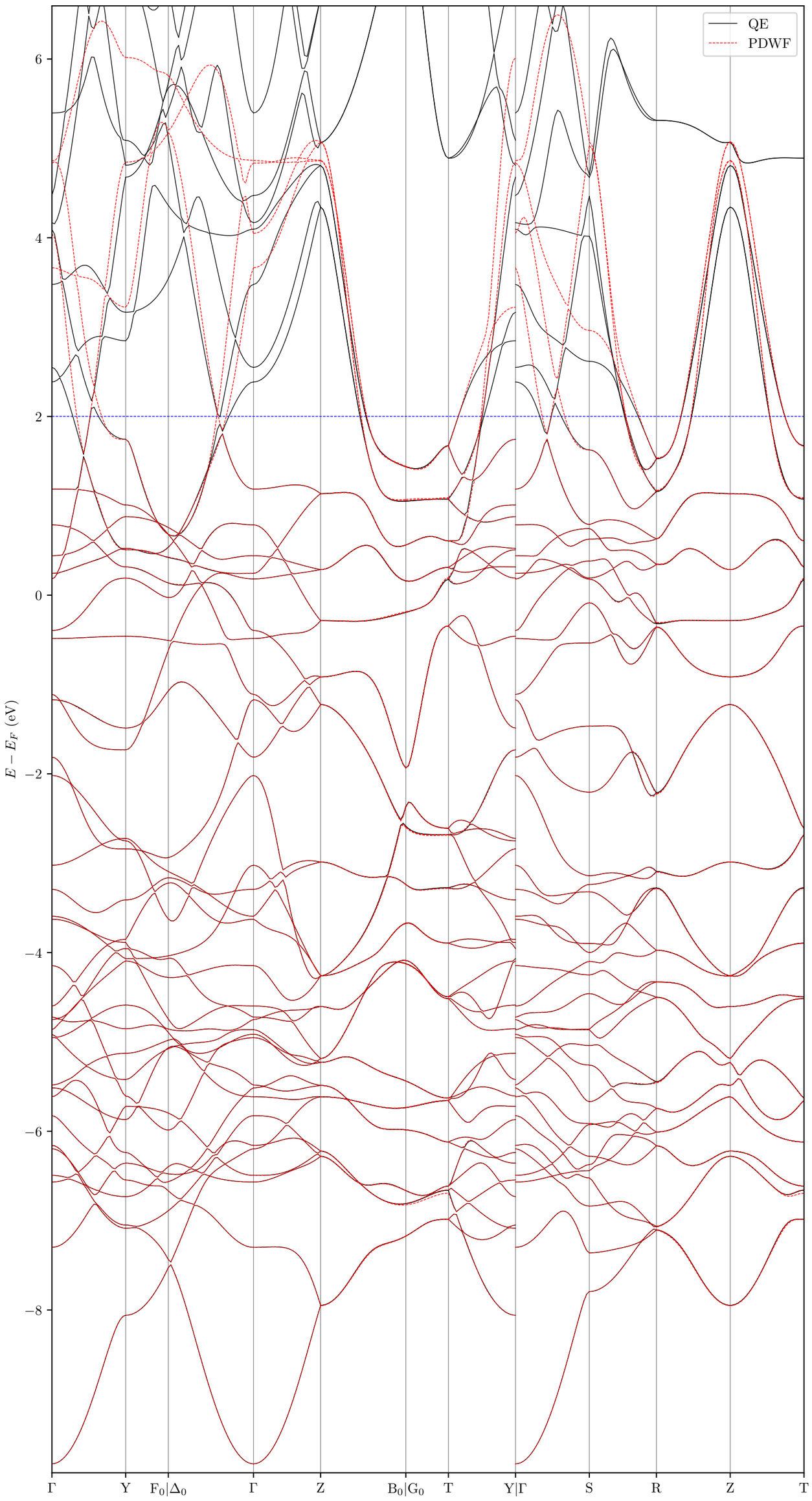

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.1 | 3.6 | 4.4 | 24.4 | 28.2 | 42.0 | 2.833 |

Hamiltonian decay



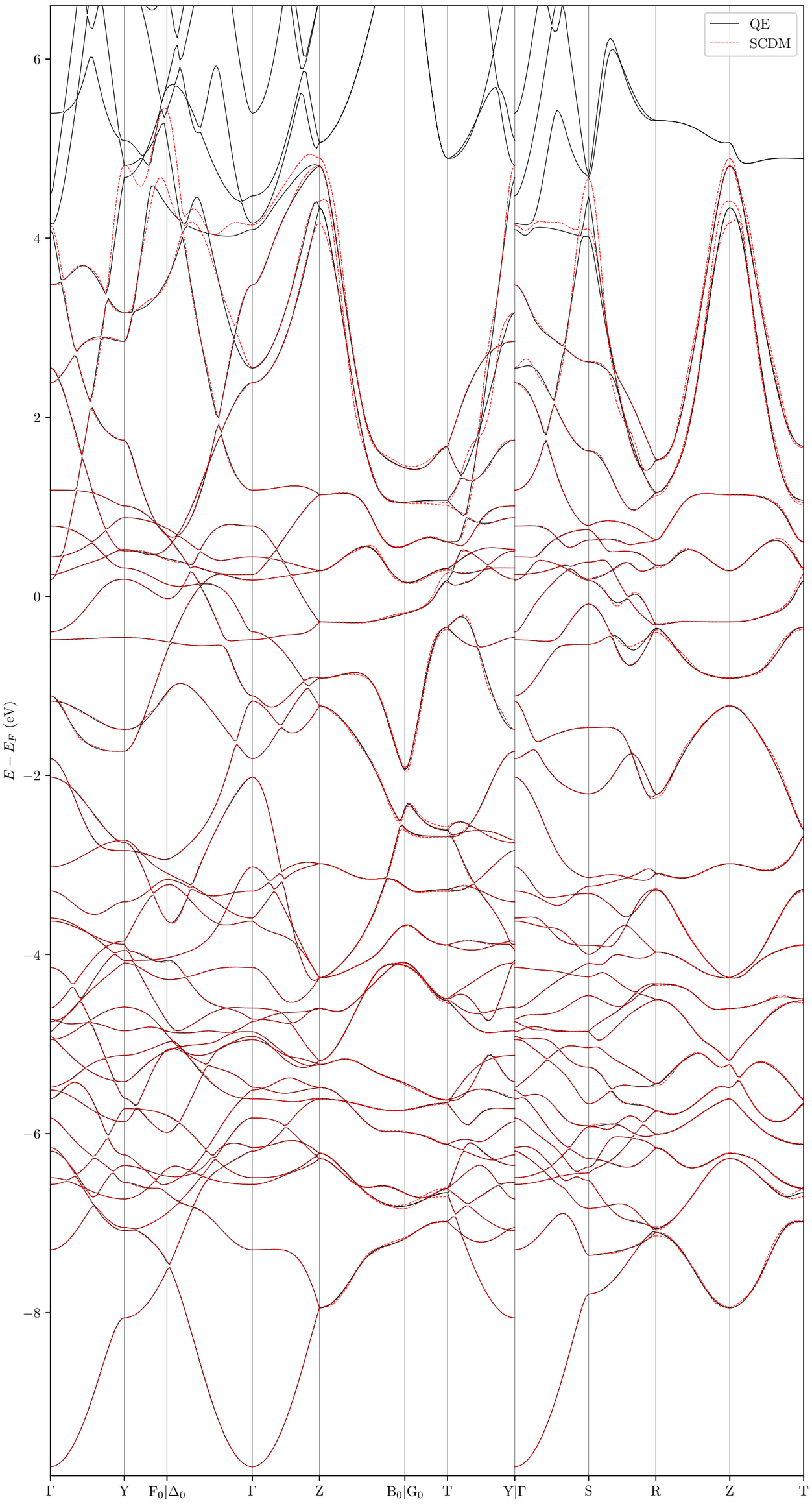
Au4V2 exclude semicore
PW=6cf556d2-4b1e-4587-bdc6-f1ee9440c094
W90=9e7e7104-e75f-40da-8672-f3cb2f880d9d




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.8 | 6.6 | 112.8 | 33.0 | 111.8 | 1256.5 | 2.118 |

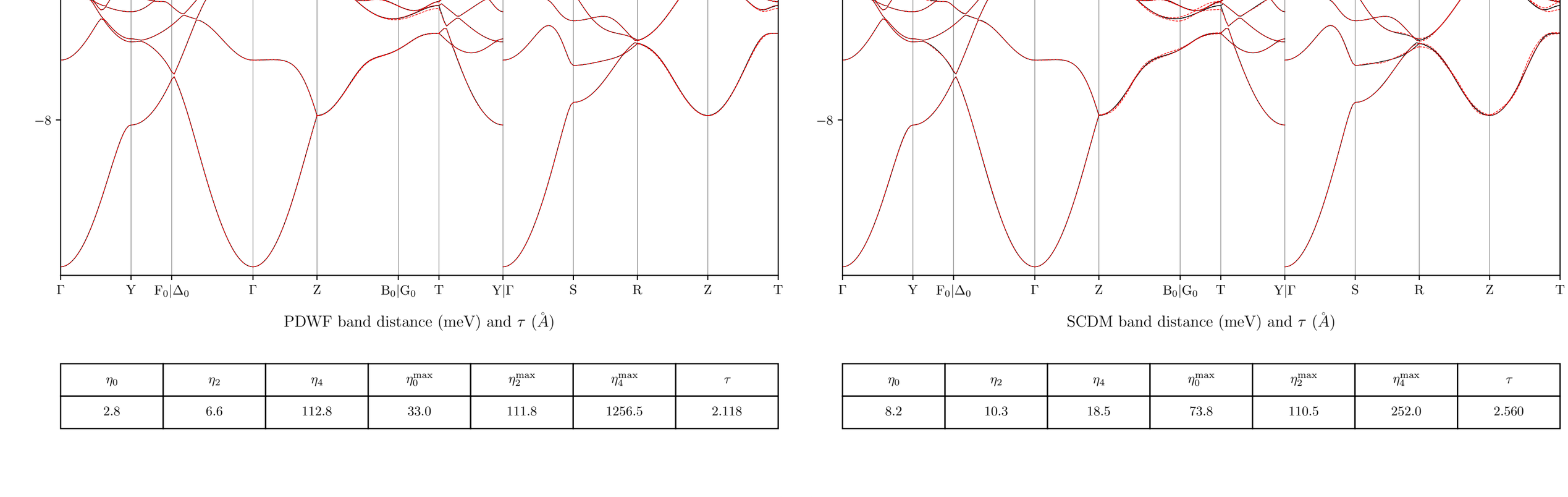
Au4V2 exclude semicore
PW=6cf556d2-4b1e-4587-bdc6-f1ee9440c094
W90=61b9da8e-7167-494e-a827-2efd41b410c2



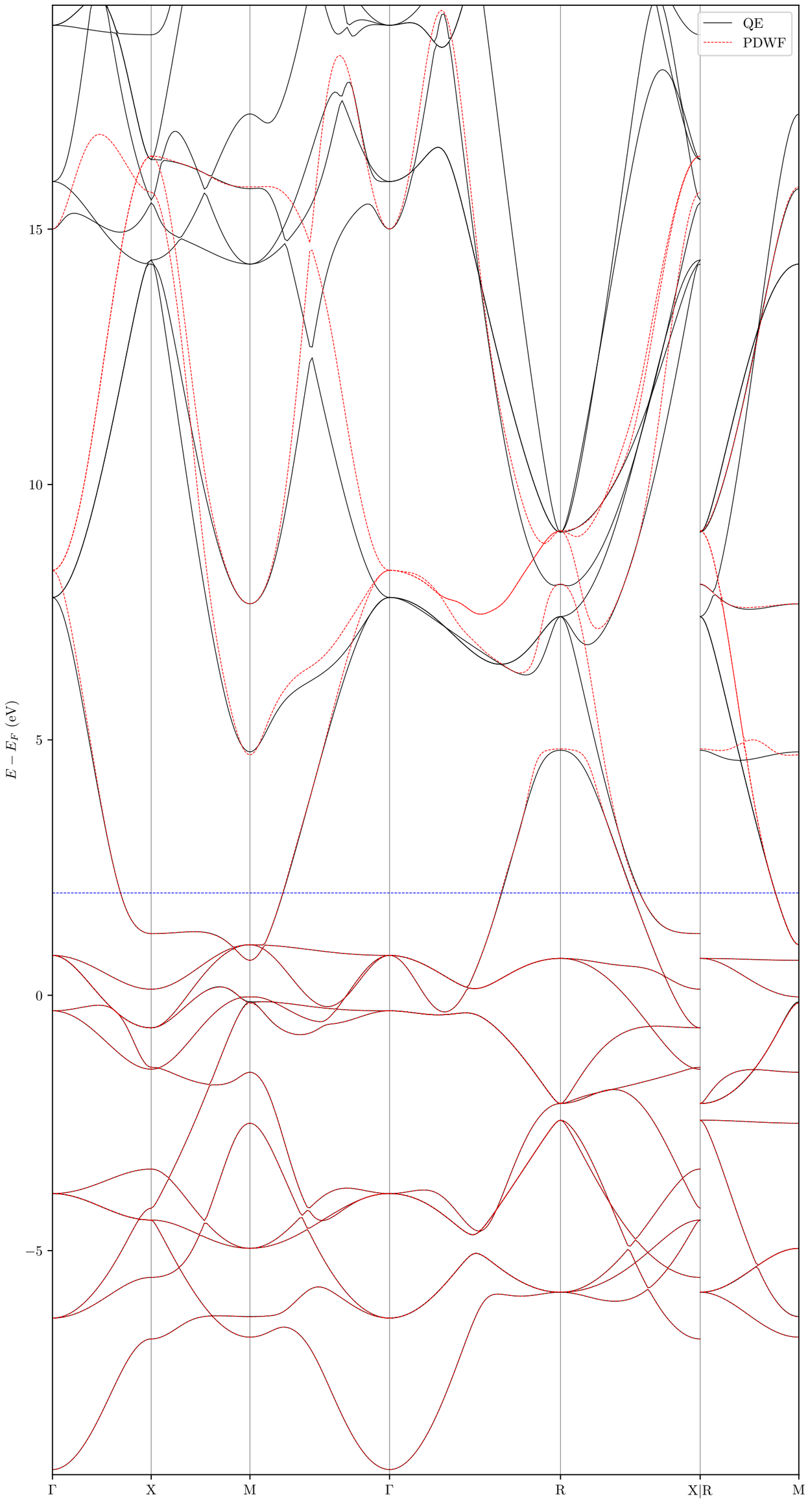

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.2 | 10.3 | 18.5 | 73.8 | 110.5 | 252.0 | 2.560 |

Hamiltonian decay



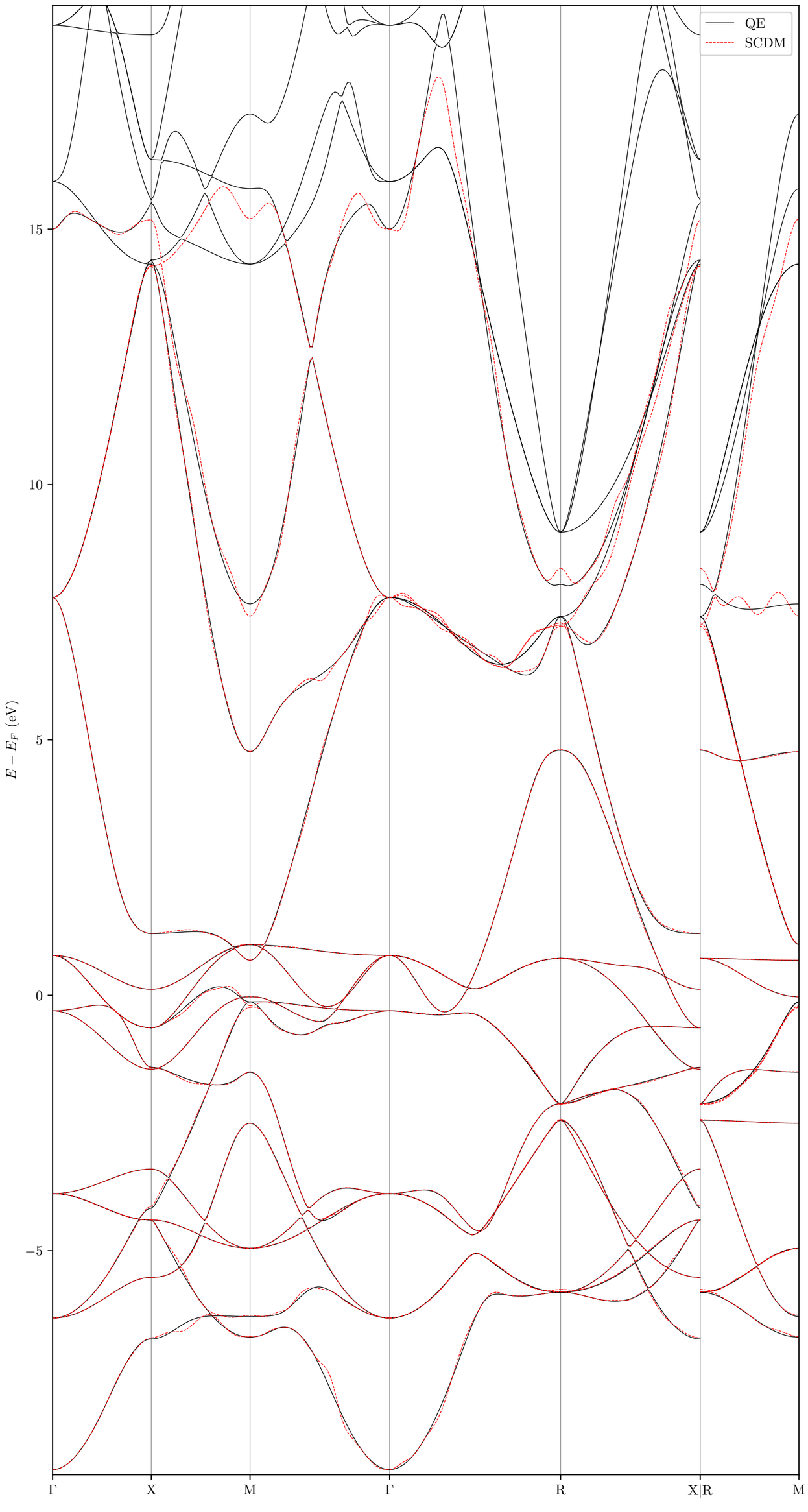
AuMn exclude semicore
PW=e12e65f9-a6f4-4a3e-9ae0-fd27c4033076
W90=e33f4606-d555-4975-8f2d-15875288a8a7




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.3 | 2.7 | 13.5 | 19.0 | 28.9 | 248.1 | 1.881 |

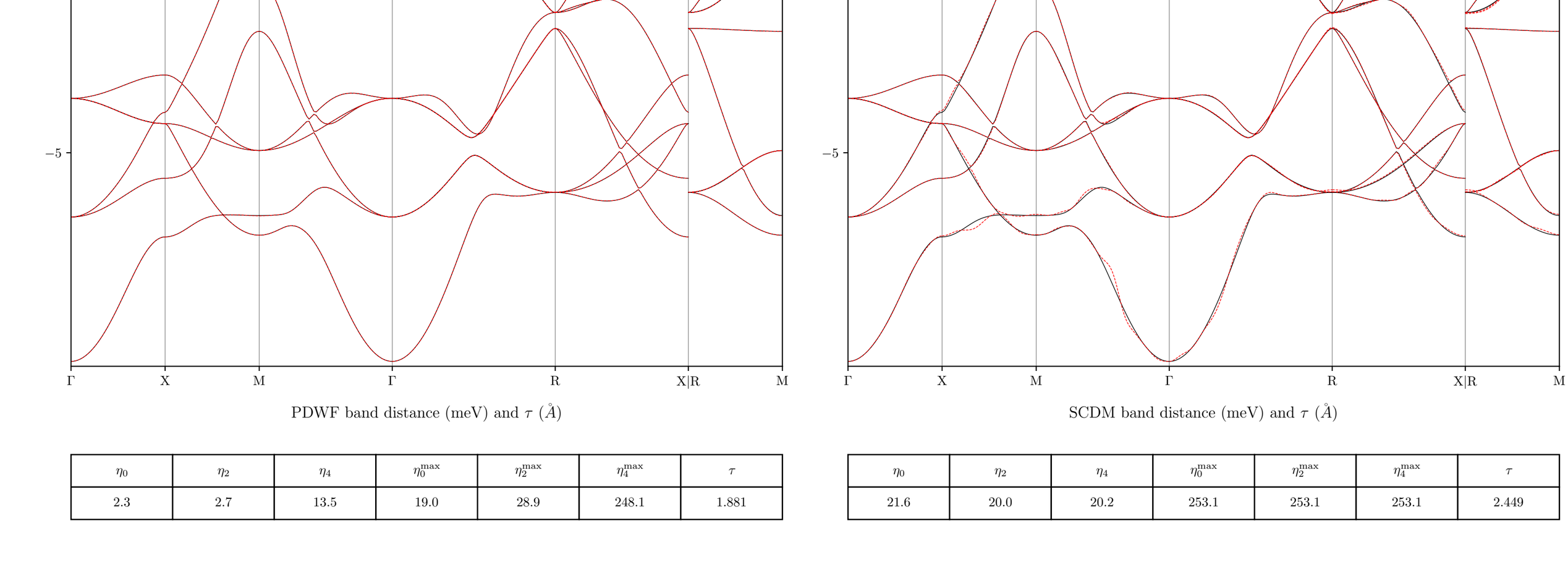
AuMn exclude semicore
PW=e12e65f9-a6f4-4a3e-9ae0-fd27c4033076
W90=f0ef9c19-0486-4f85-af0f-82745751eb1f




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 21.6 | 20.0 | 20.2 | 253.1 | 253.1 | 253.1 | 2.449 |

Hamiltonian decay



B16Mg4 exclude semicore
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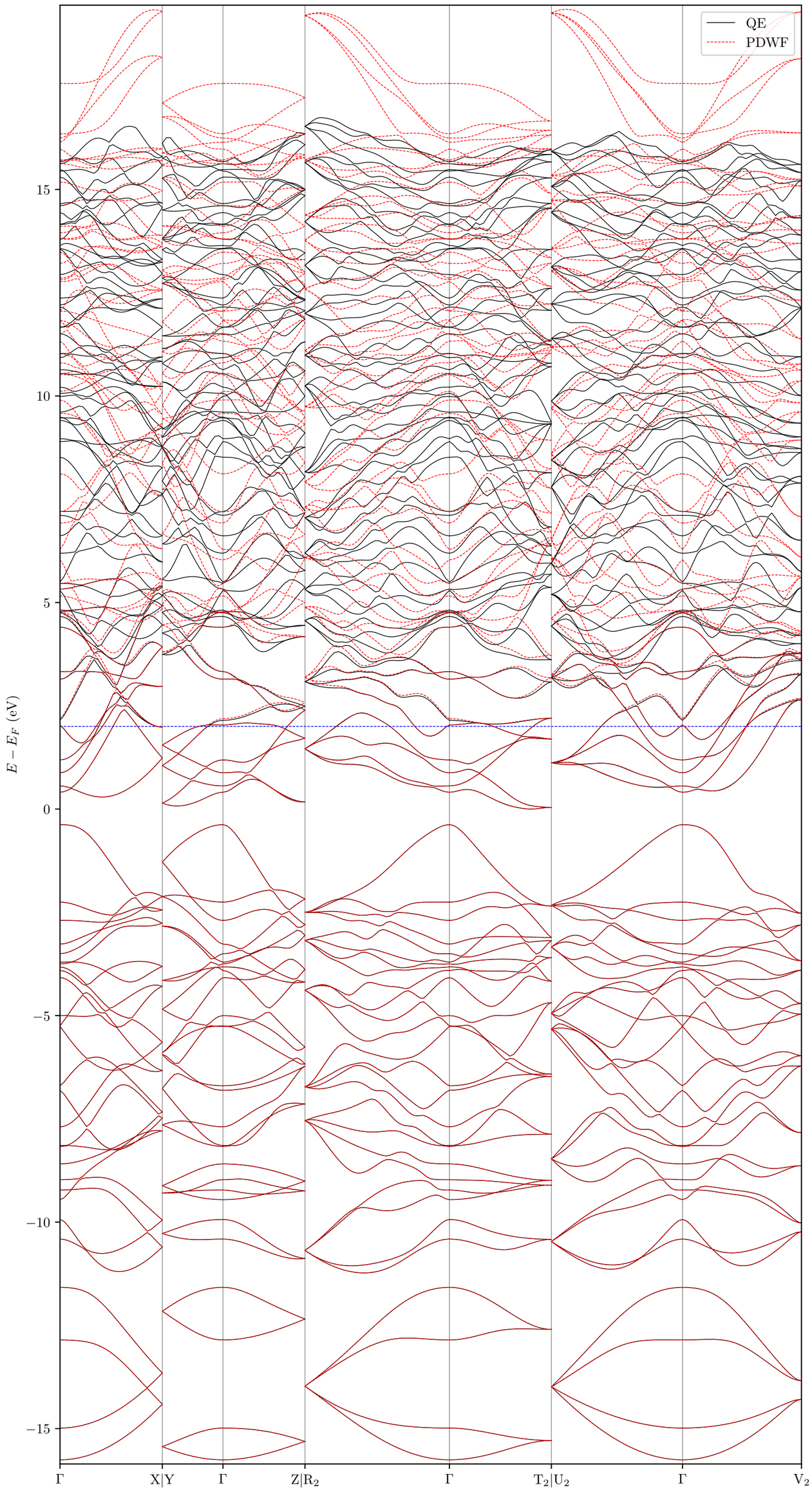
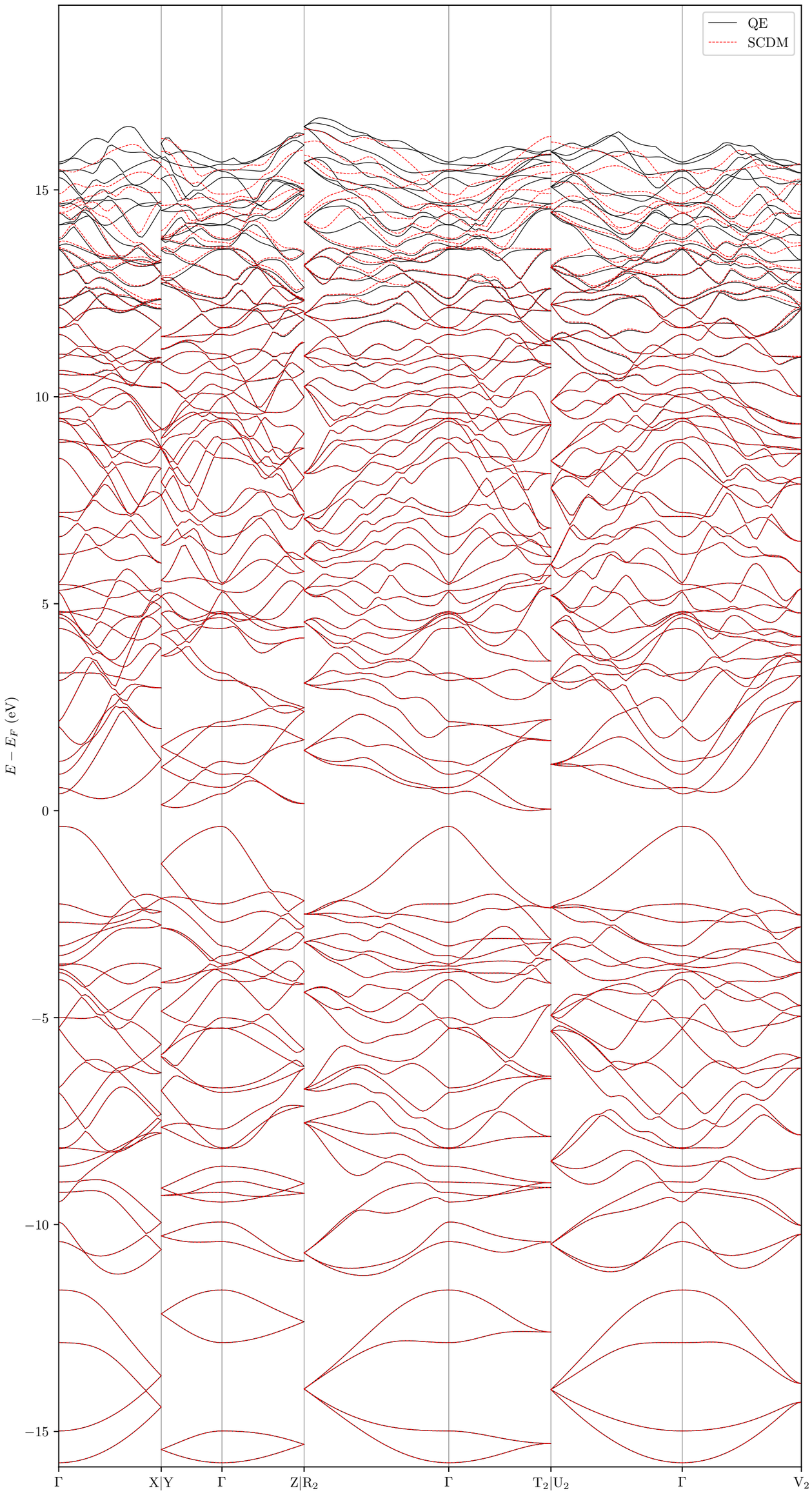
W90=0a8ad666-9520-425d-b2b6-403440086269




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.5 | 1.9 | 19.8 | 8.5 | 10.1 | 208.5 | 2.591 |

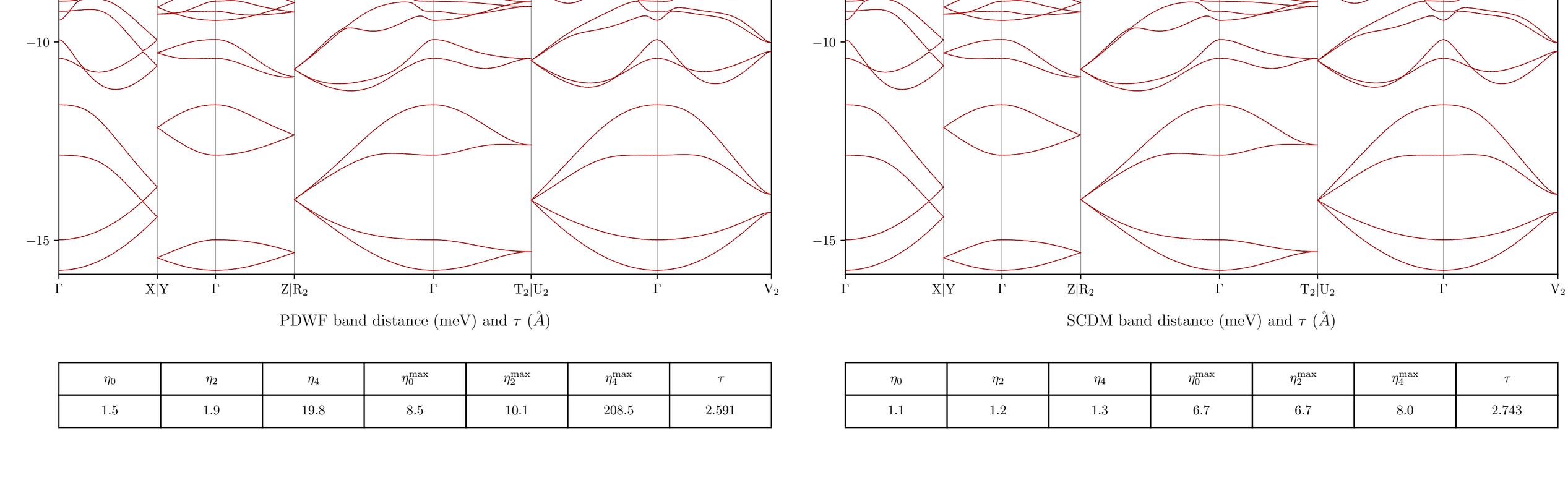
B16Mg4 exclude semicore
PW=27d40827-a39b-41cb-9fe7-936b5d4d2586
W90=926ba297-3d02-4084-af09-4f1873512e82




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.2 | 1.3 | 6.7 | 6.7 | 8.0 | 2.743 |

Hamiltonian decay



B2Cr exclude semicore
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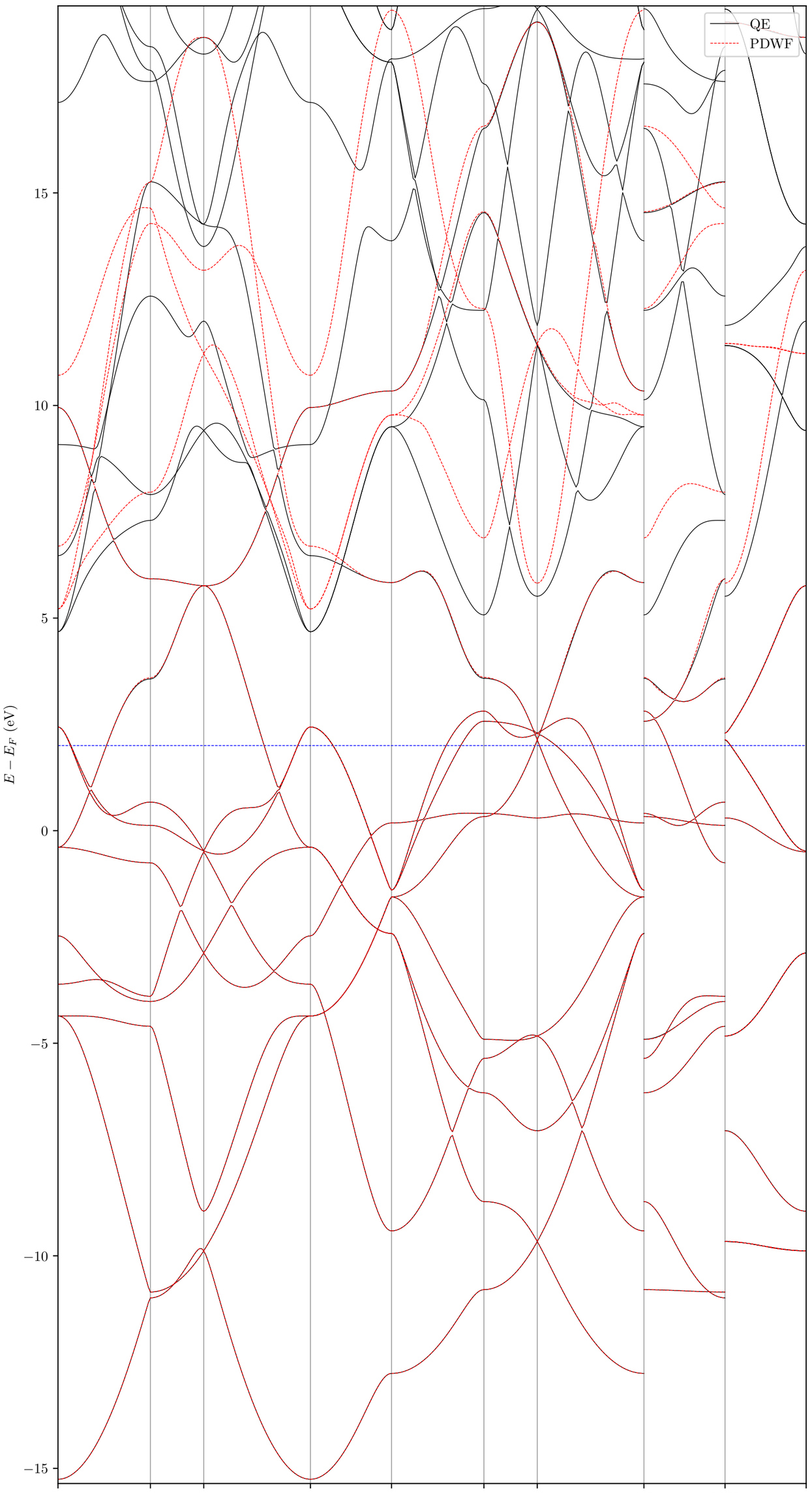
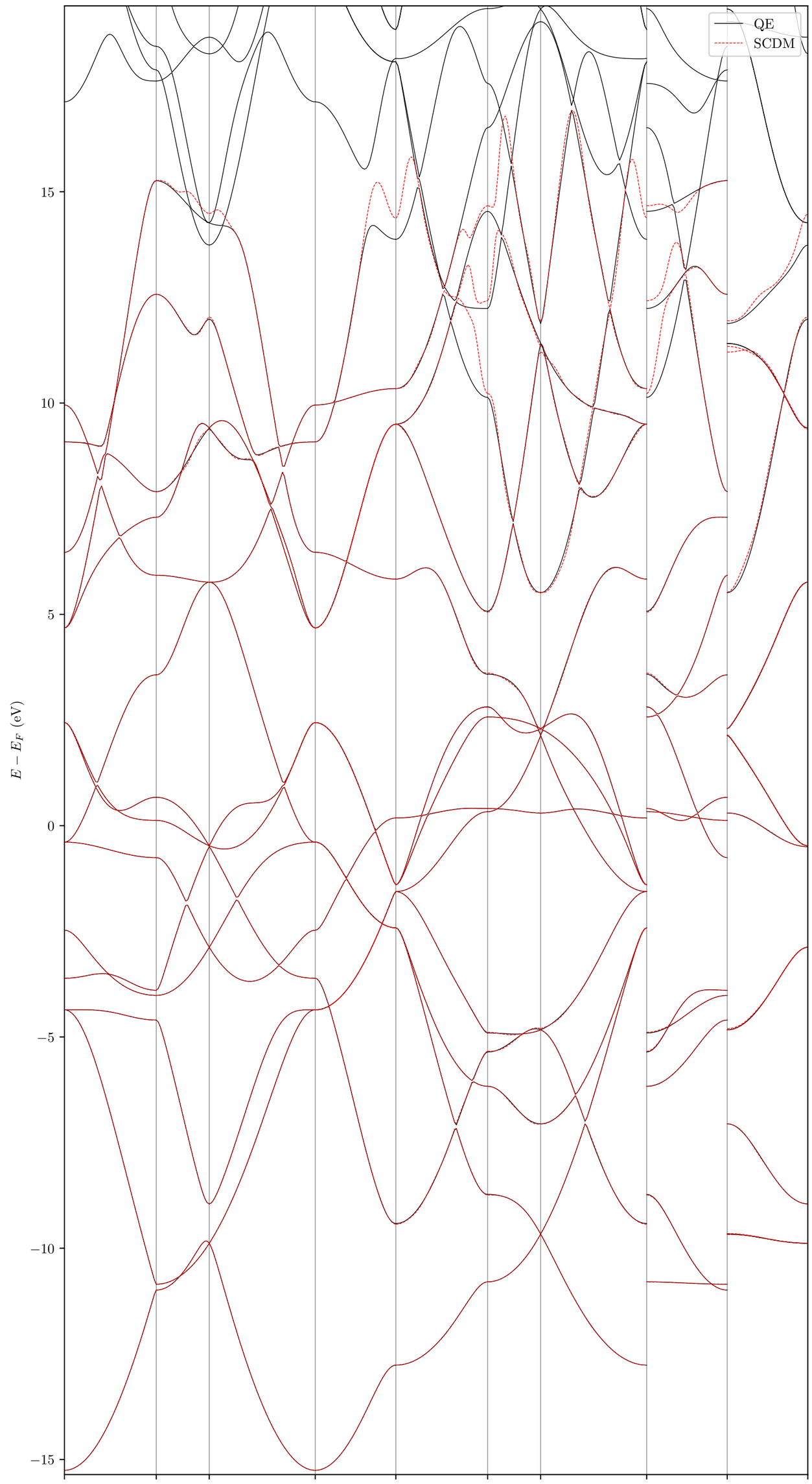
W90=93f69500-af67-4d1b-9177-6c9f3a610bf7




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.6 | 1.6 | 3.8 | 11.5 | 11.5 | 44.9 | 1.925 |

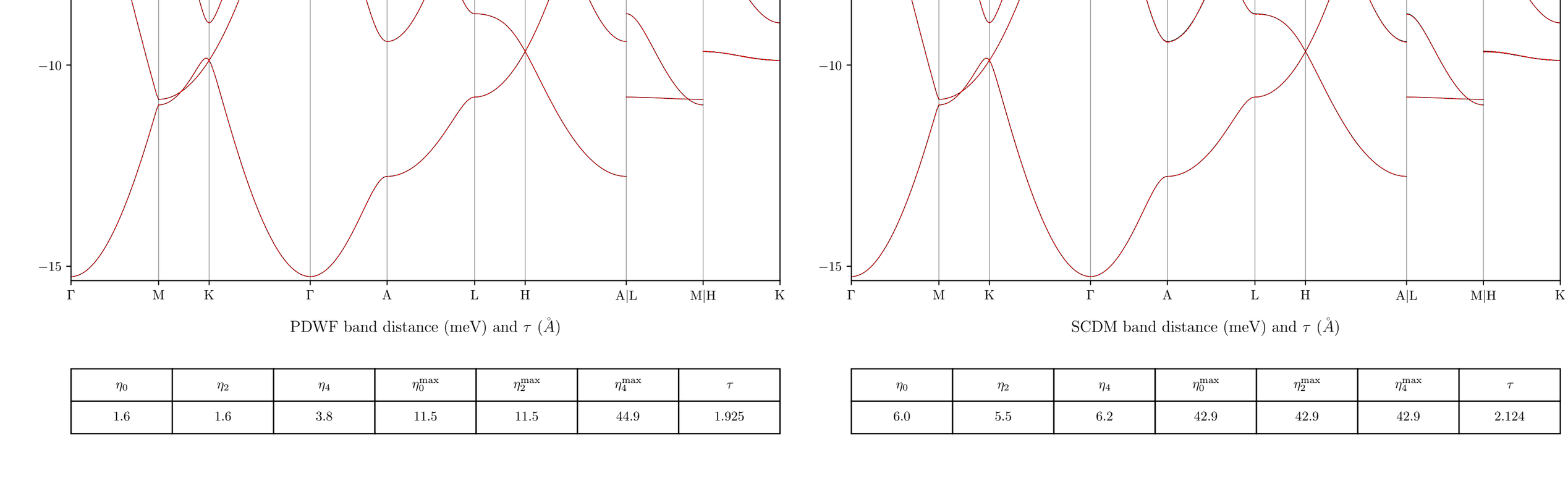
B2Cr exclude semicore
PW=21e67c10-682e-4f49-8b67-d37473cc2bdb
W90=ab6916de-974b-4030-9382-4dc78e042200



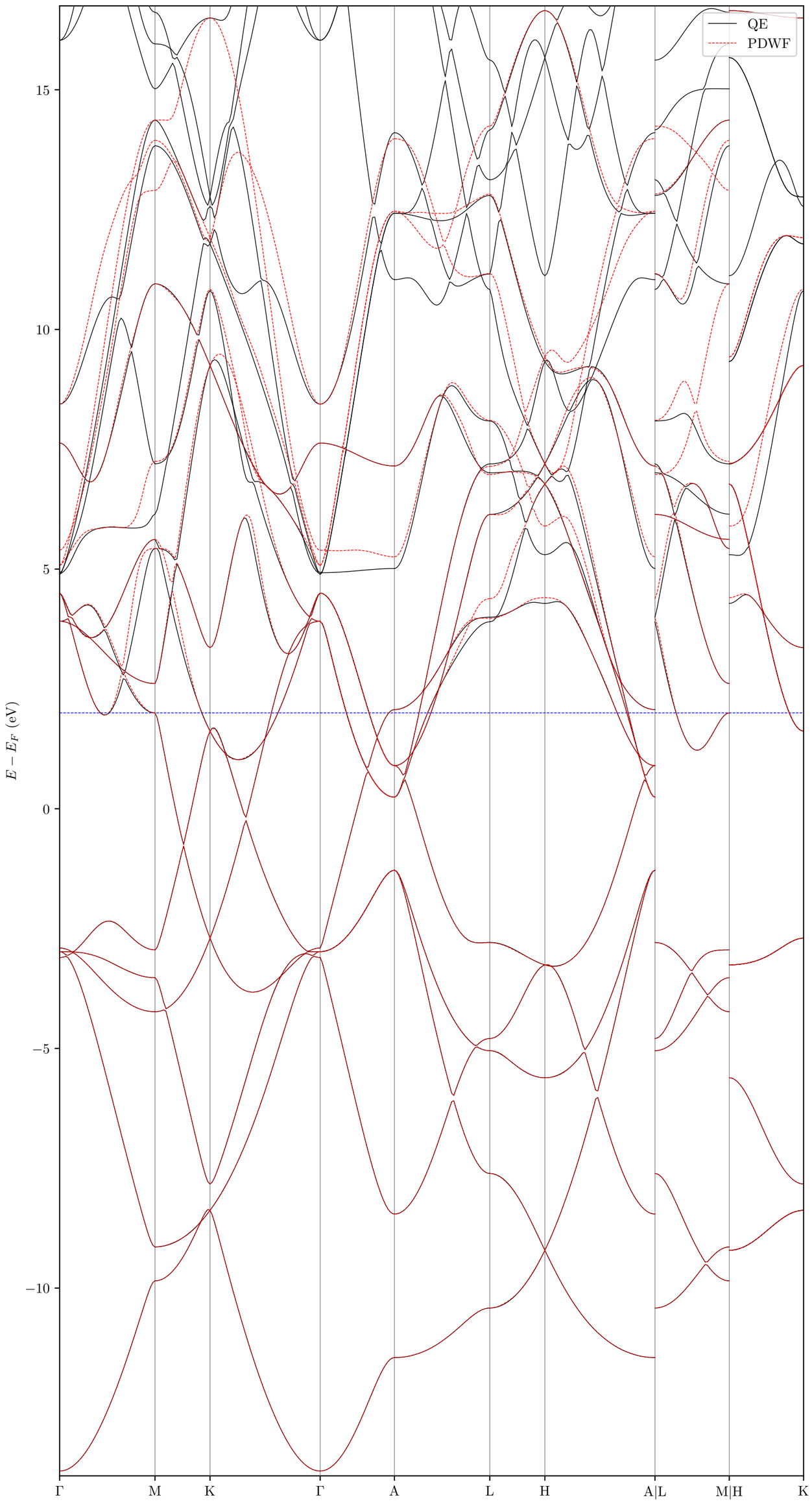

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.0 | 5.5 | 6.2 | 42.9 | 42.9 | 42.9 | 2.124 |

Hamiltonian decay



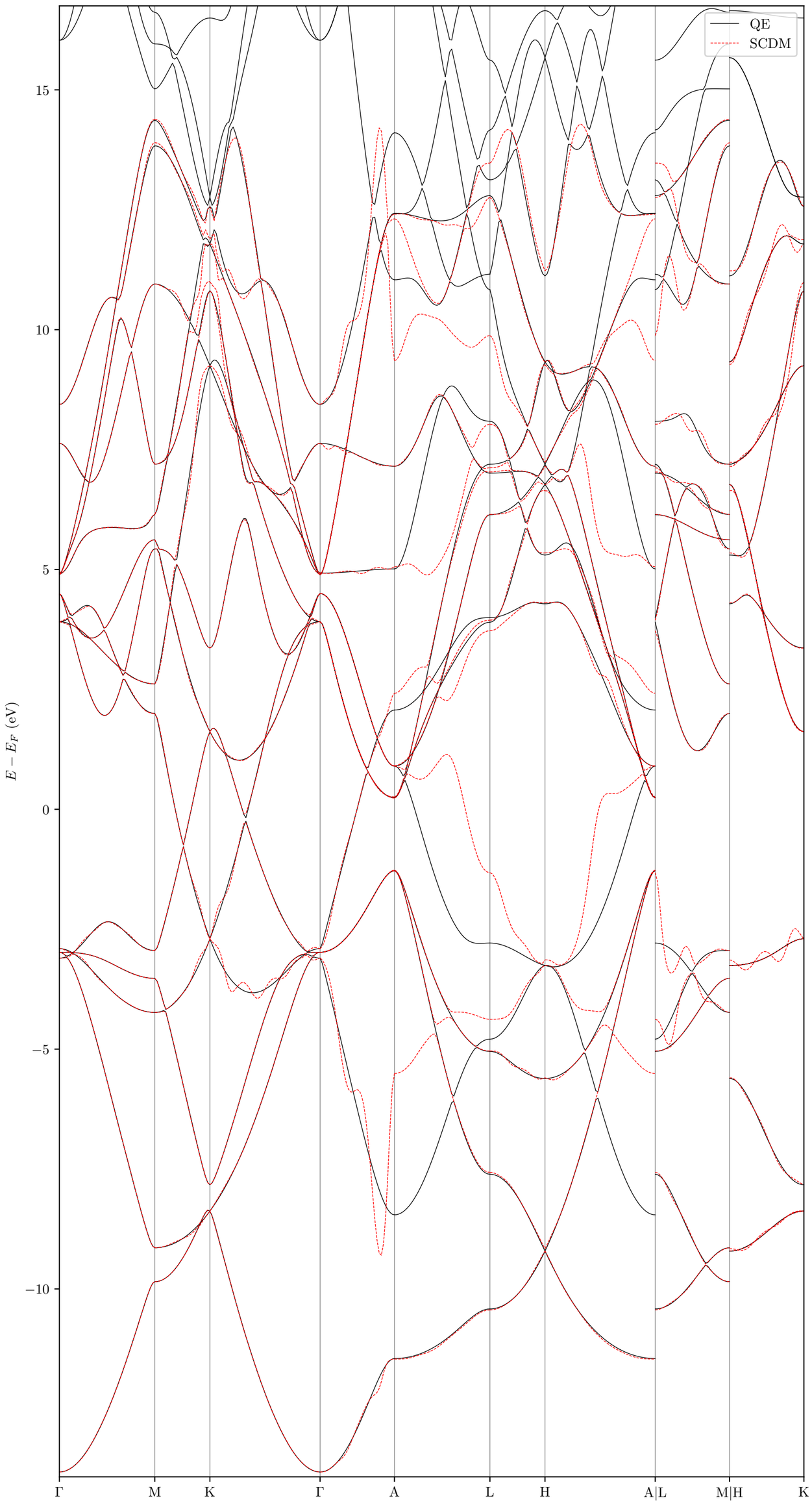
B2Hf exclude semicore
PW=be27a286-3233-4a8b-8659-a2989ab0b72b
W90=2c4dacb9-427b-438f-a6a0-549167984c97




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.3 | 3.9 | 31.6 | 14.4 | 21.7 | 510.7 | 2.095 |

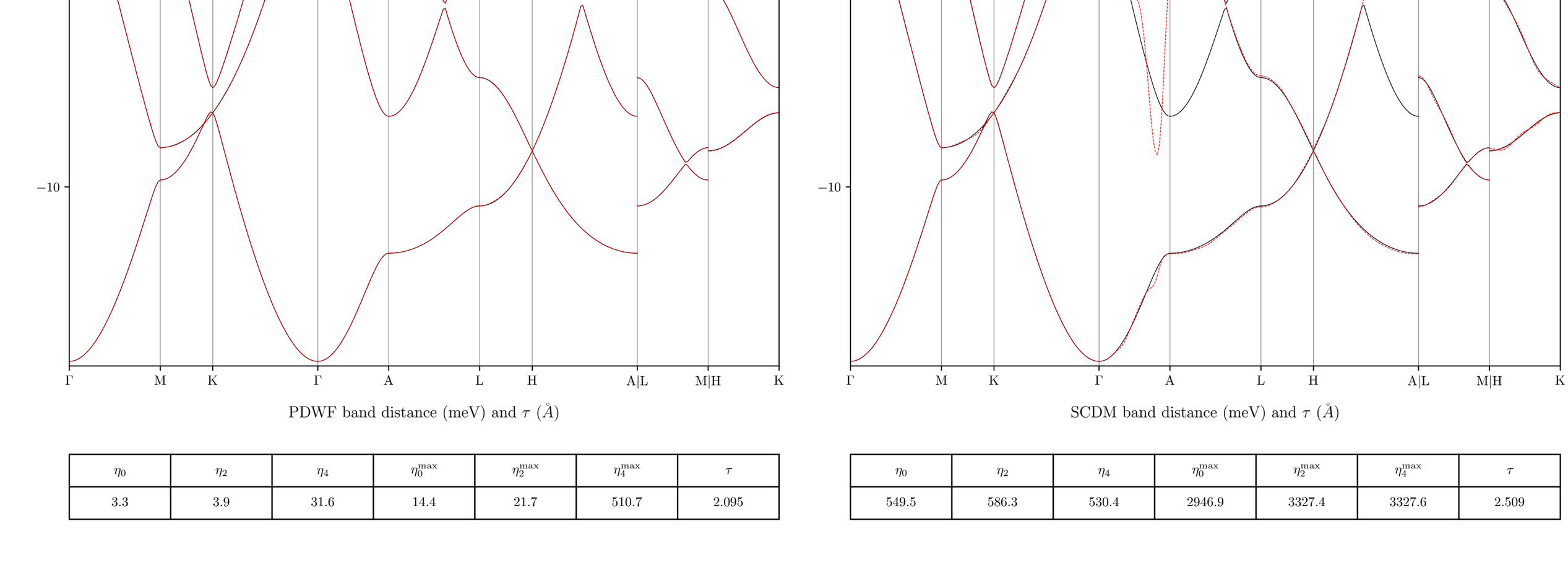
B2Hf exclude semicore
PW=be27a286-3233-4a8b-8659-a2989ab0b72b
W90=768e43c8-f627-4c4d-b7a7-78e190dd0399



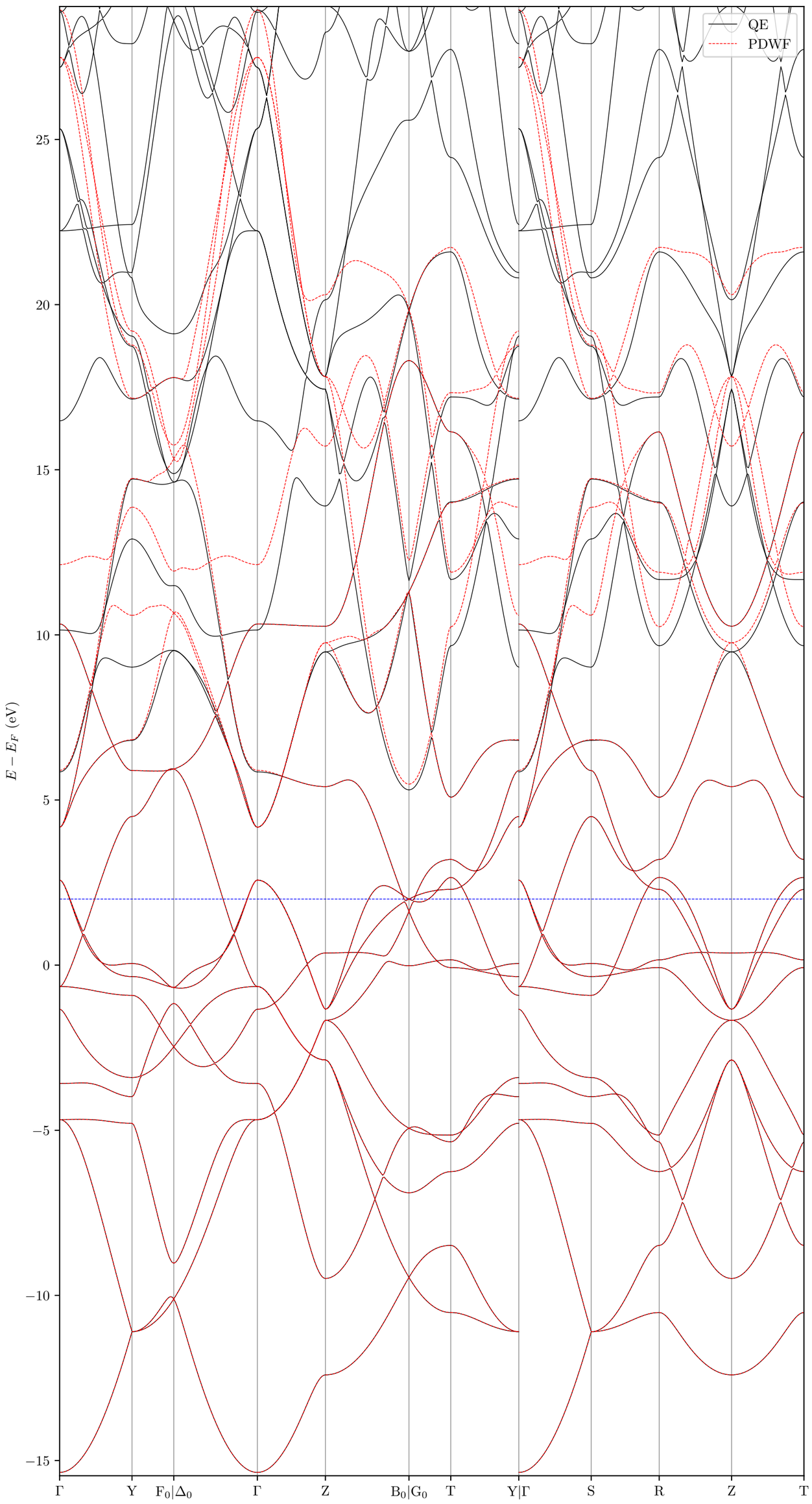

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 549.5 | 586.3 | 530.4 | 2946.9 | 3327.4 | 3327.6 | 2.509 |

Hamiltonian decay



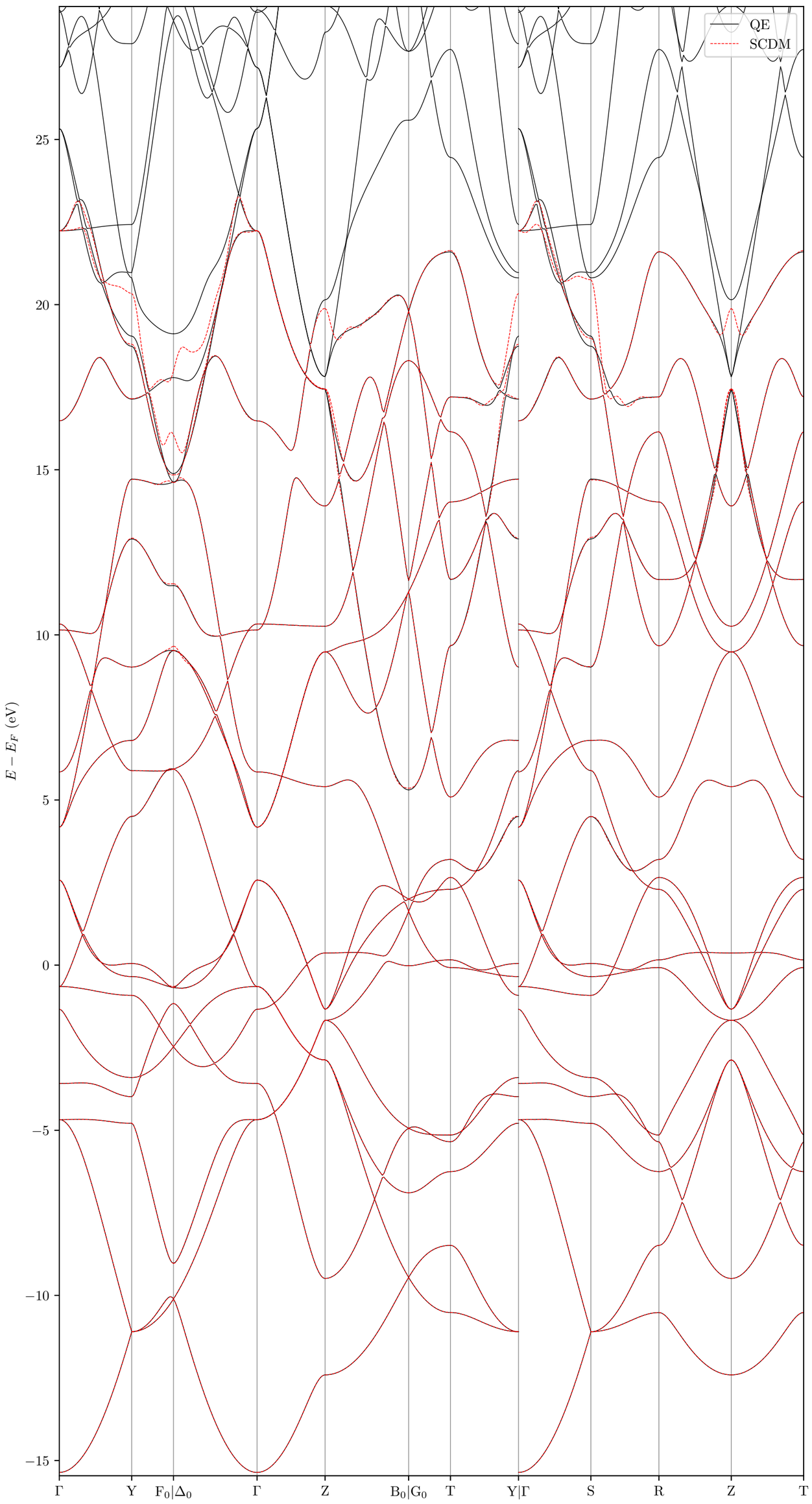
B2Mn exclude semicore
PW=1f23b5c4-a17a-4b9c-96f2-6976ab734028
W90=7dd1daef-69ae-447e-9741-5a7e8af9039e




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.4 | 1.4 | 1.4 | 6.4 | 7.3 | 7.3 | 1.910 |

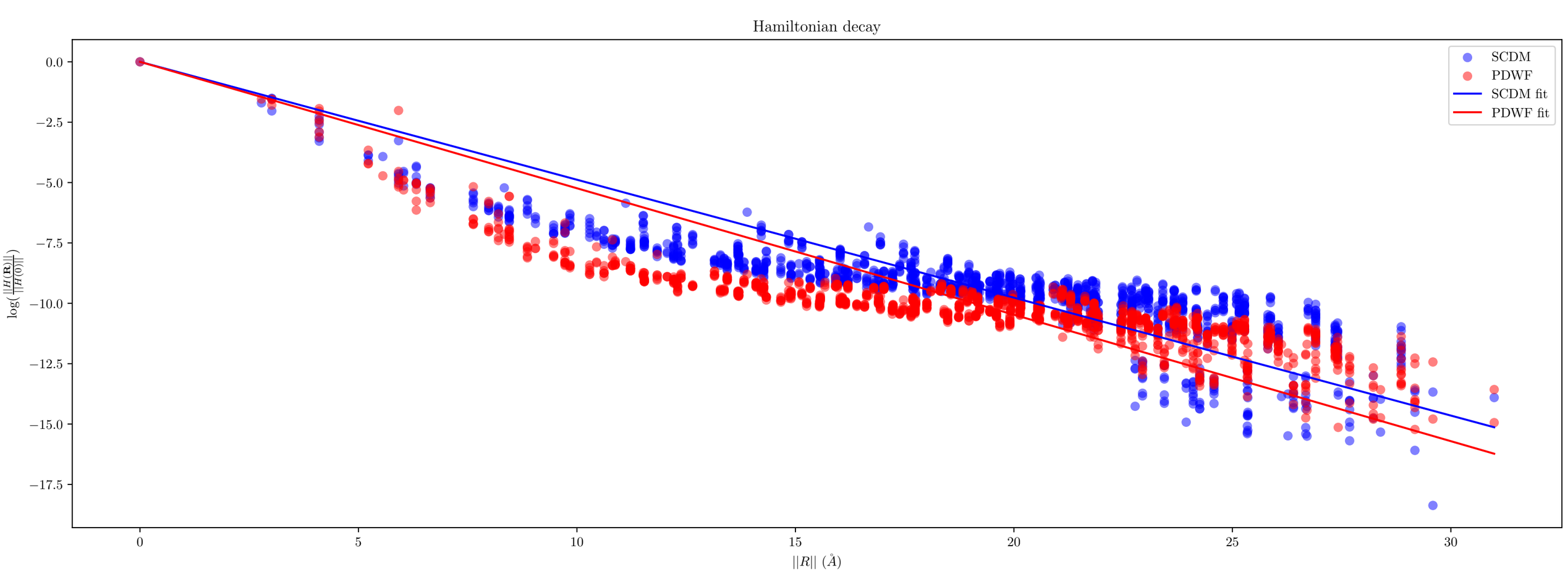
B2Mn exclude semicore
PW=1f23b5c4-a17a-4b9c-96f2-6976ab734028
W90=6bee2cd5-24c1-40a3-be43-42b0ceec2d4f




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.6 | 2.4 | 3.1 | 31.8 | 31.9 | 37.6 | 2.048 |

Hamiltonian decay



B2Ta exclude semicore
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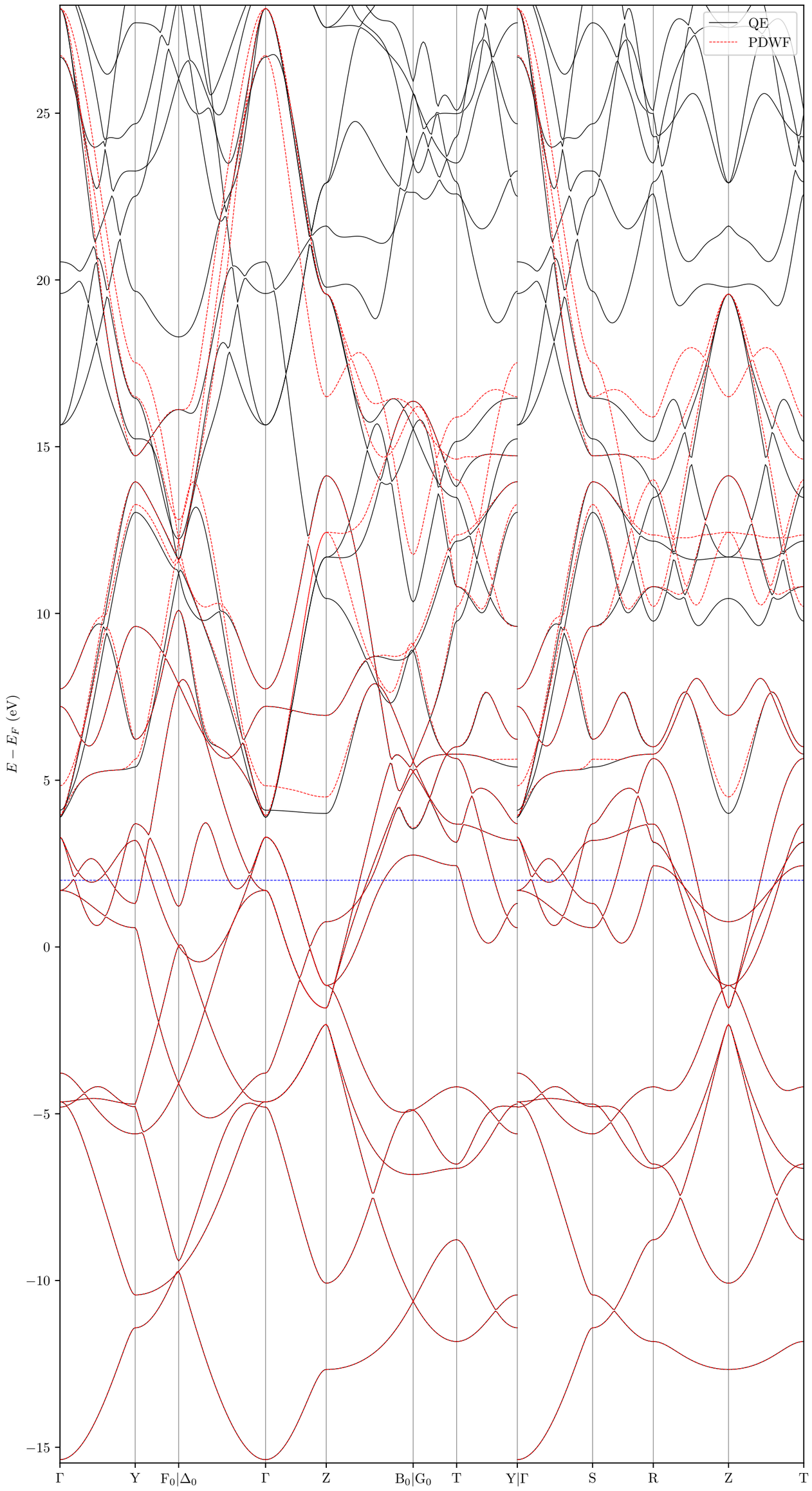
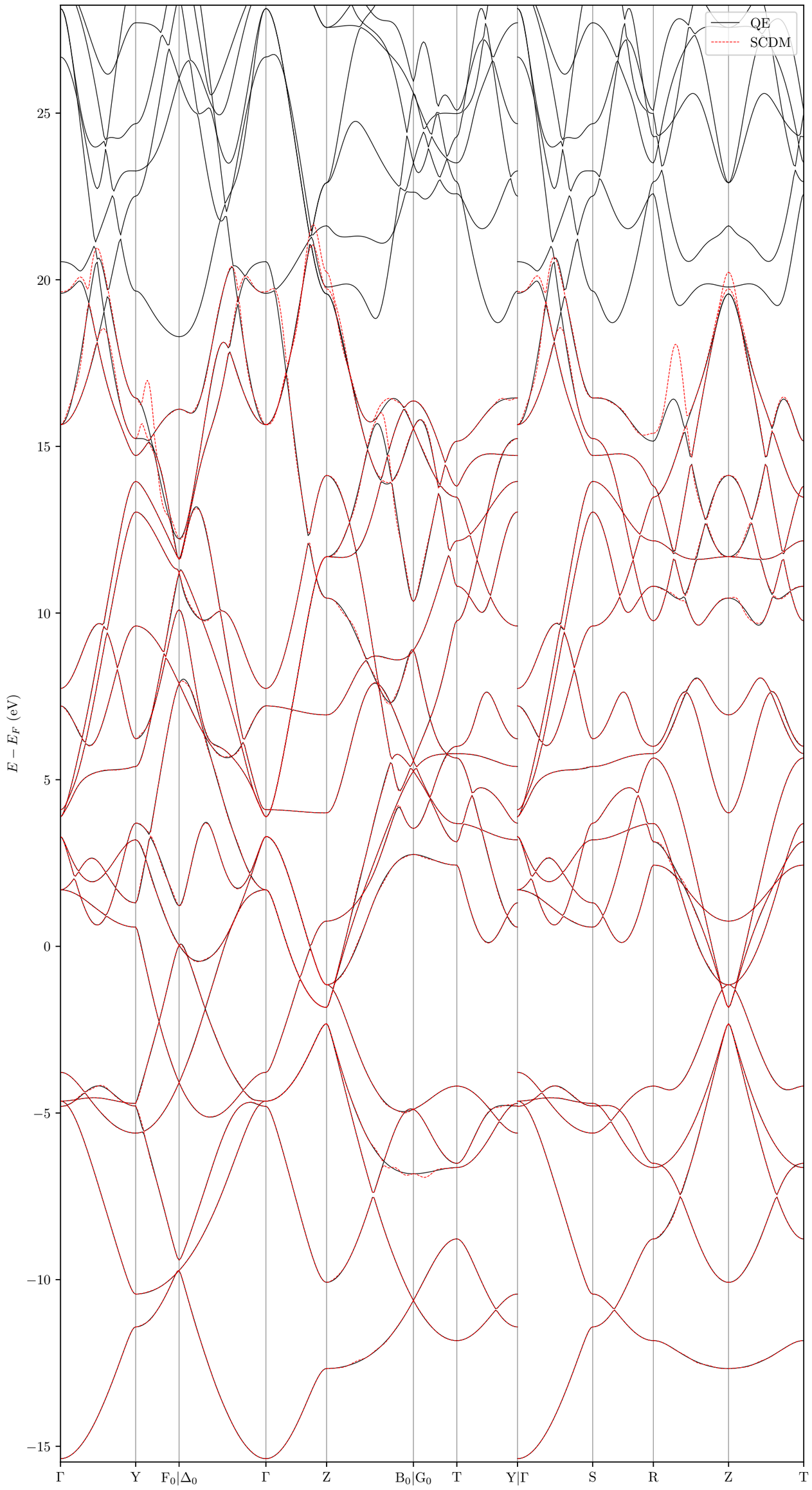
W90=45c47276-8196-4f2f-bcca-40a24380cfee




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.2 | 11.7 | 7.2 | 8.0 | 34.4 | 1.897 |

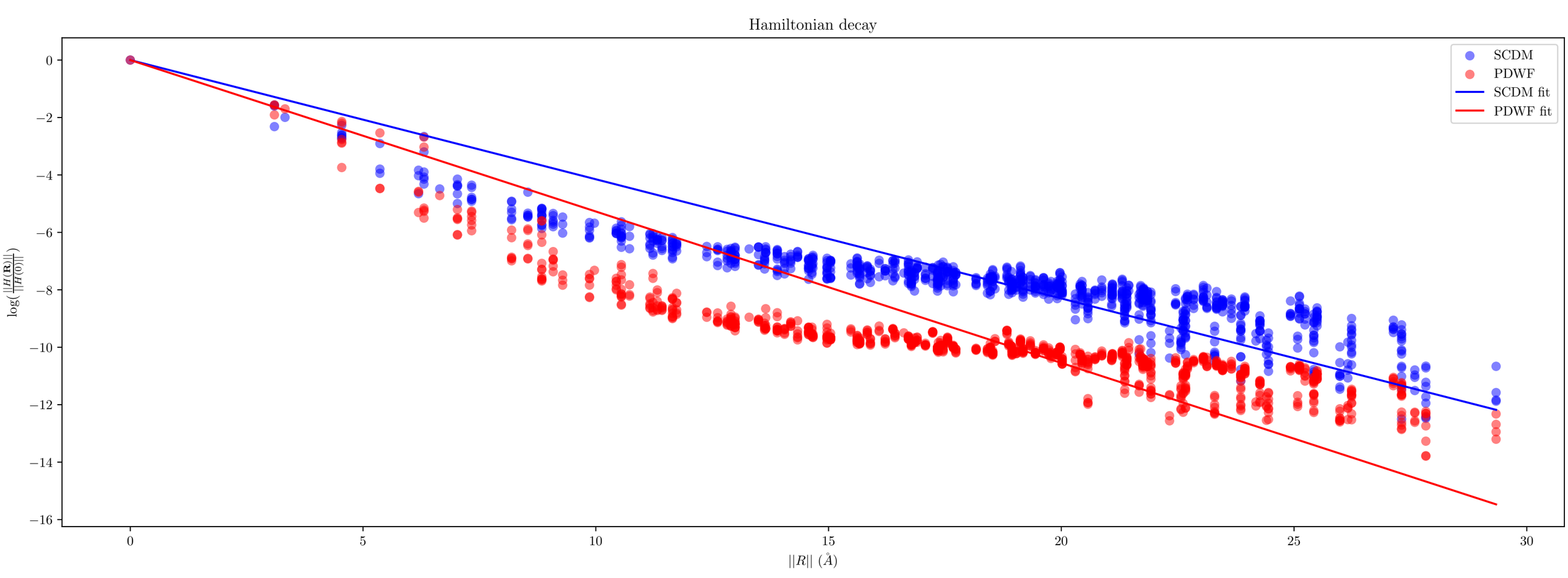
B2Ta exclude semicore
PW=7ac0cdc4-5ec1-4c08-8e29-362eede7cc85
W90=051bd8e6-c343-479d-9ad3-f9d67035ed83



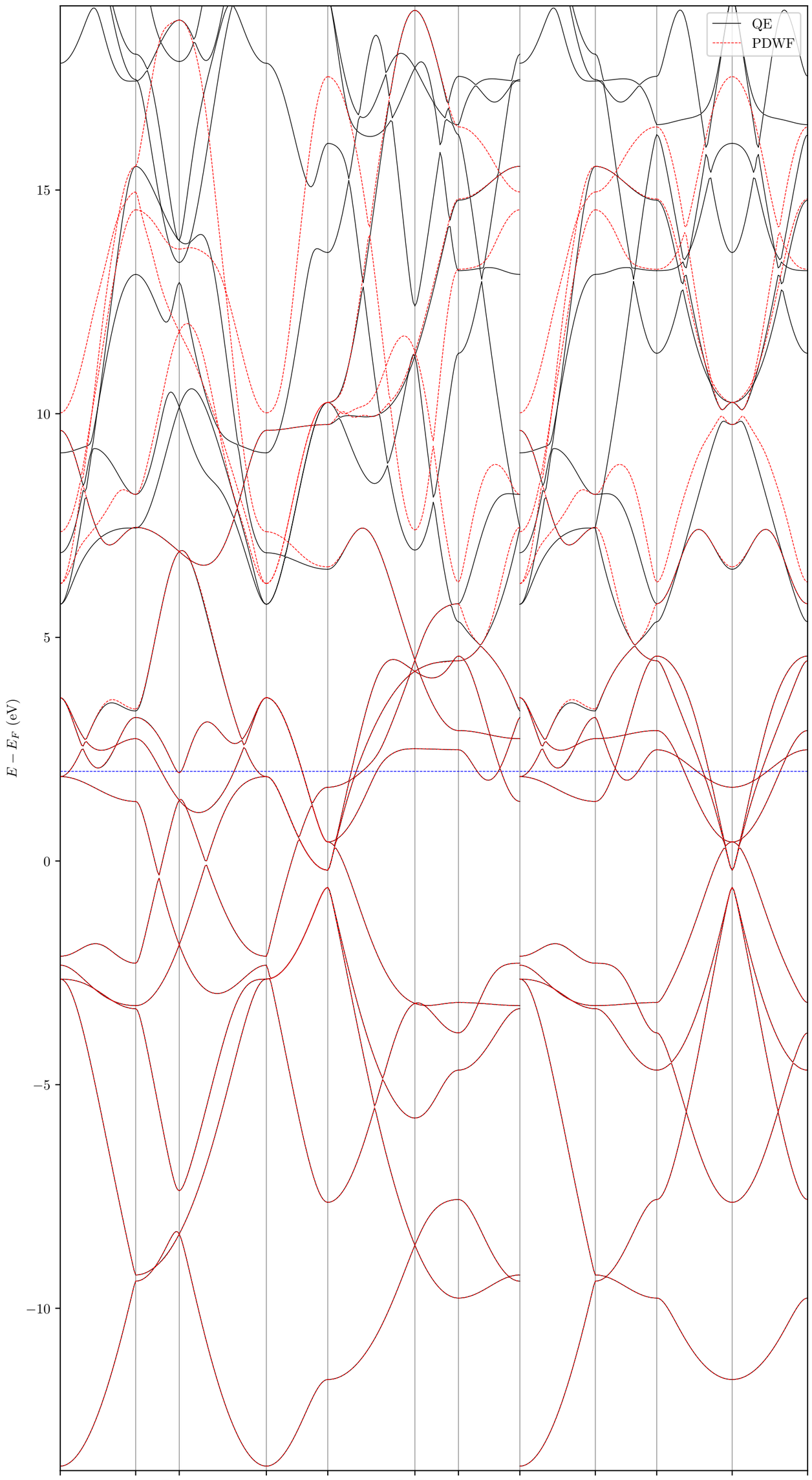

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 13.4 | 13.9 | 14.3 | 138.7 | 138.7 | 138.7 | 2.409 |

Hamiltonian decay



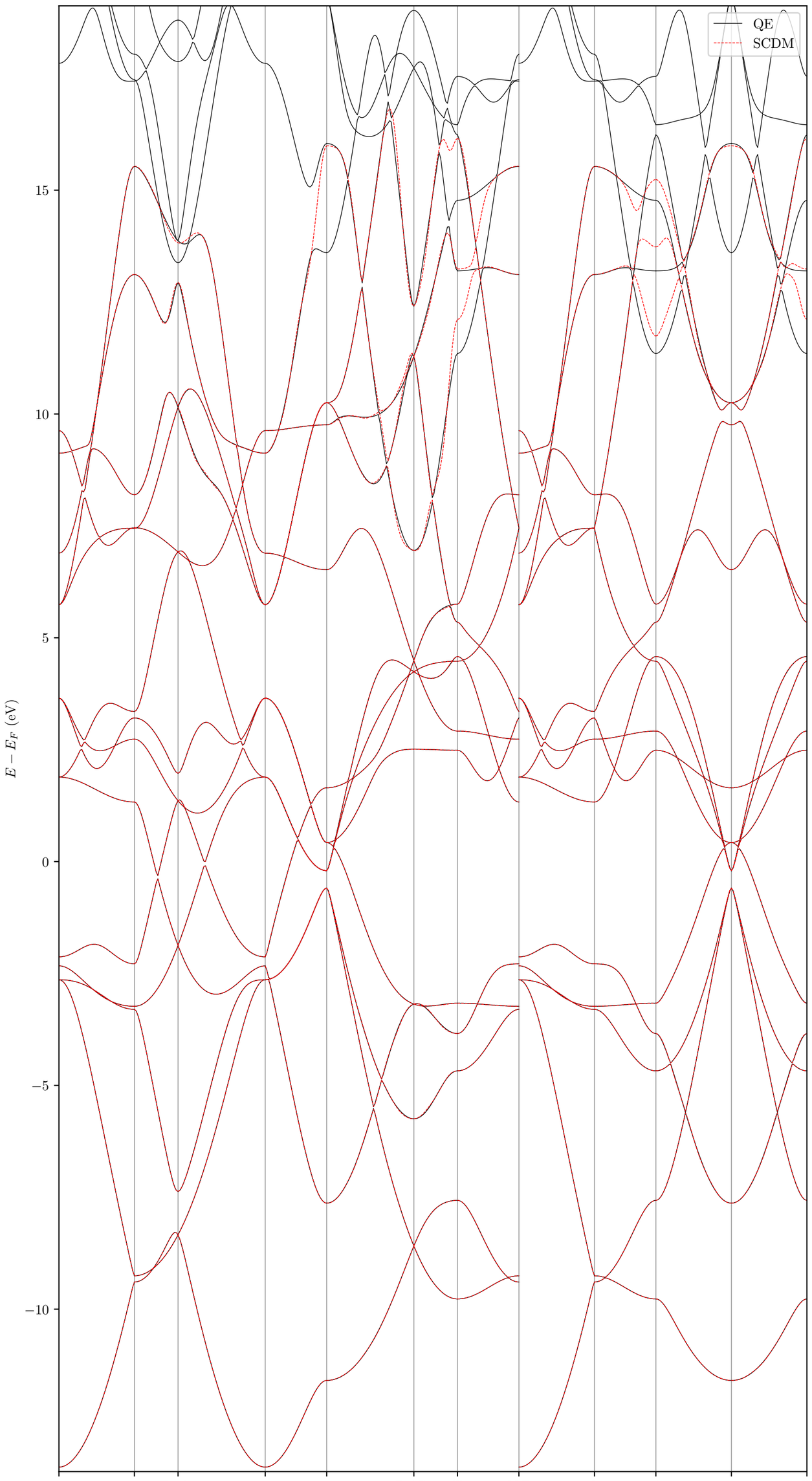
B2Ti exclude semicore
PW=c3a671c5-328a-4c24-81a1-8dd25fcb2f76
W90=ecd1ef01-bfb5-452f-976e-5cfca6e0ec8d




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.5 | 1.5 | 6.9 | 12.5 | 12.5 | 74.7 | 1.931 |

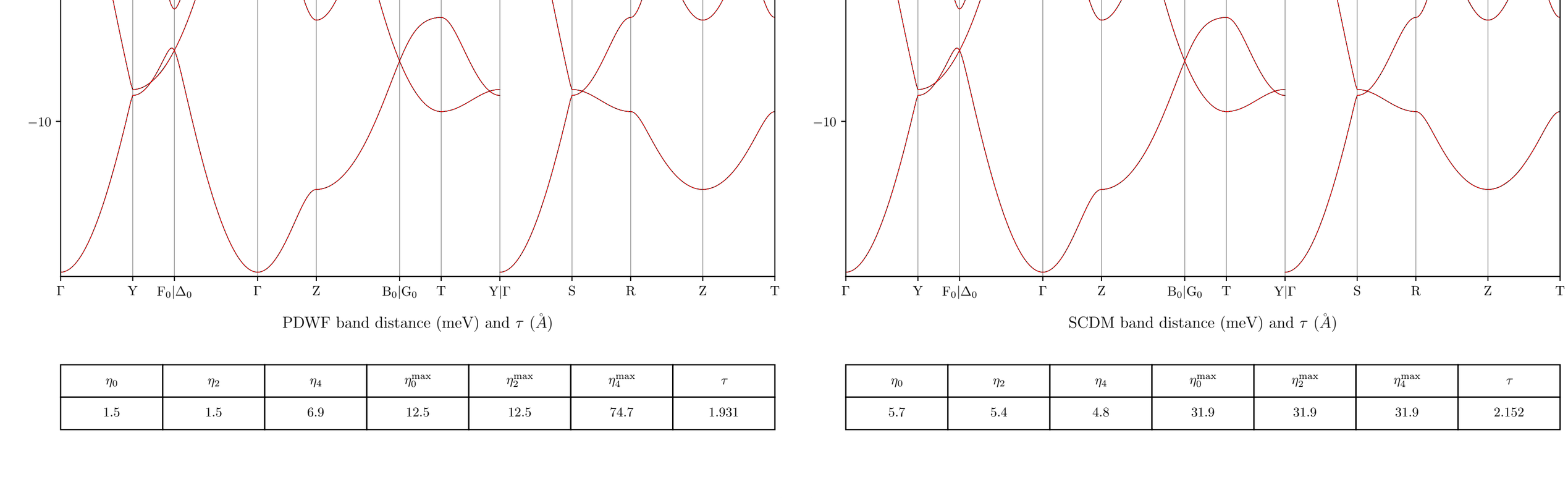
B2Ti exclude semicore
PW=c3a671c5-328a-4c24-81a1-8dd25fcb2f76
W90=be14ccc5-7096-4aa4-8f0c-8d432404f1be

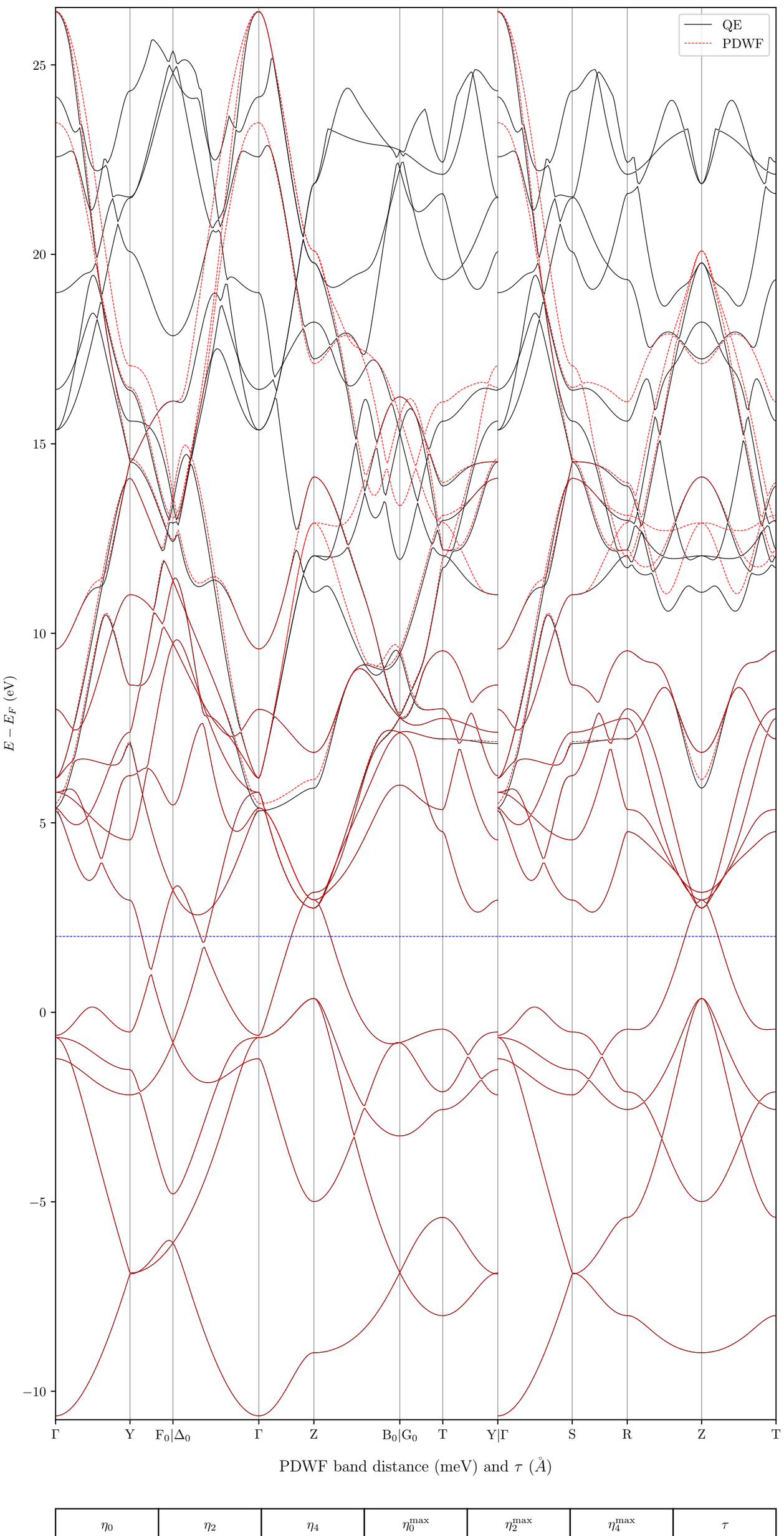



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.7 | 5.4 | 4.8 | 31.9 | 31.9 | 31.9 | 2.152 |

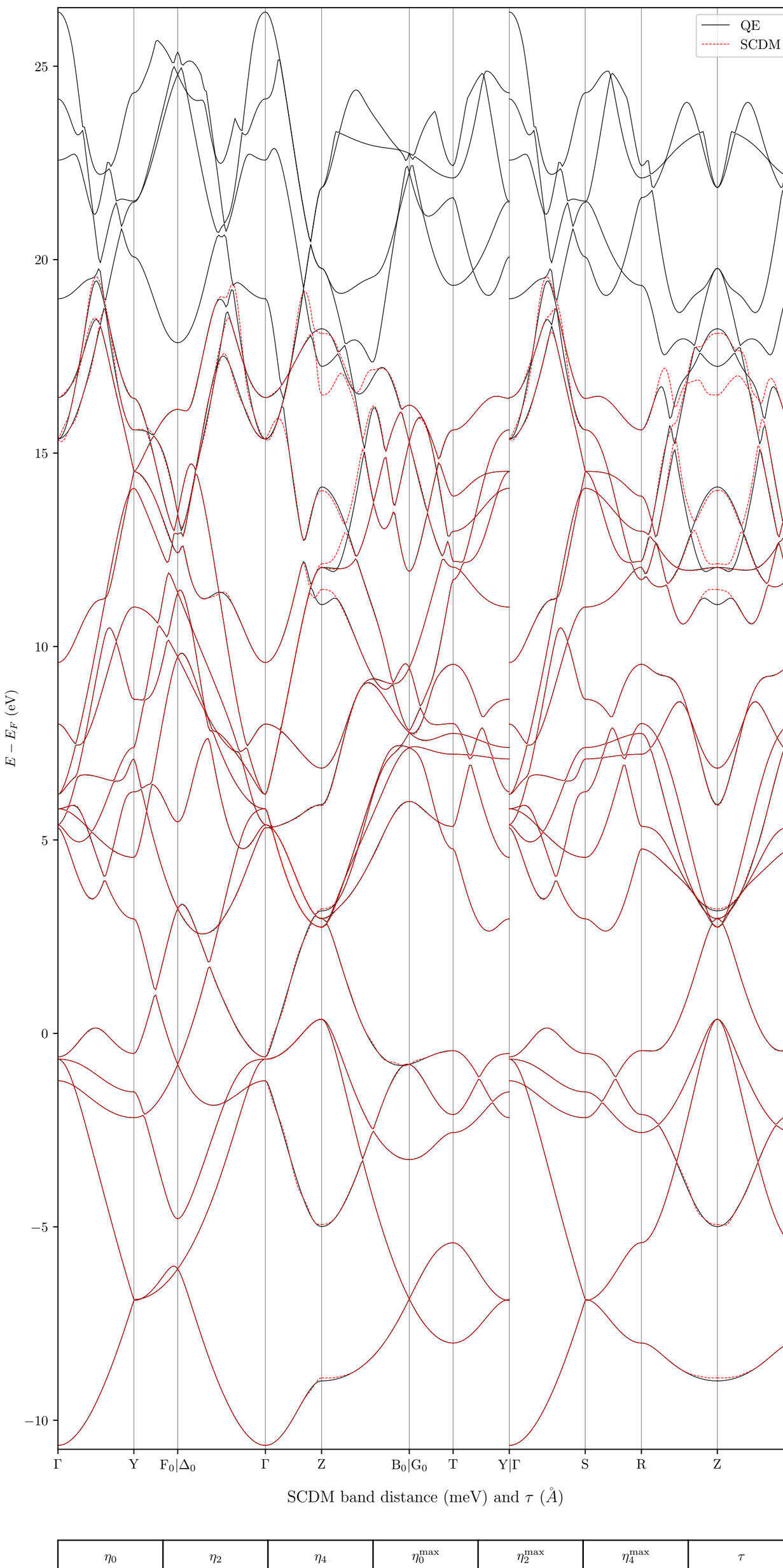
Hamiltonian decay





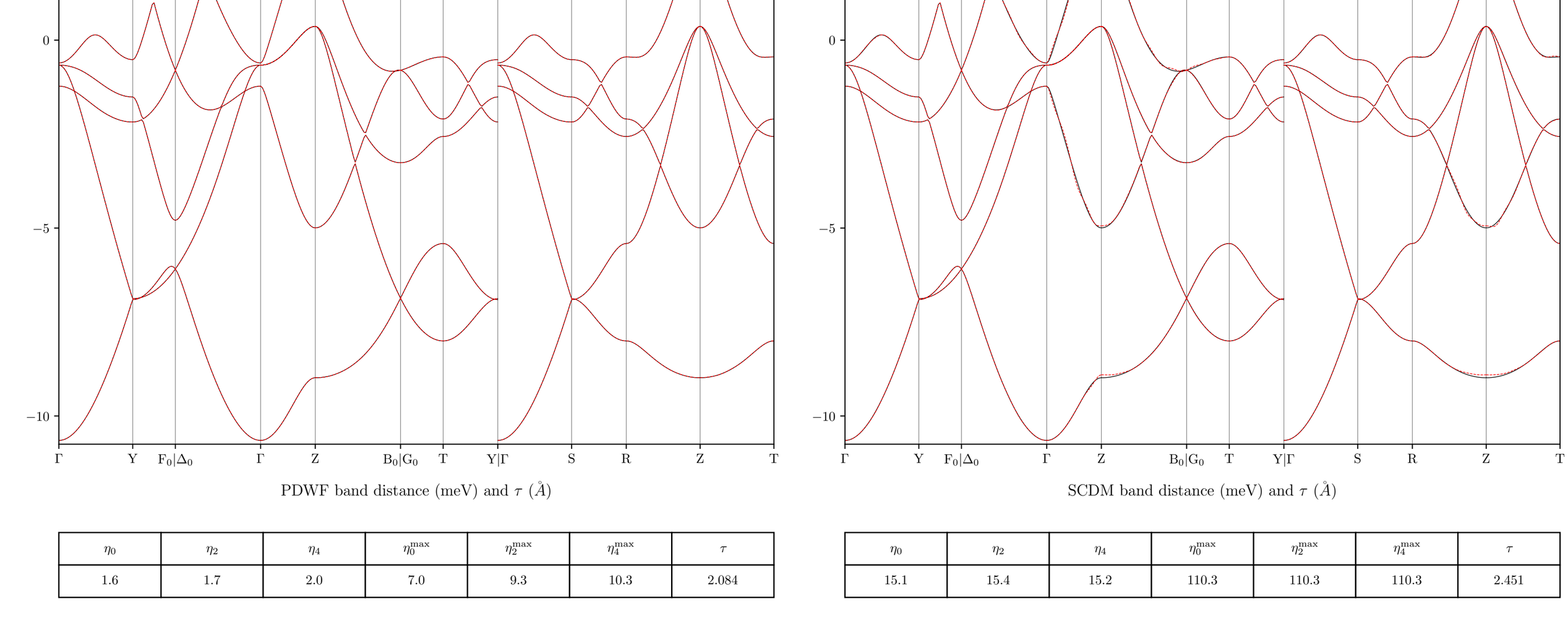

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.6 | 1.7 | 2.0 | 7.0 | 9.3 | 10.3 | 2.084 |

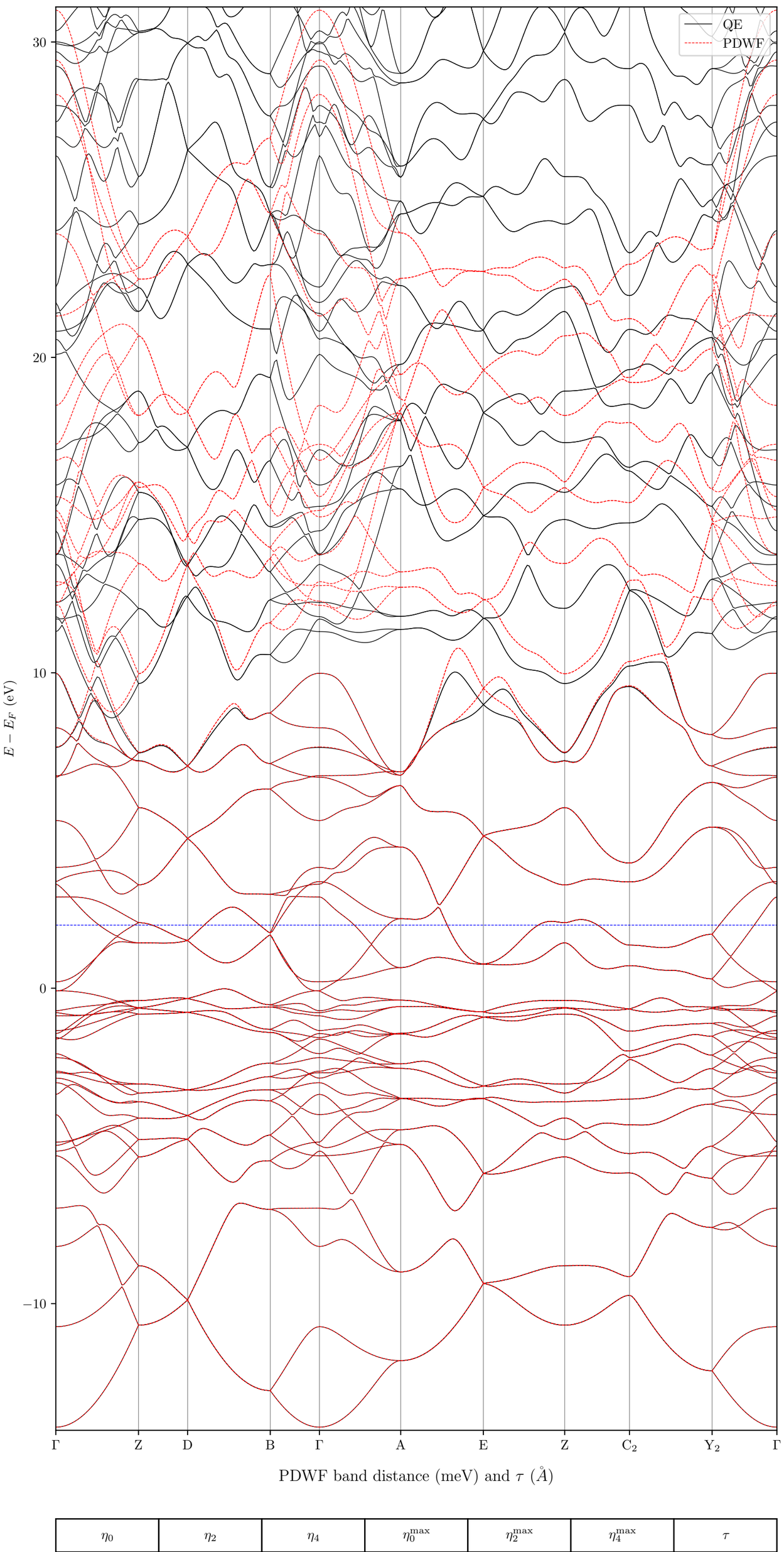



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 15.1 | 15.4 | 15.2 | 110.3 | 110.3 | 110.3 | 2.451 |



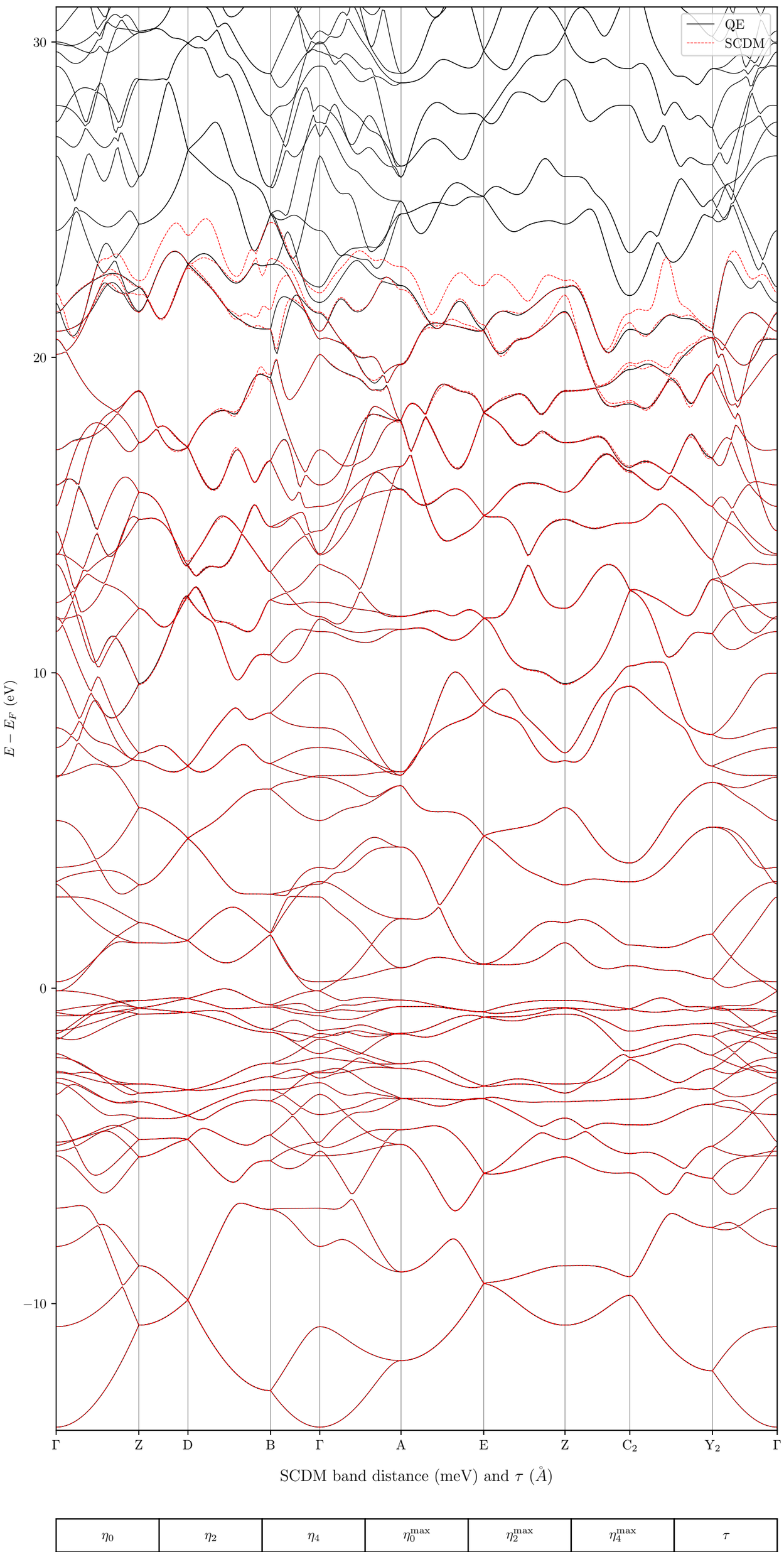
B4Co4 exclude semicore
PW=56fbd965-453e-48a1-be00-5f28f8b1c0f0
W90=5848c031-42ba-4c50-9e47-c8921edb89bf




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 0.7 | 4.4 | 4.4 | 5.1 | 2.029 |

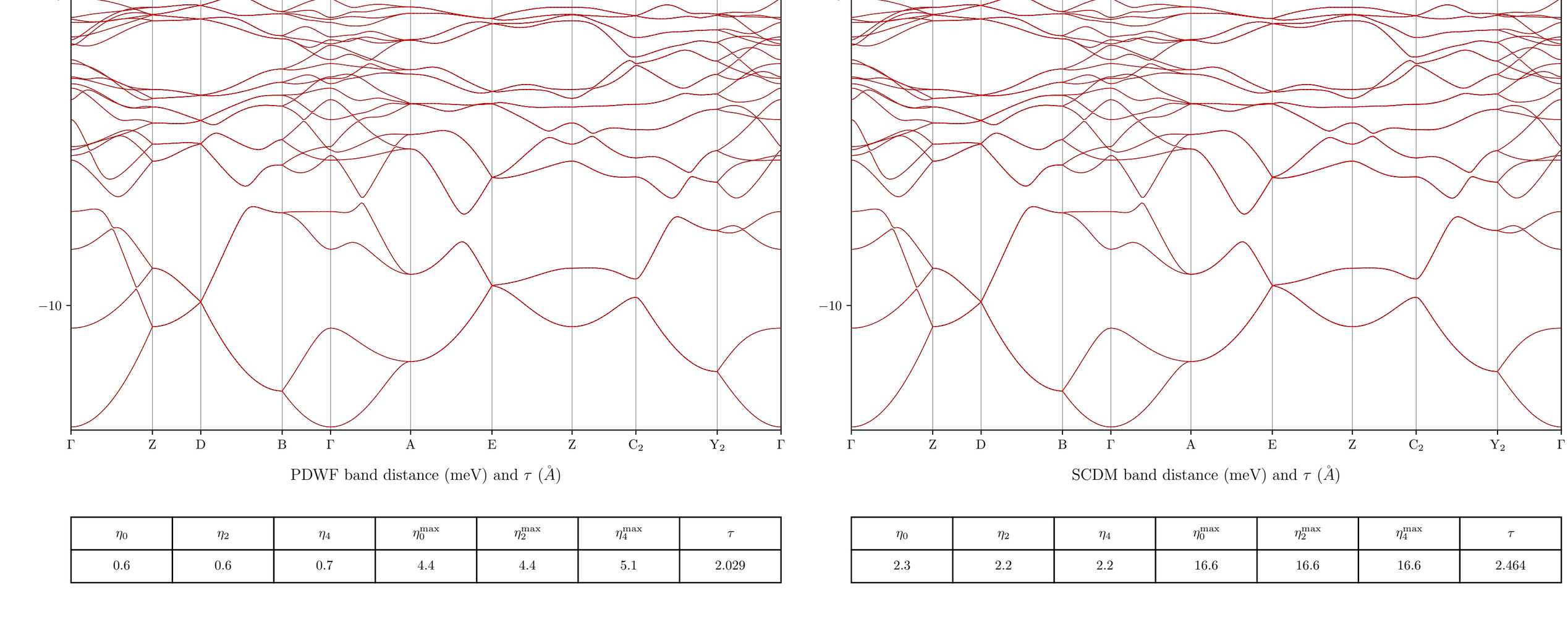
B4Co4 exclude semicore
PW=56fbd965-453e-48a1-be00-5f28f8b1c0f0
W90=2e4fea18-8af6-4a17-964f-9c3421950062



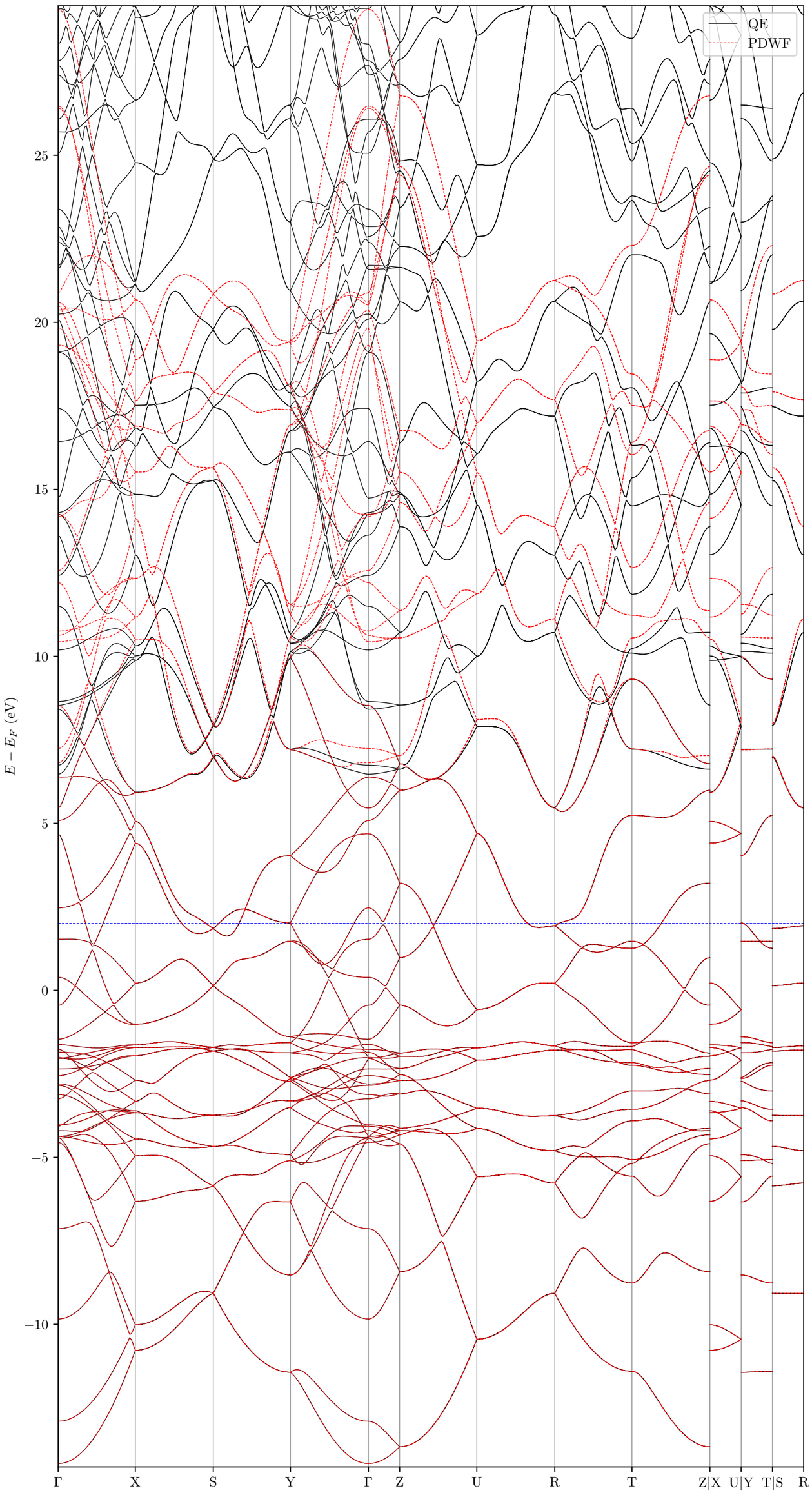

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.3 | 2.2 | 2.2 | 16.6 | 16.6 | 16.6 | 2.464 |

Hamiltonian decay



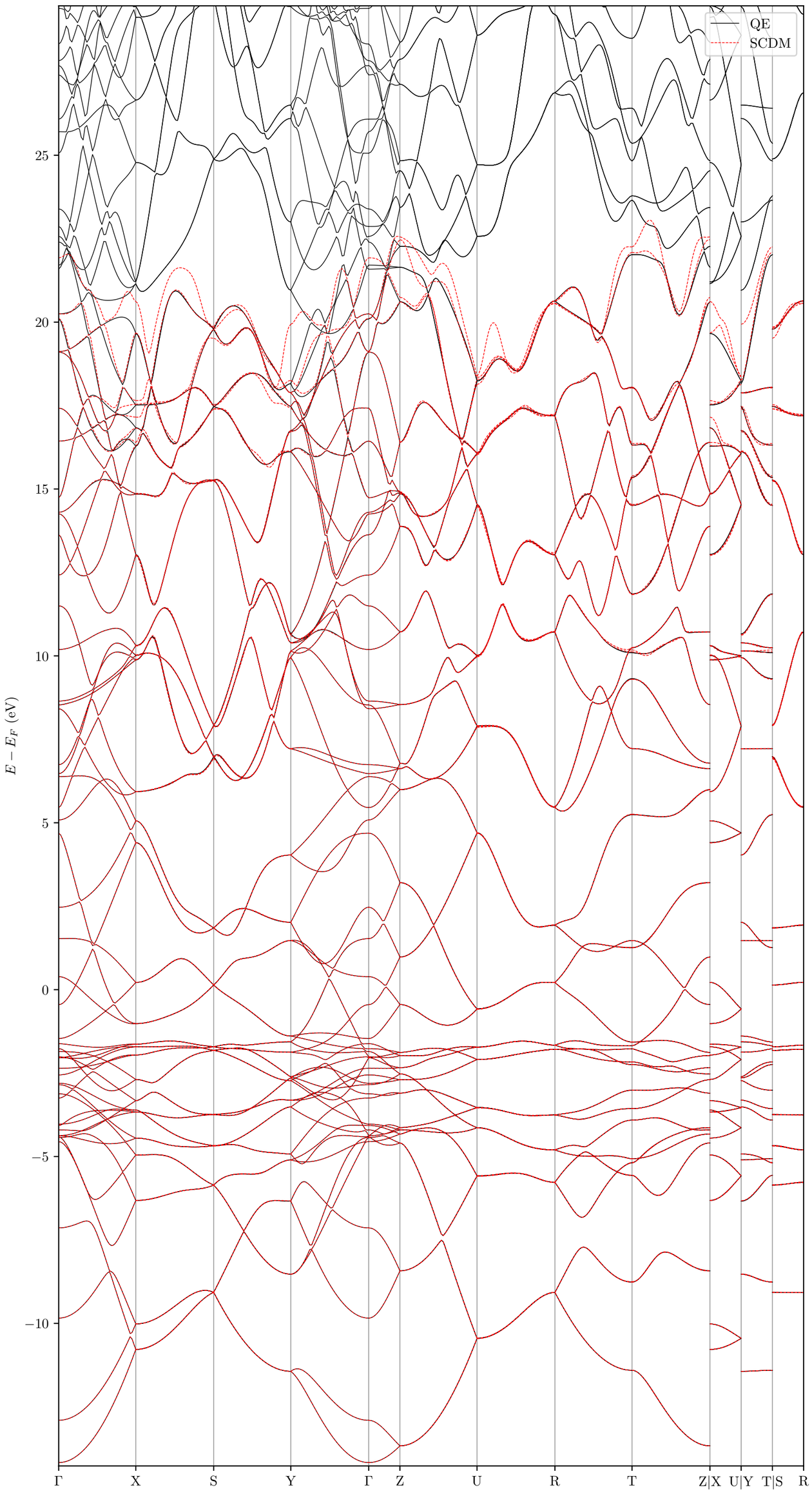
B4Ni4 exclude semicore
PW=81b84c87-f49c-46a1-9c0d-da21157cf47c
W90=77e39593-a244-4a39-9fc1-14092ca7a3b5




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.9 | 1.0 | 1.0 | 5.5 | 6.4 | 8.2 | 2.104 |

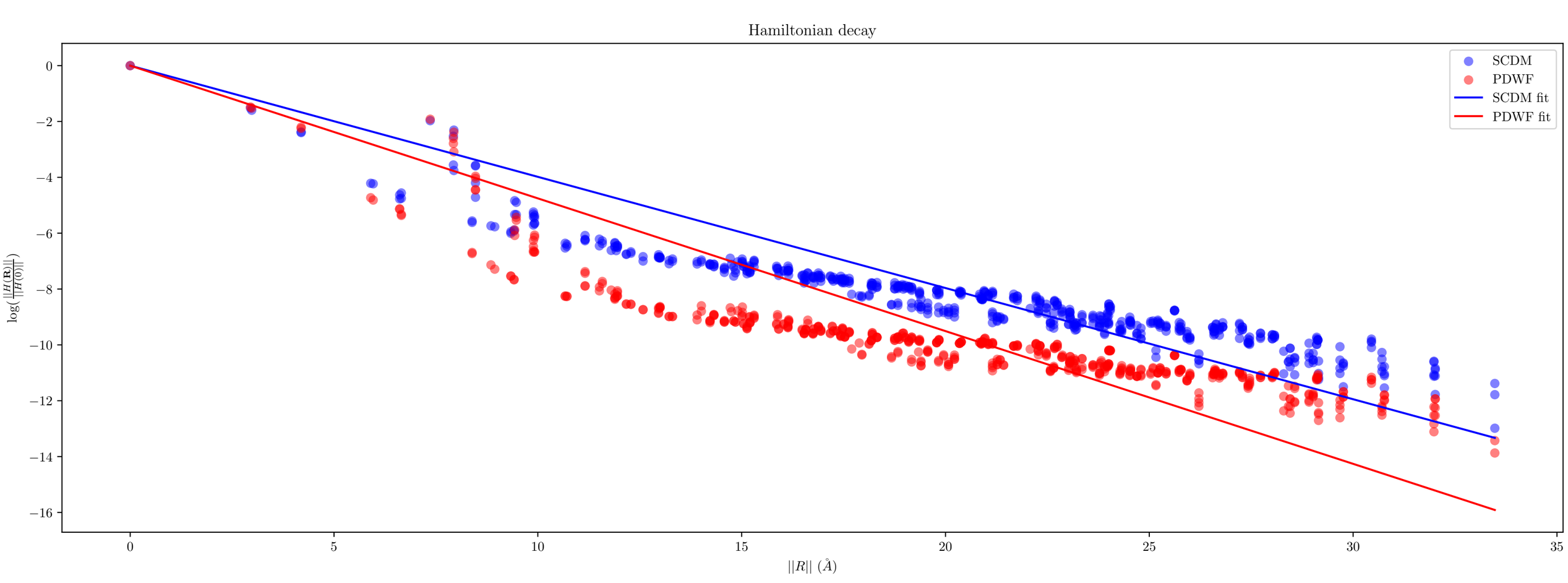
B4Ni4 exclude semicore
PW=81b84c87-f49c-46a1-9c0d-da21157cf47c
W90=4203a12d-503a-482b-b04a-75bd52191c64



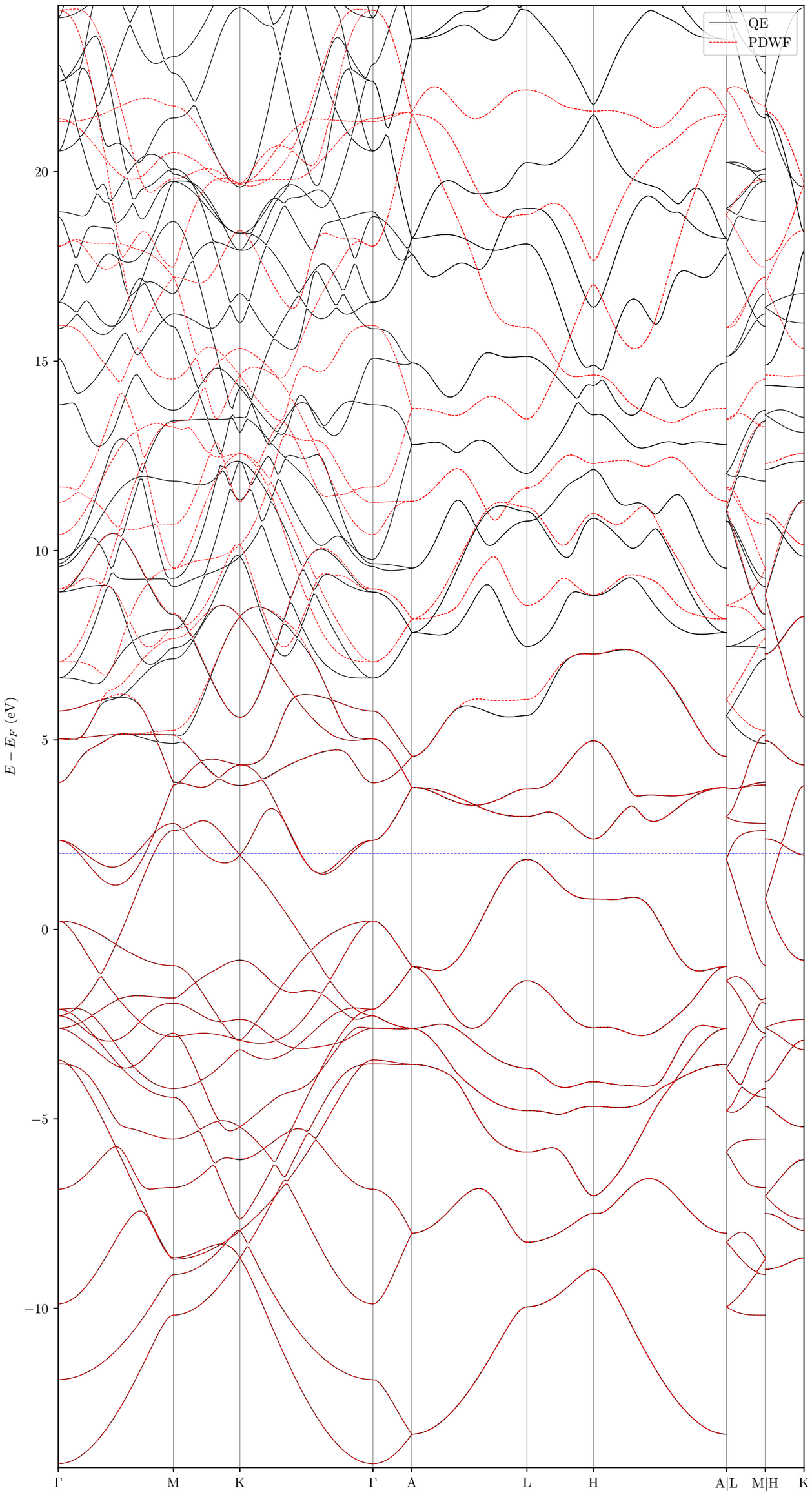

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.2 | 3.2 | 3.3 | 19.5 | 22.2 | 22.3 | 2.511 |

Hamiltonian decay



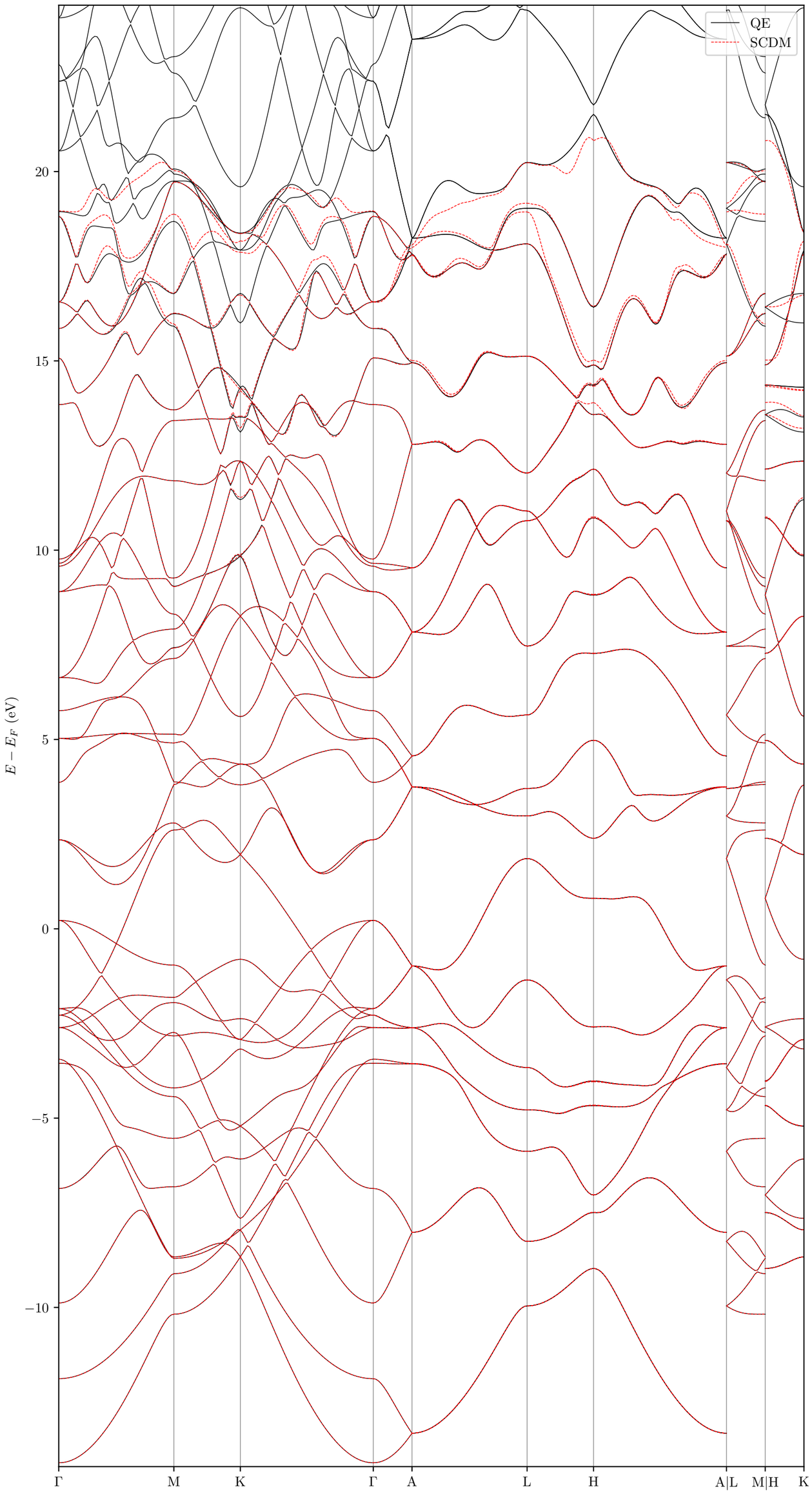
B4Re2 exclude semicore
PW=721fde27-79a7-4ce6-ada4-b262aa549239
W90=5cae9b63-1c4b-4bf3-be84-5a7fdaca2a4c




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.1 | 3.3 | 3.4 | 22.3 | 22.3 | 22.3 | 2.256 |

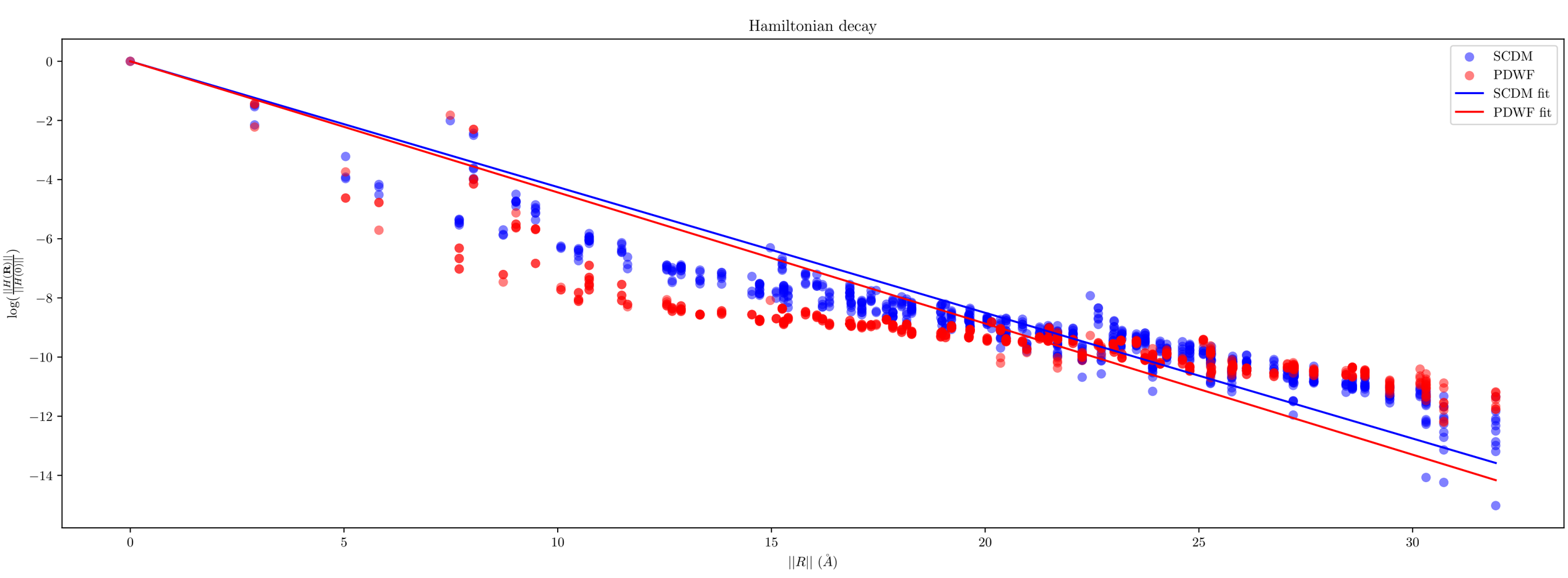
B4Re2 exclude semicore
PW=721fde27-79a7-4ce6-ada4-b262aa549239
W90=1b61aa70-303d-4d3b-bb2f-c85f418fe438



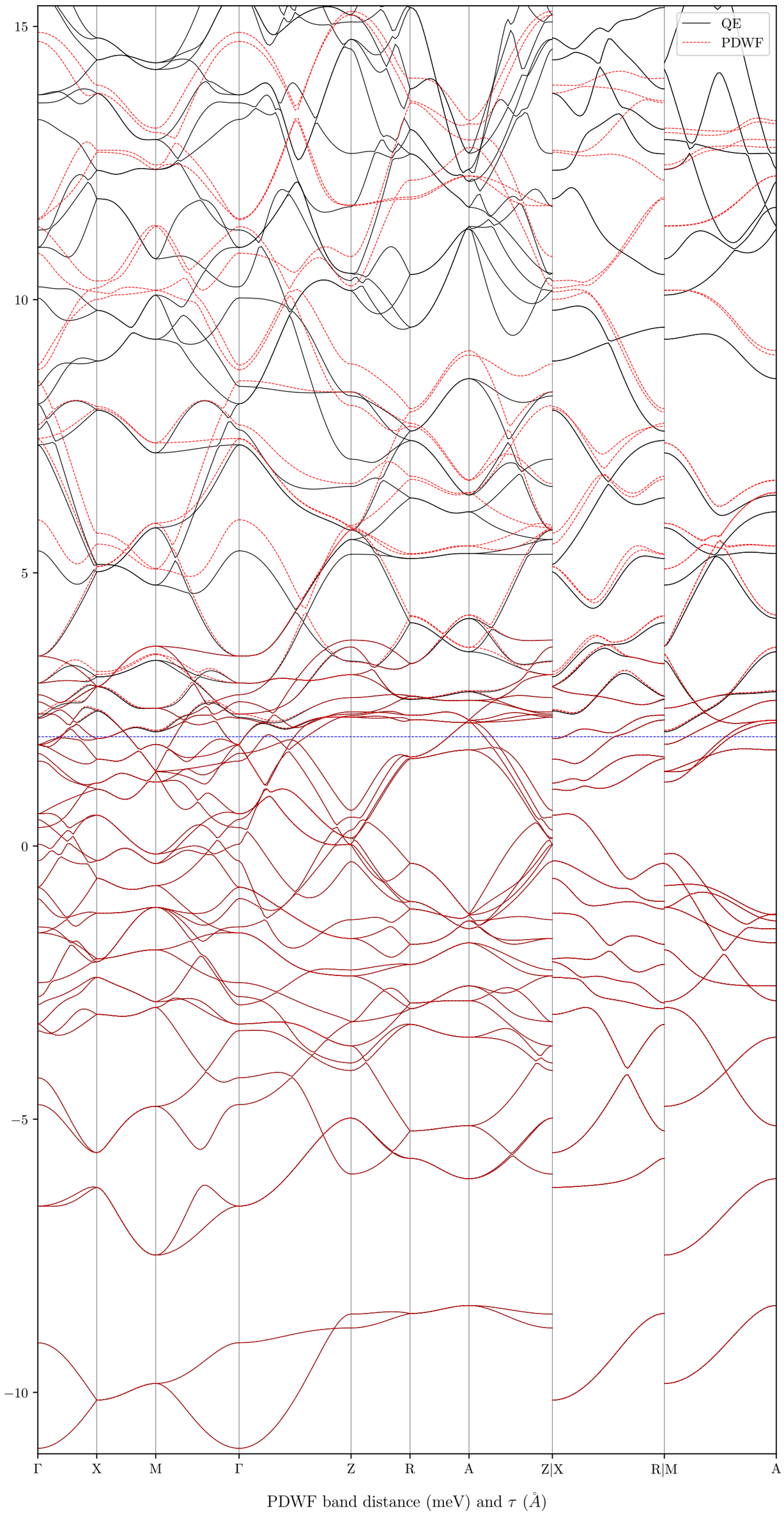

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.0 | 2.9 | 2.8 | 22.9 | 22.9 | 22.9 | 2.352 |

Hamiltonian decay



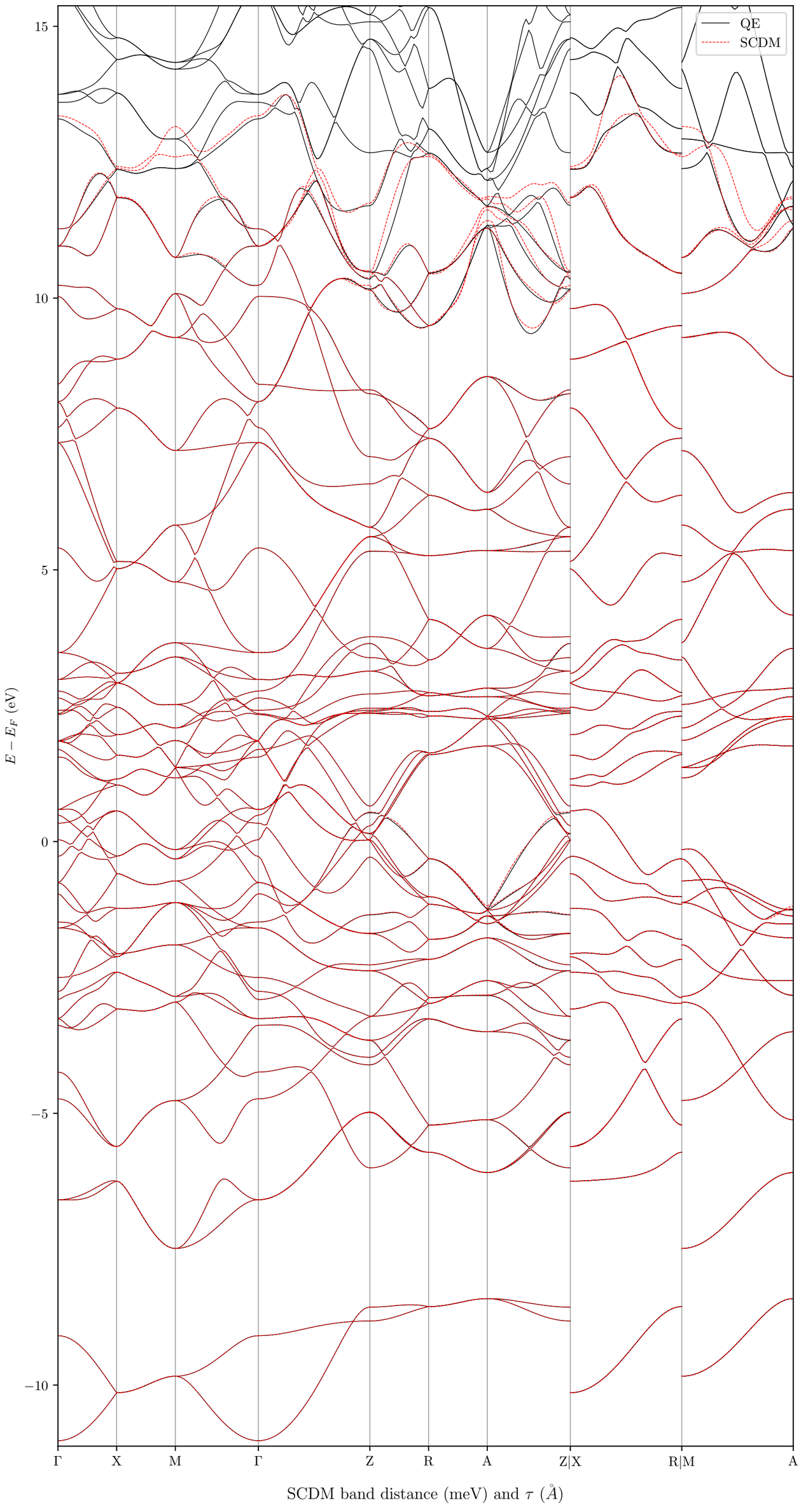
B4V6 exclude semicore
PW=d8354294-b7f4-4df8-a711-9308c8d04cf7
W90=5f82675b-8fb3-411a-b91a-46f28b4f3058




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.4 | 1.2 | 16.2 | 2.4 | 7.1 | 134.5 | 1.925 |

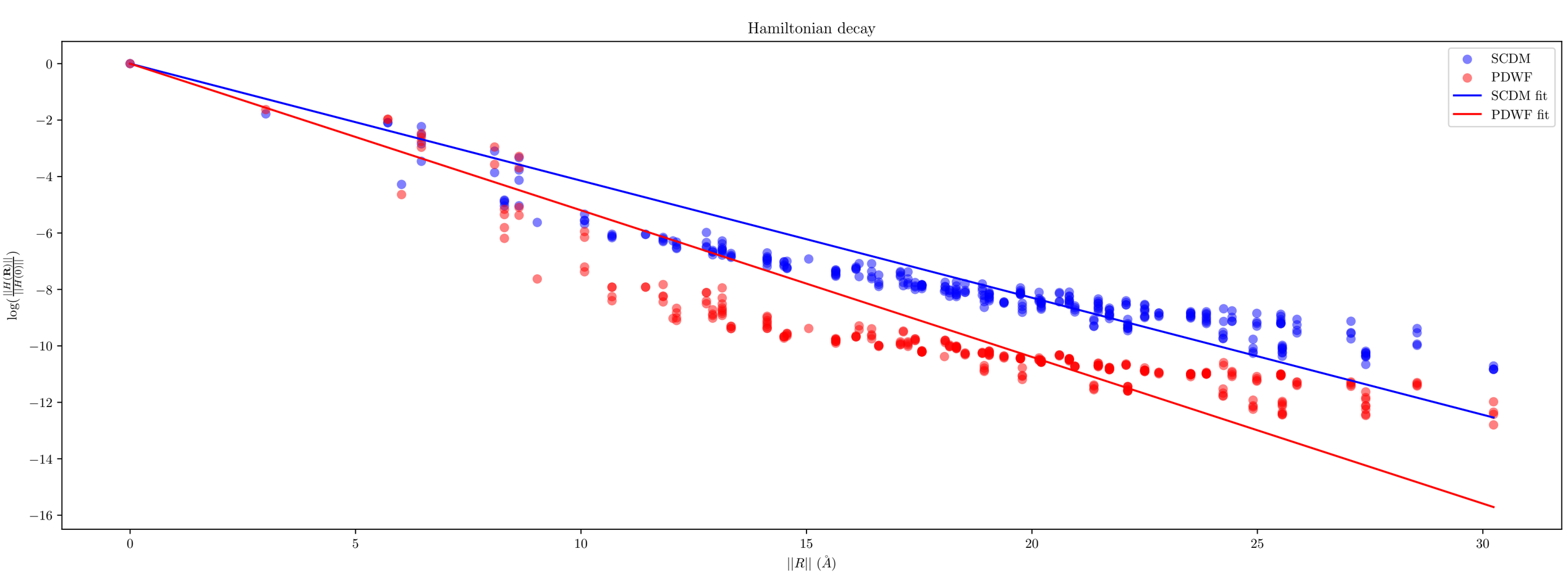
B4V6 exclude semicore
PW=d8354294-b7f4-4df8-a711-9308c8d04cf7
W90=7c67540d-56fe-4880-99e3-badc27e2fe5f

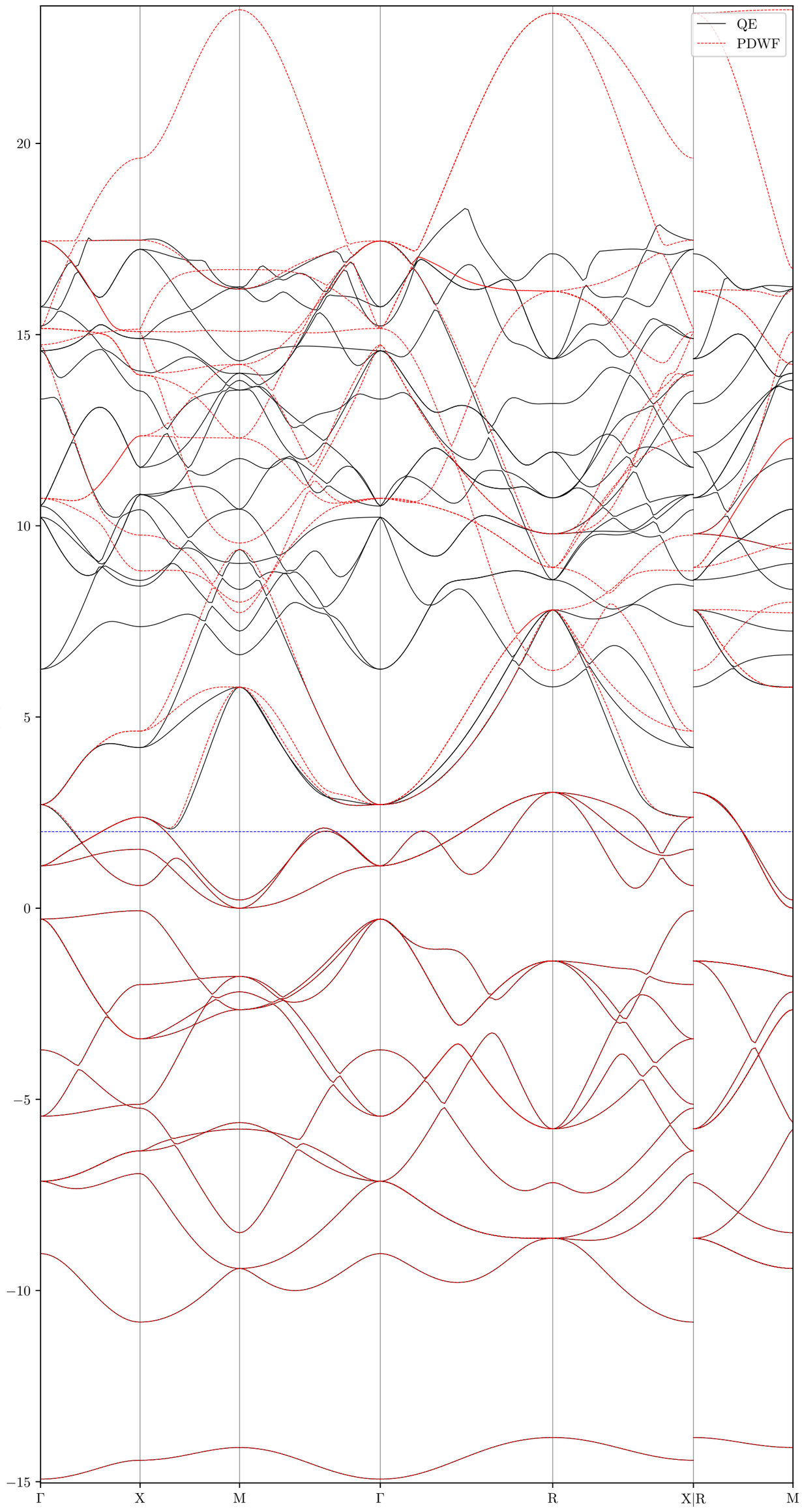



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.4 | 4.2 | 3.7 | 60.9 | 61.5 | 61.5 | 2.412 |

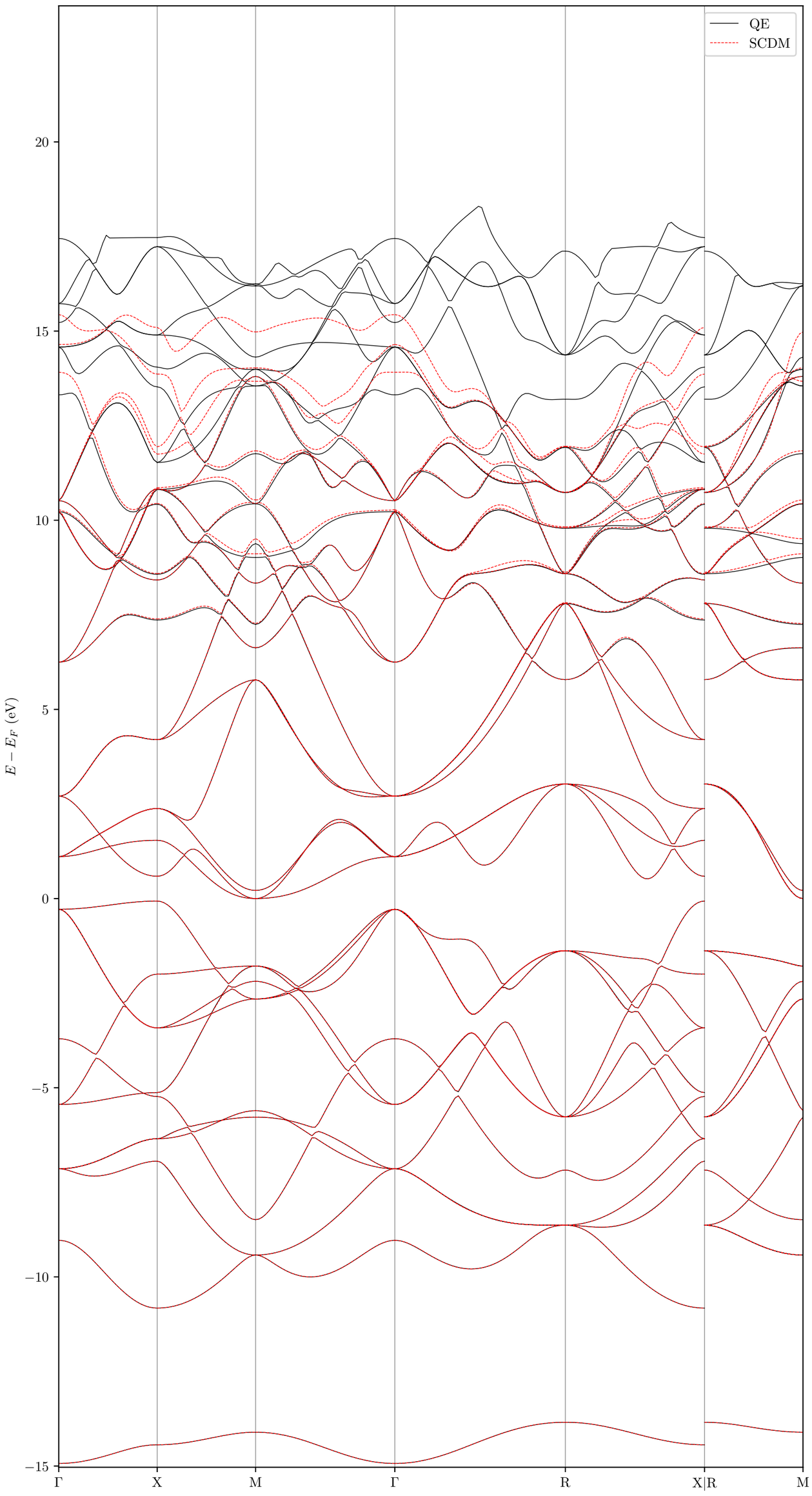
Hamiltonian decay





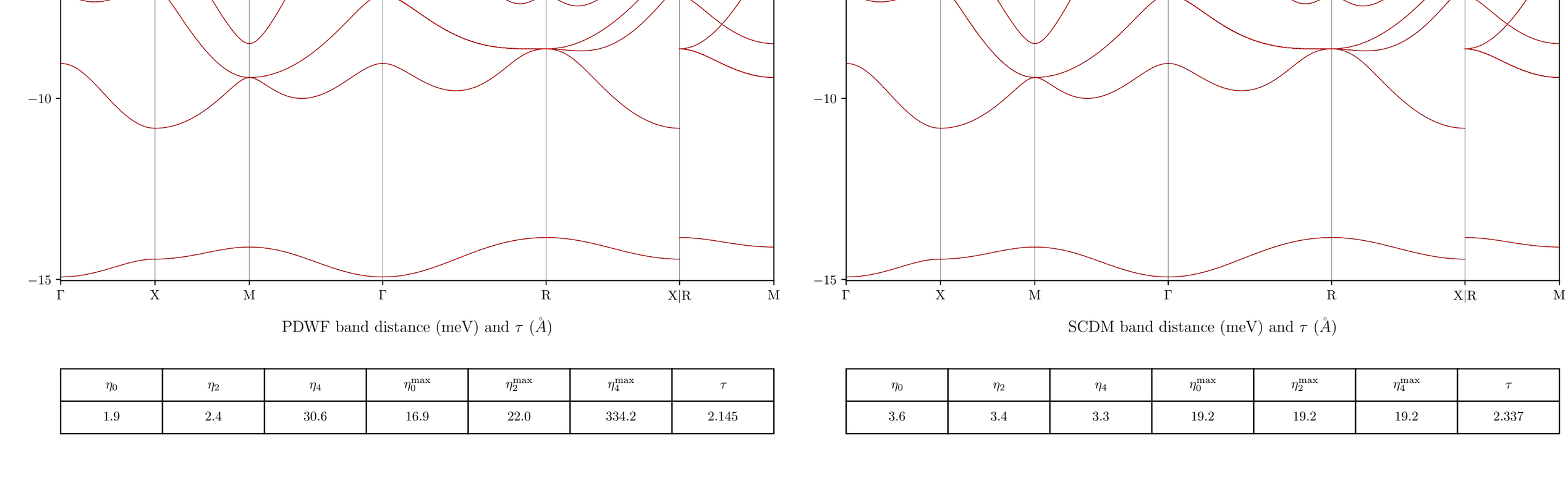

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.9 | 2.4 | 30.6 | 16.9 | 22.0 | 334.2 | 2.145 |

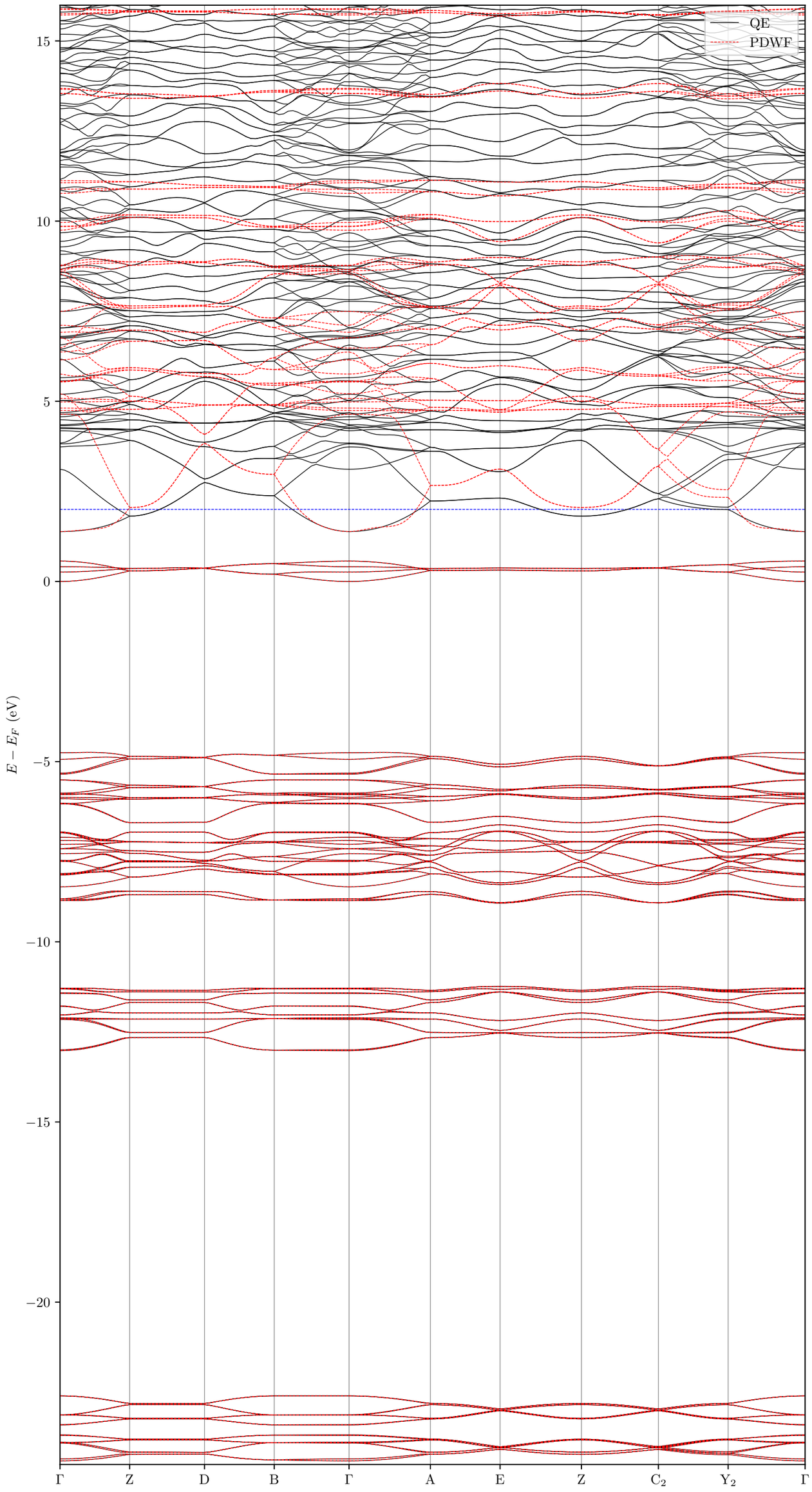



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.6 | 3.4 | 3.3 | 19.2 | 19.2 | 19.2 | 2.337 |



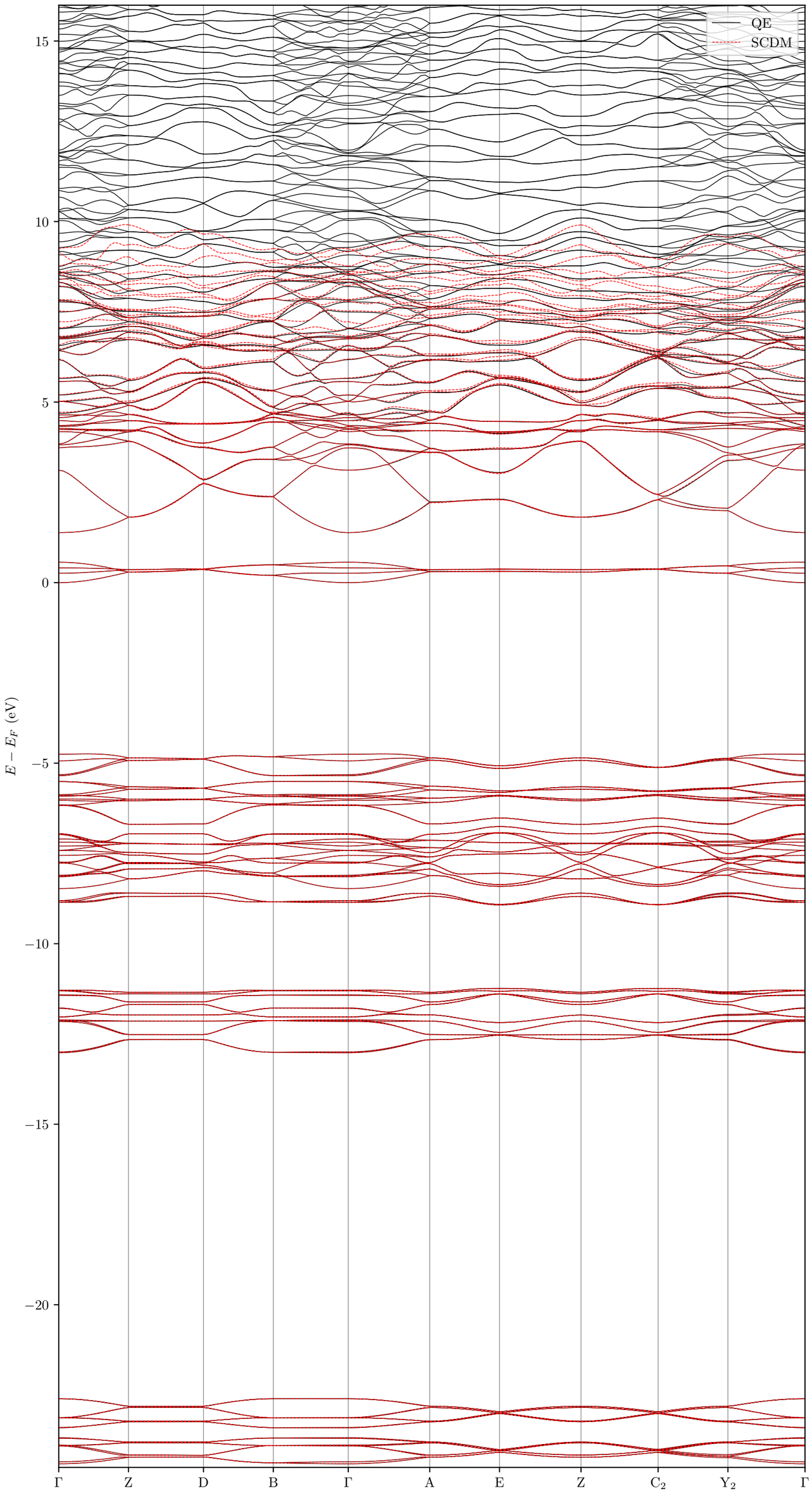
B8H16O16 exclude semicore
PW=96e339df-e901-400f-b0b2-fa494cb7e2bd
W90=7c16c833-c91d-49be-9e6b-a7a16b8f992a




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 13.7 | 2.3 | 2.3 | 142.7 | 2.703 |

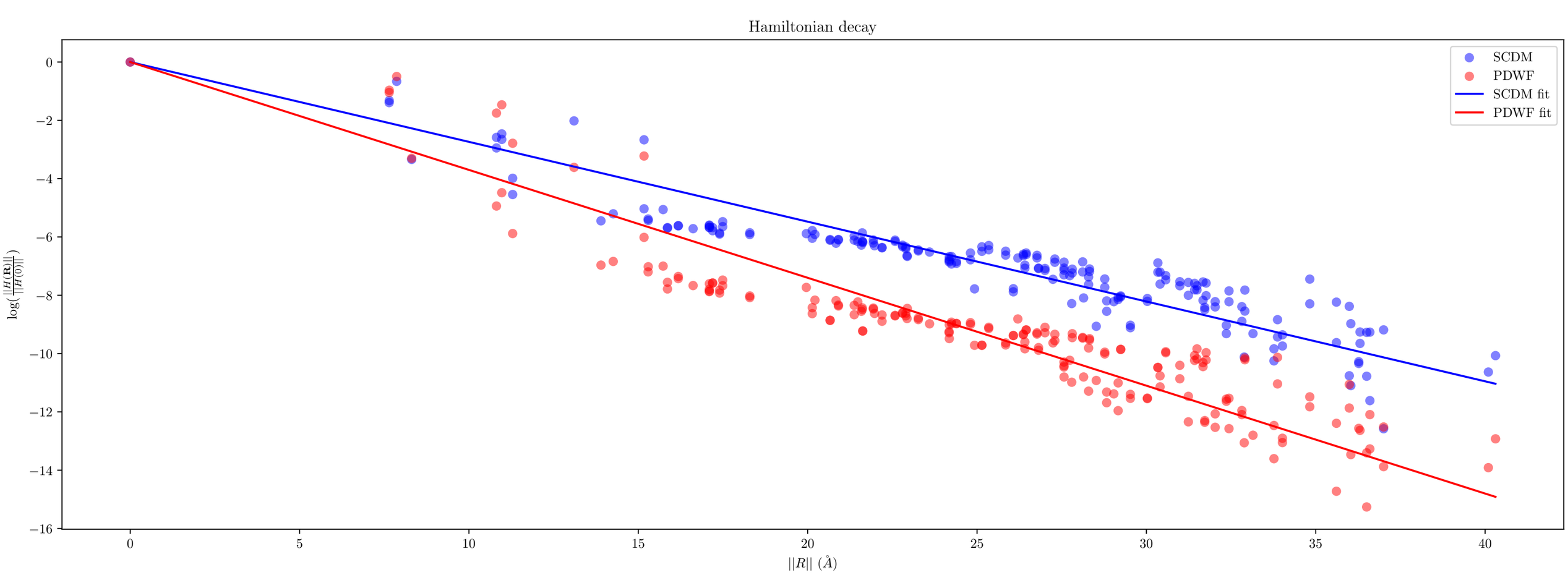
B8H16O16 exclude semicore
PW=96e339df-e901-400f-b0b2-fa494cb7e2bd
W90=7ec02dcc-e7ba-43ac-b8f3-0064684a0612

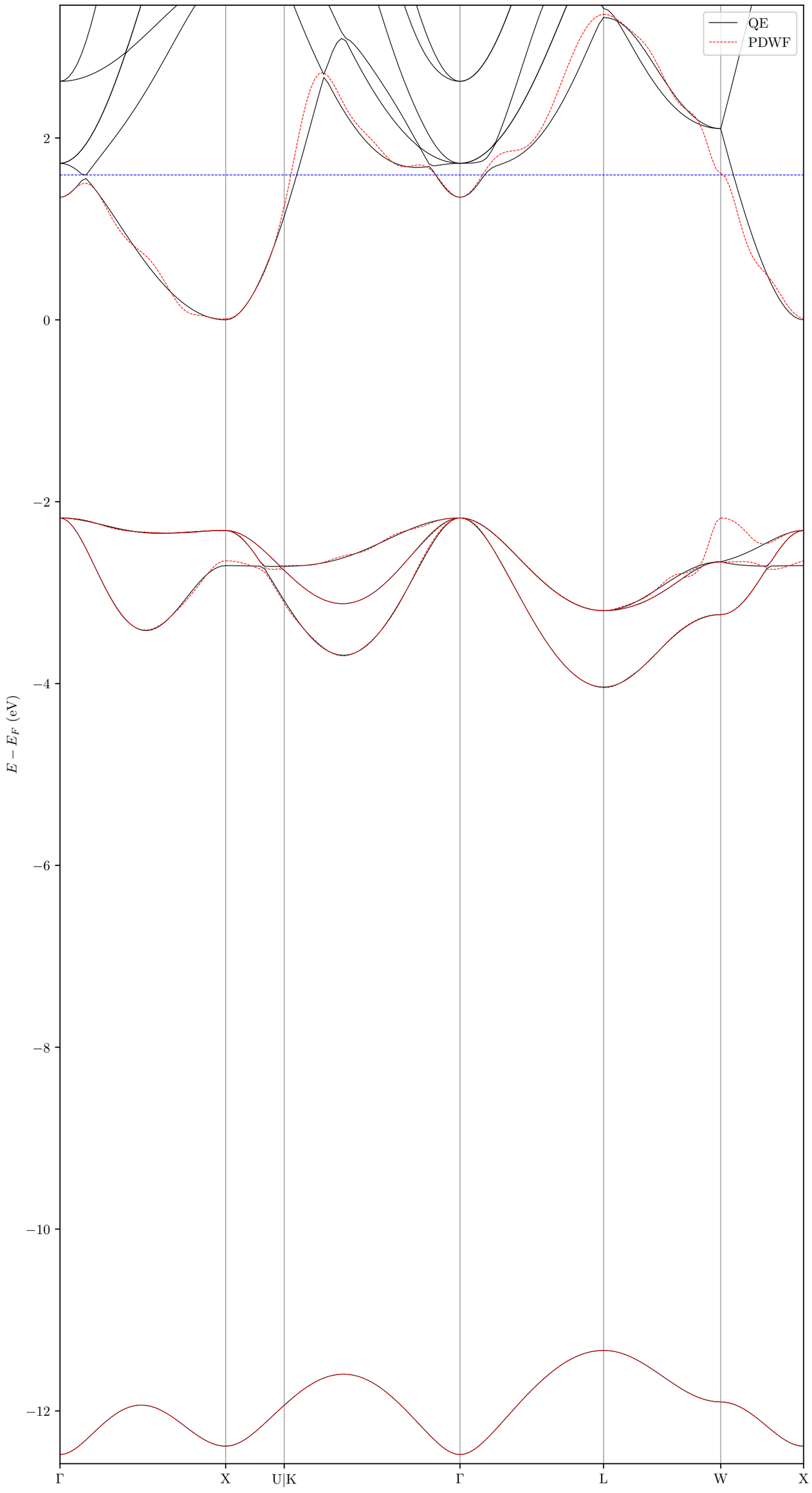



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.3 | 1.4 | 1.8 | 7.1 | 7.1 | 16.4 | 3.653 |

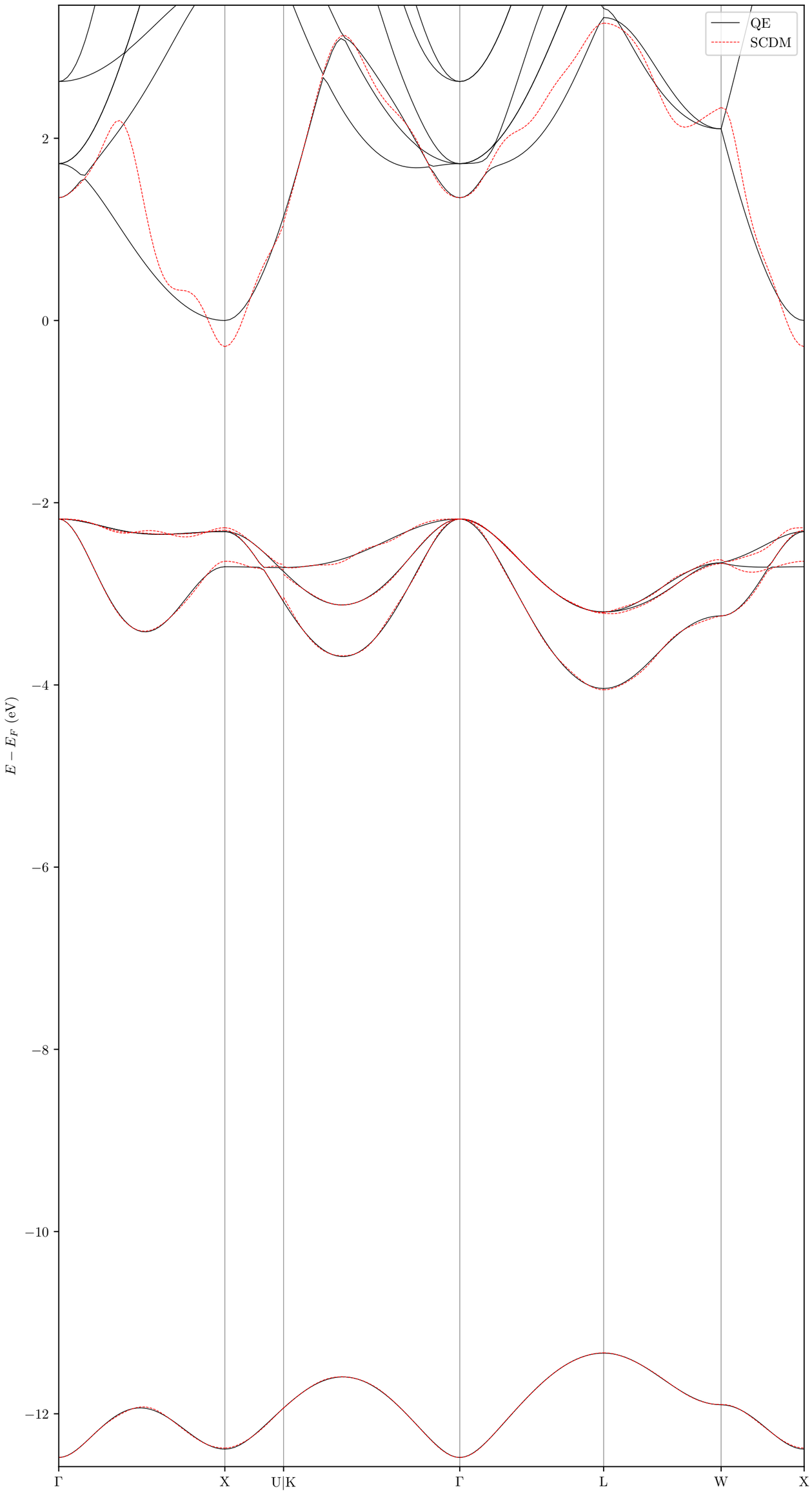
Hamiltonian decay





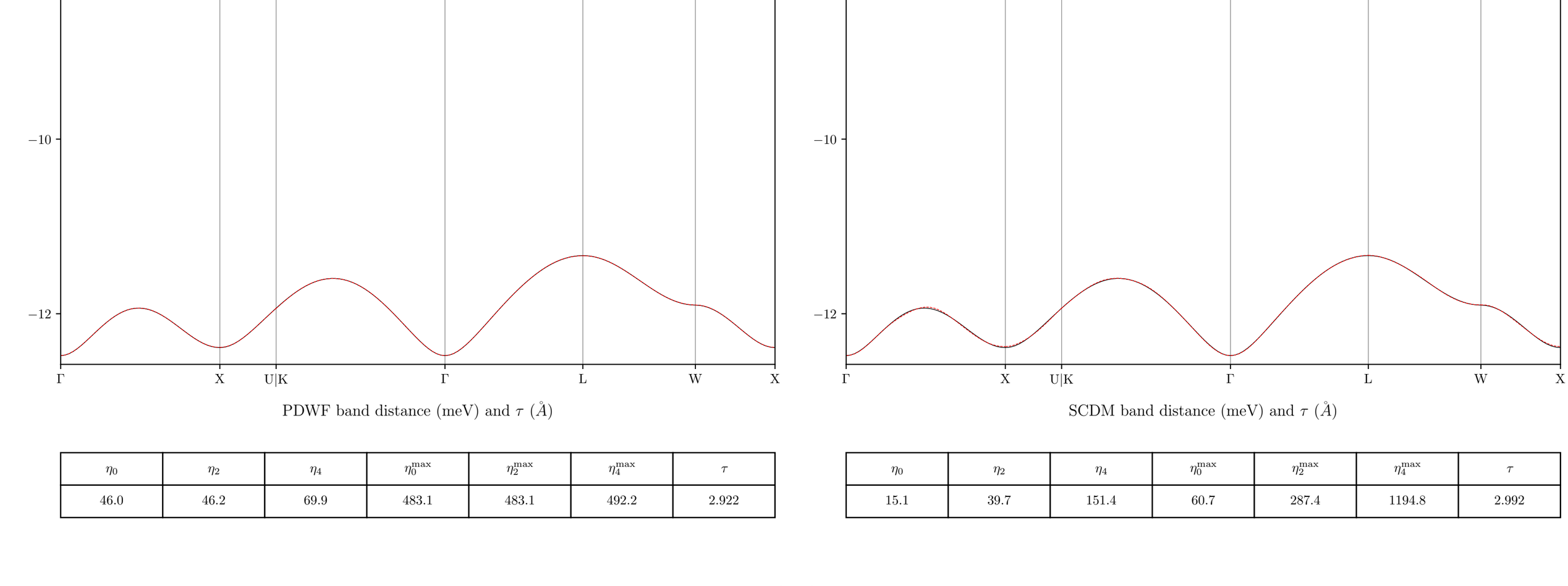

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 46.0 | 46.2 | 69.9 | 483.1 | 483.1 | 492.2 | 2.922 |

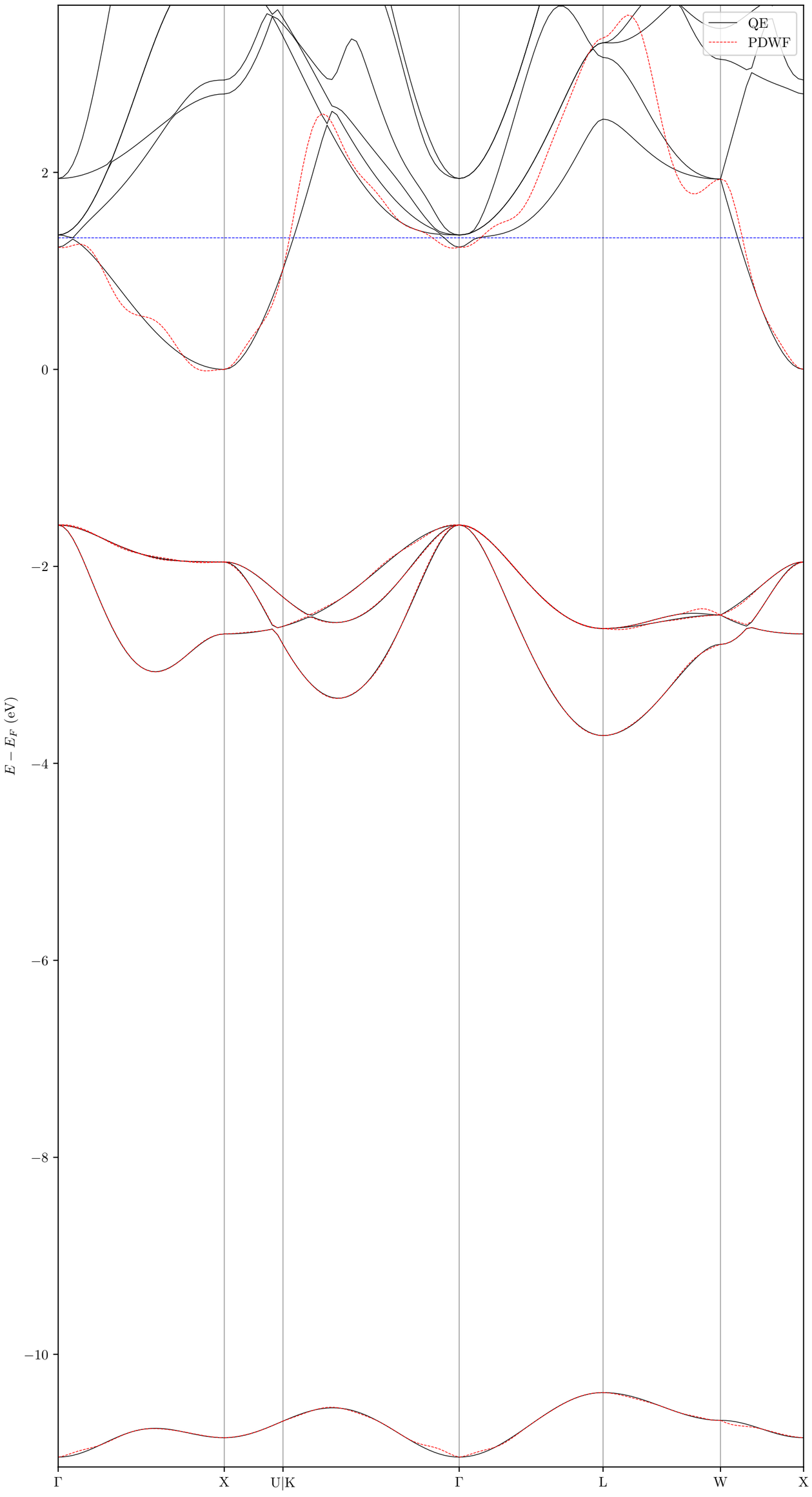



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 15.1 | 39.7 | 151.4 | 60.7 | 287.4 | 1194.8 | 2.992 |



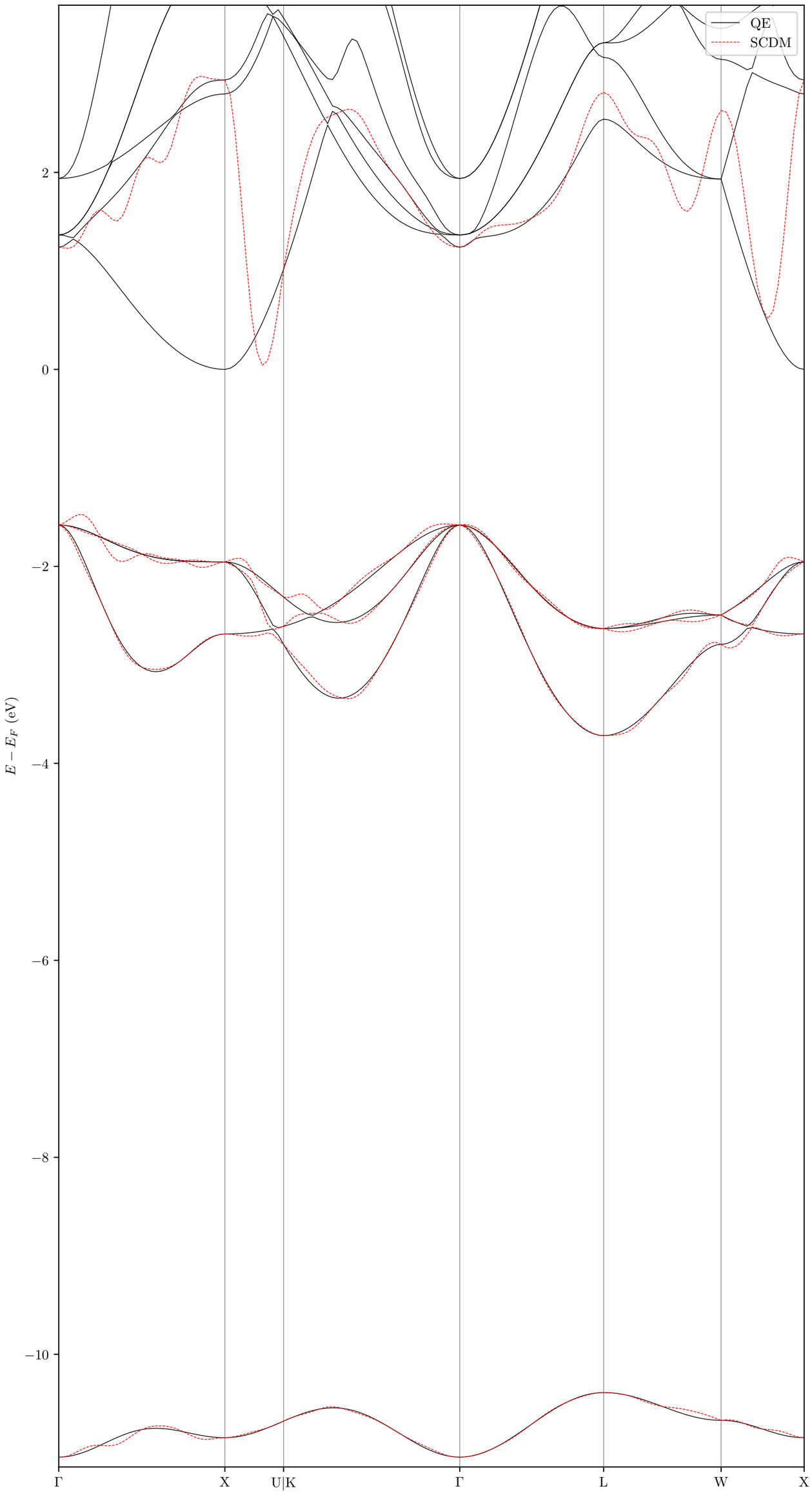
BaTe exclude semicore
PW=a1e46b91-0fee-4045-8764-44205249a373
W90=ef9e0a3c-fe10-4ac7-b86b-e3be92cbdf8f




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 9.0 | 21.1 | 128.2 | 50.2 | 130.9 | 798.0 | 2.931 |

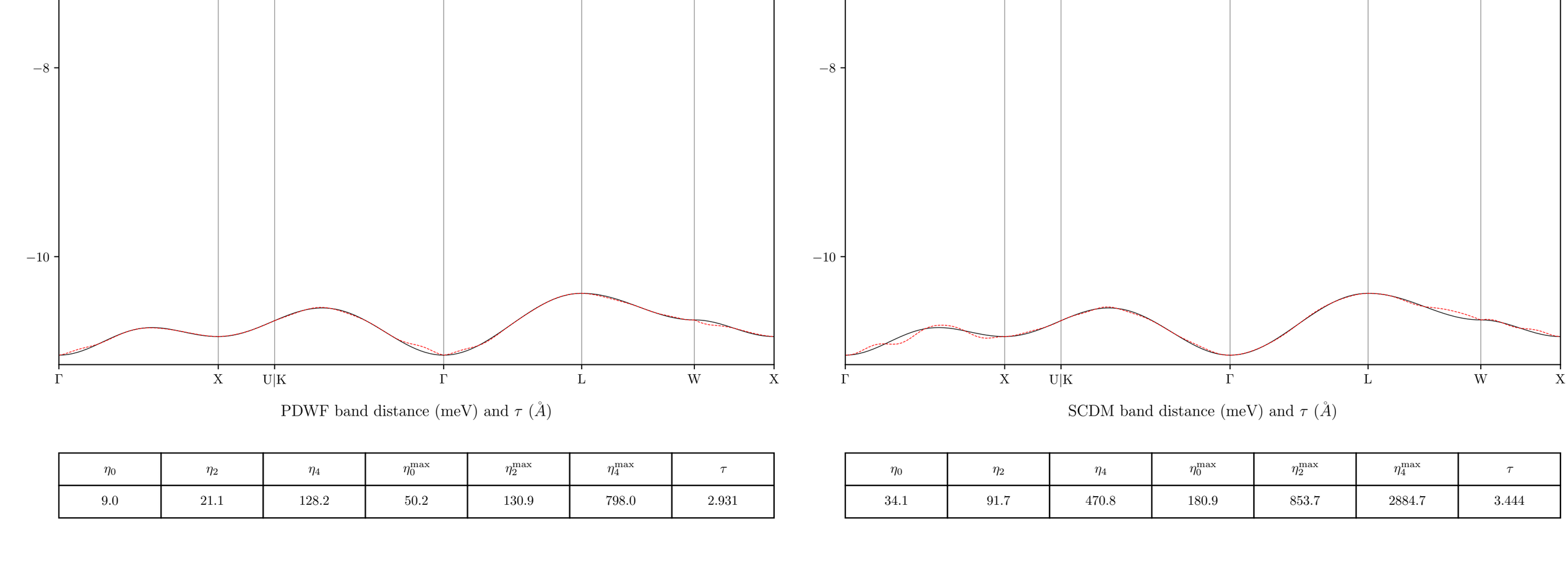
BaTe exclude semicore
PW=a1e46b91-0fee-4045-8764-44205249a373
W90=aafc23dd-6bb0-4831-86fd-de3852a6c701



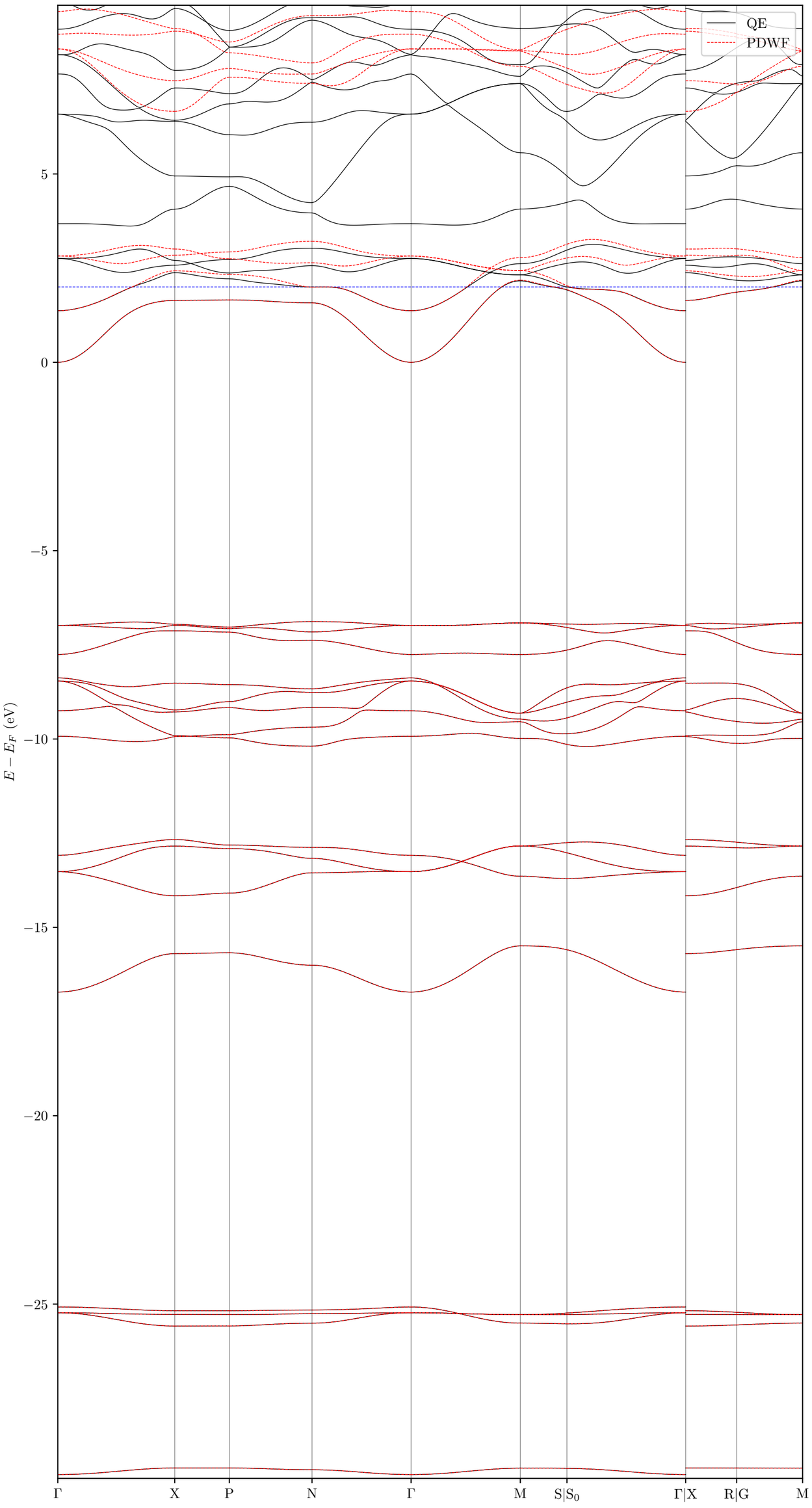

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 34.1 | 91.7 | 470.8 | 180.9 | 853.7 | 2884.7 | 3.444 |

Hamiltonian decay



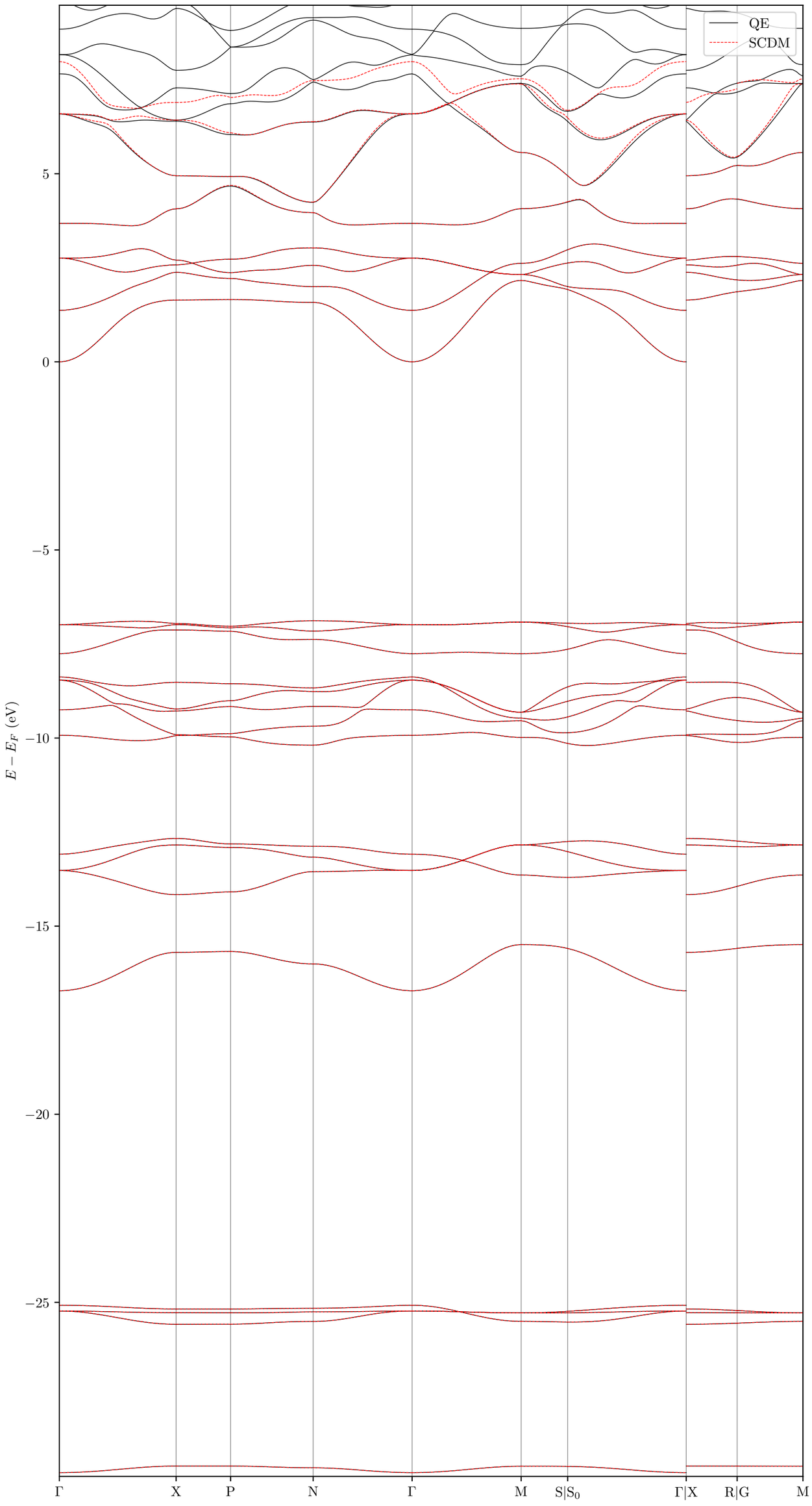
BeO4S exclude semicore
PW=da1e7885-9c89-4f71-bc77-65331a8d6a19
W90=1e5dab89-0759-4850-9d94-a2768454c232




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.2 | 1.4 | 1.4 | 1.4 | 4.8 | 2.291 |

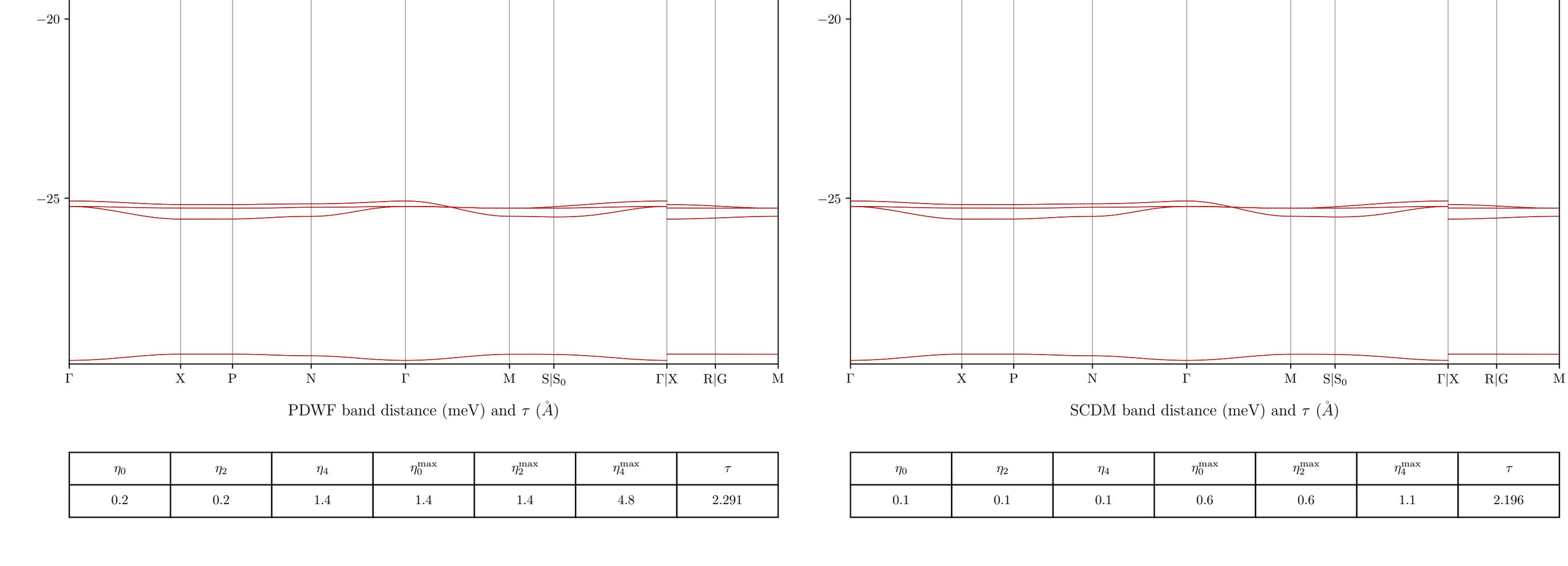
BeO4S exclude semicore
PW=da1e7885-9c89-4f71-bc77-65331a8d6a19
W90=755f3914-aa78-4779-9b5c-f73480c9340d



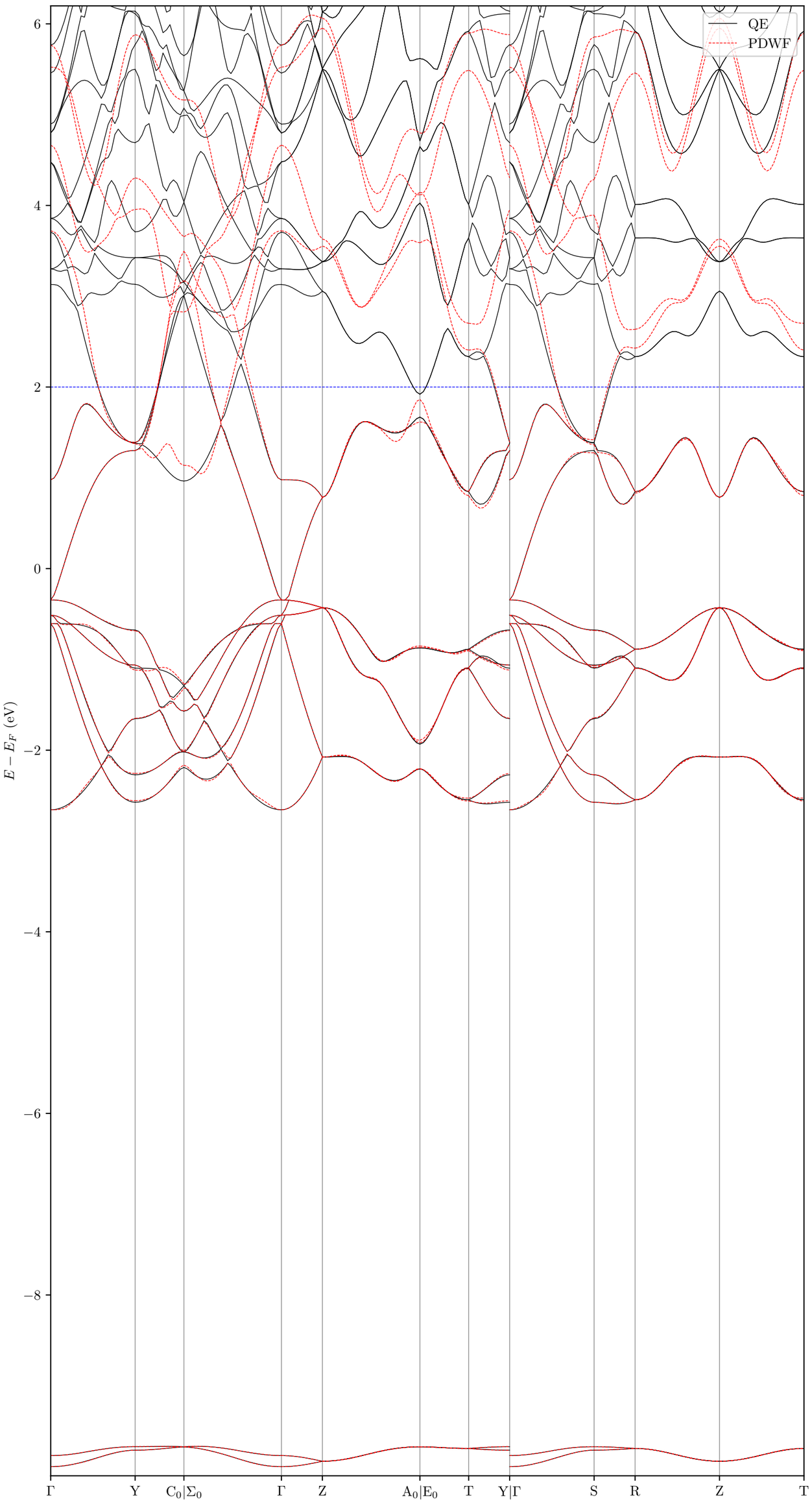

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.1 | 0.1 | 0.6 | 0.6 | 1.1 | 2.196 |

Hamiltonian decay



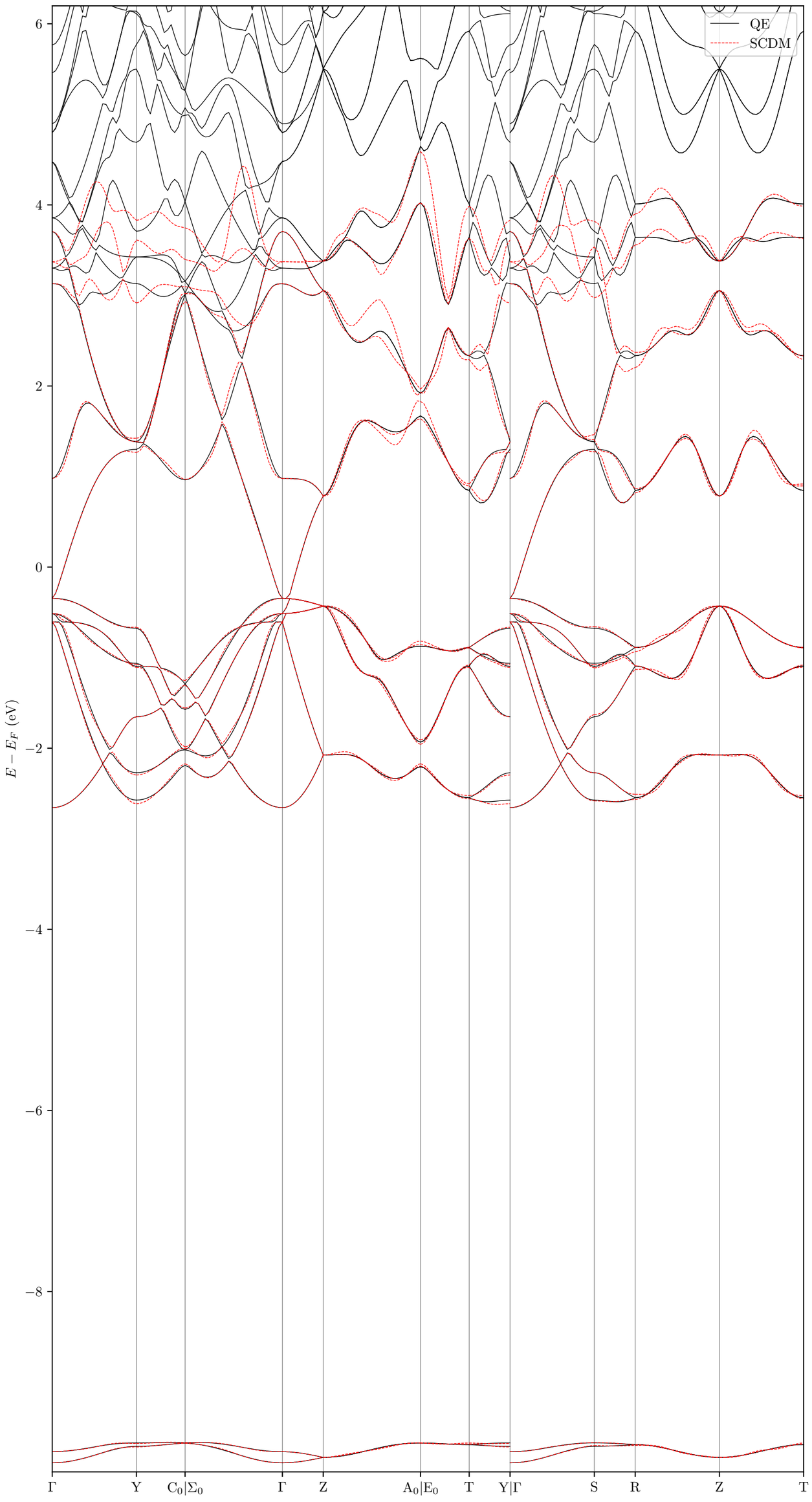
Bi2Na6 exclude semicore
PW=13f522cf-417b-44cb-beda-1db9cc7a56e3
W90=f1216349-310c-4e2b-8779-bbe2ee2521f5




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.6 | 21.8 | 254.3 | 45.0 | 312.6 | 1652.3 | 3.480 |

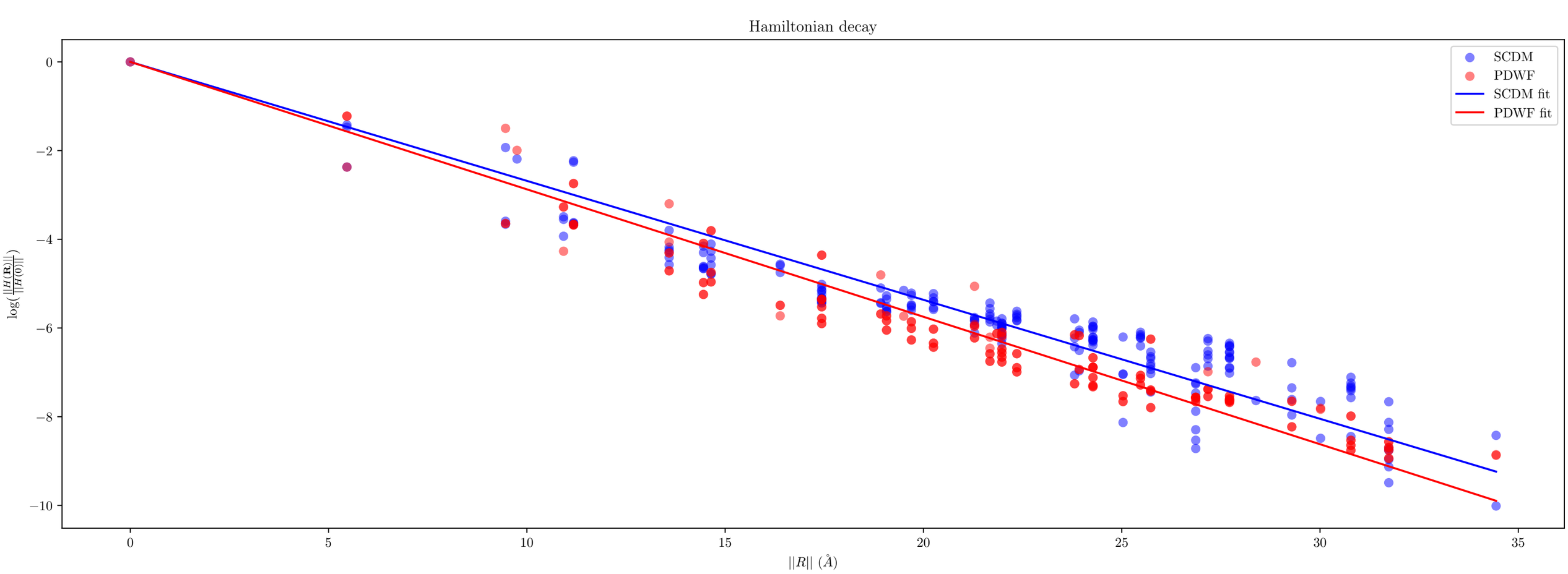
Bi2Na6 exclude semicore
PW=13f522cf-417b-44cb-beda-1db9cc7a56e3
W90=295fe79b-a447-42ea-859f-2860674dfa2d

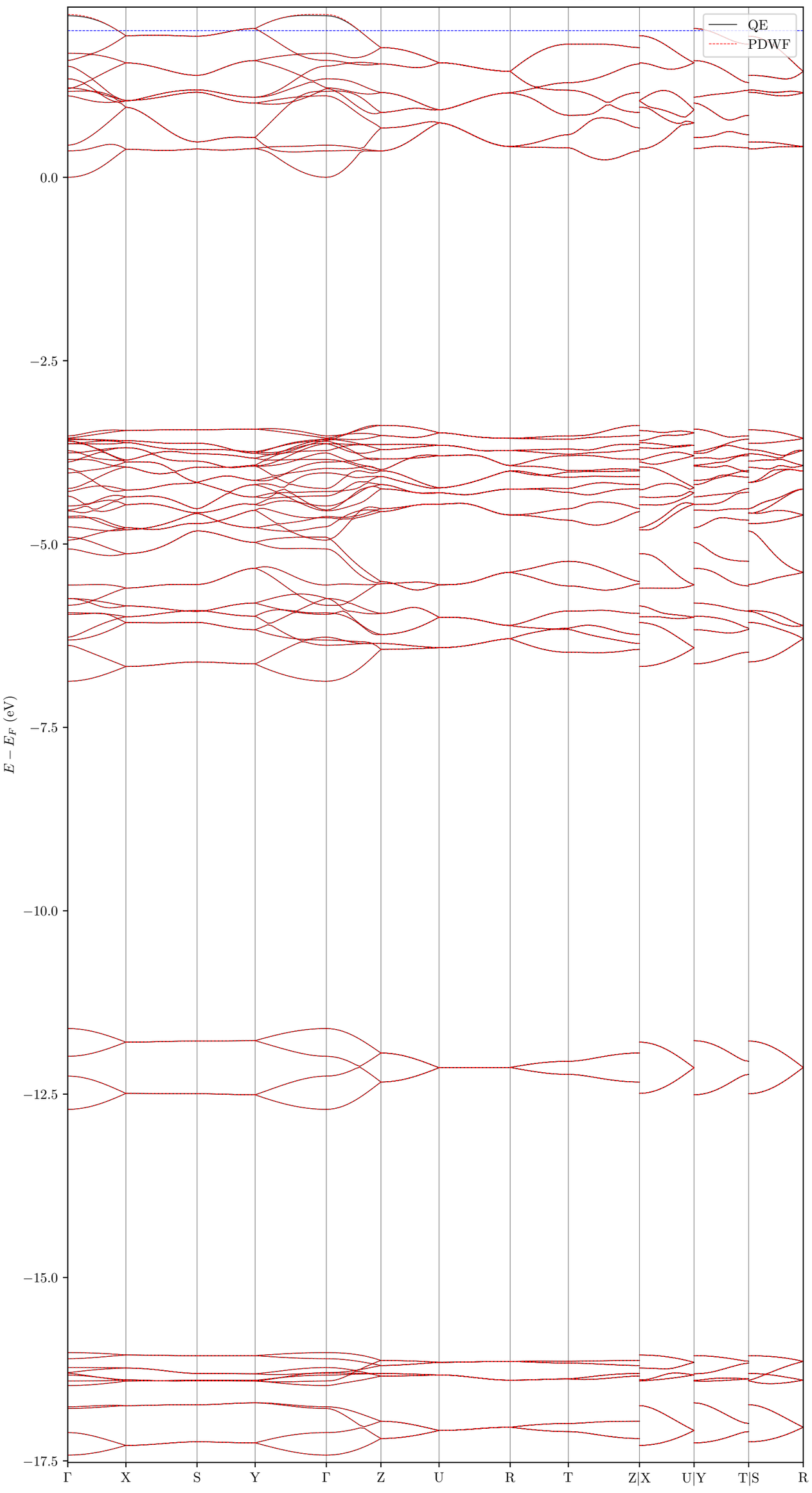



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 13.0 | 21.2 | 95.1 | 55.9 | 163.8 | 564.3 | 3.728 |

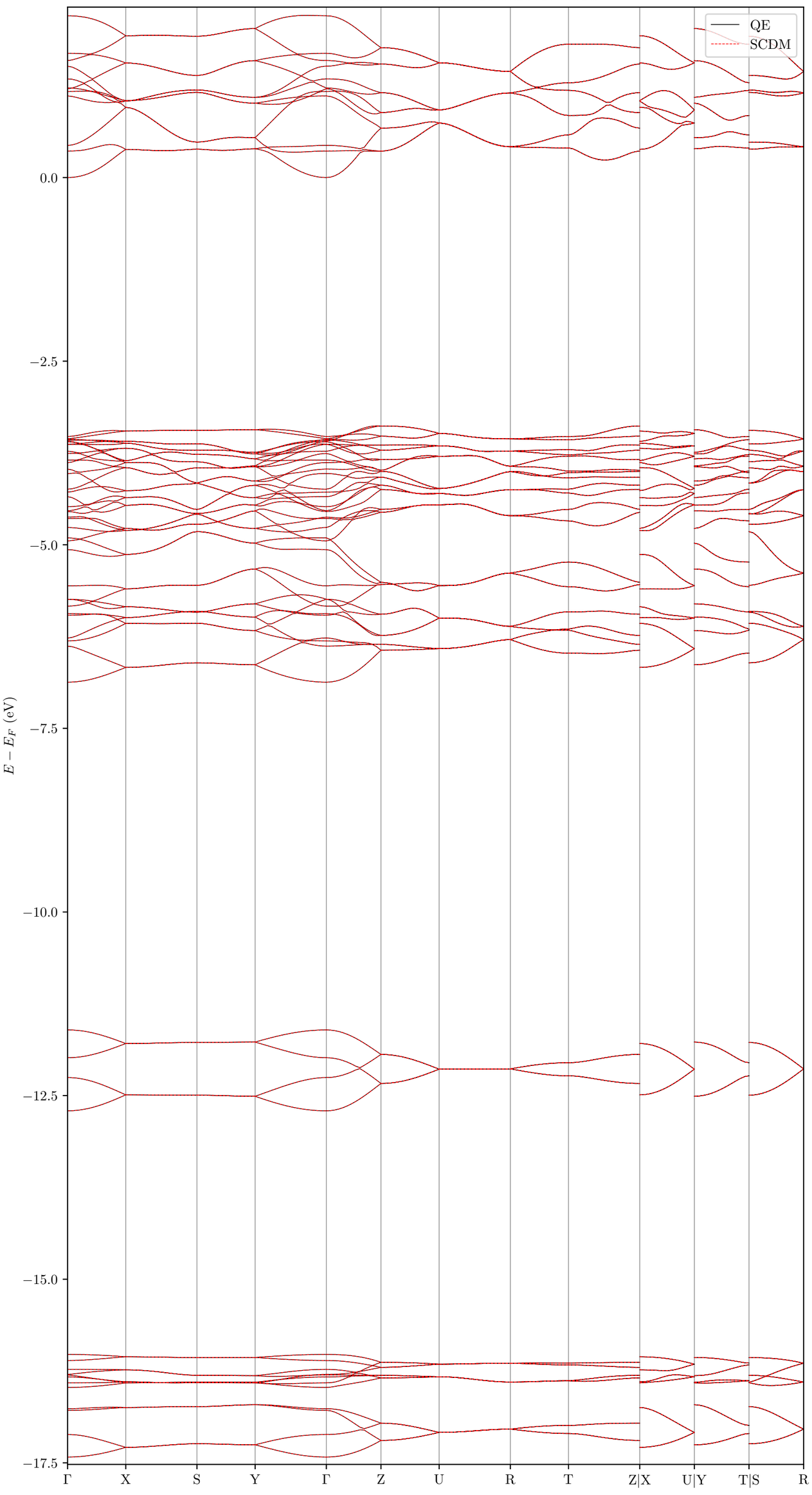
Hamiltonian decay





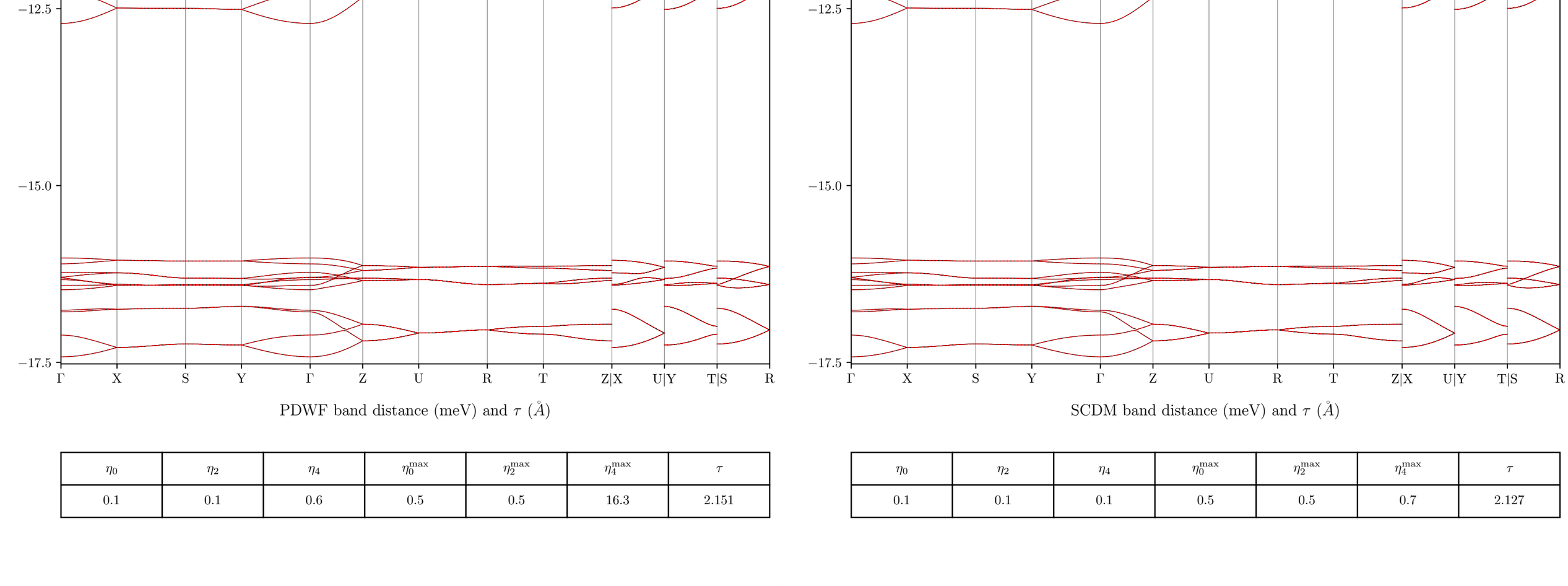

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

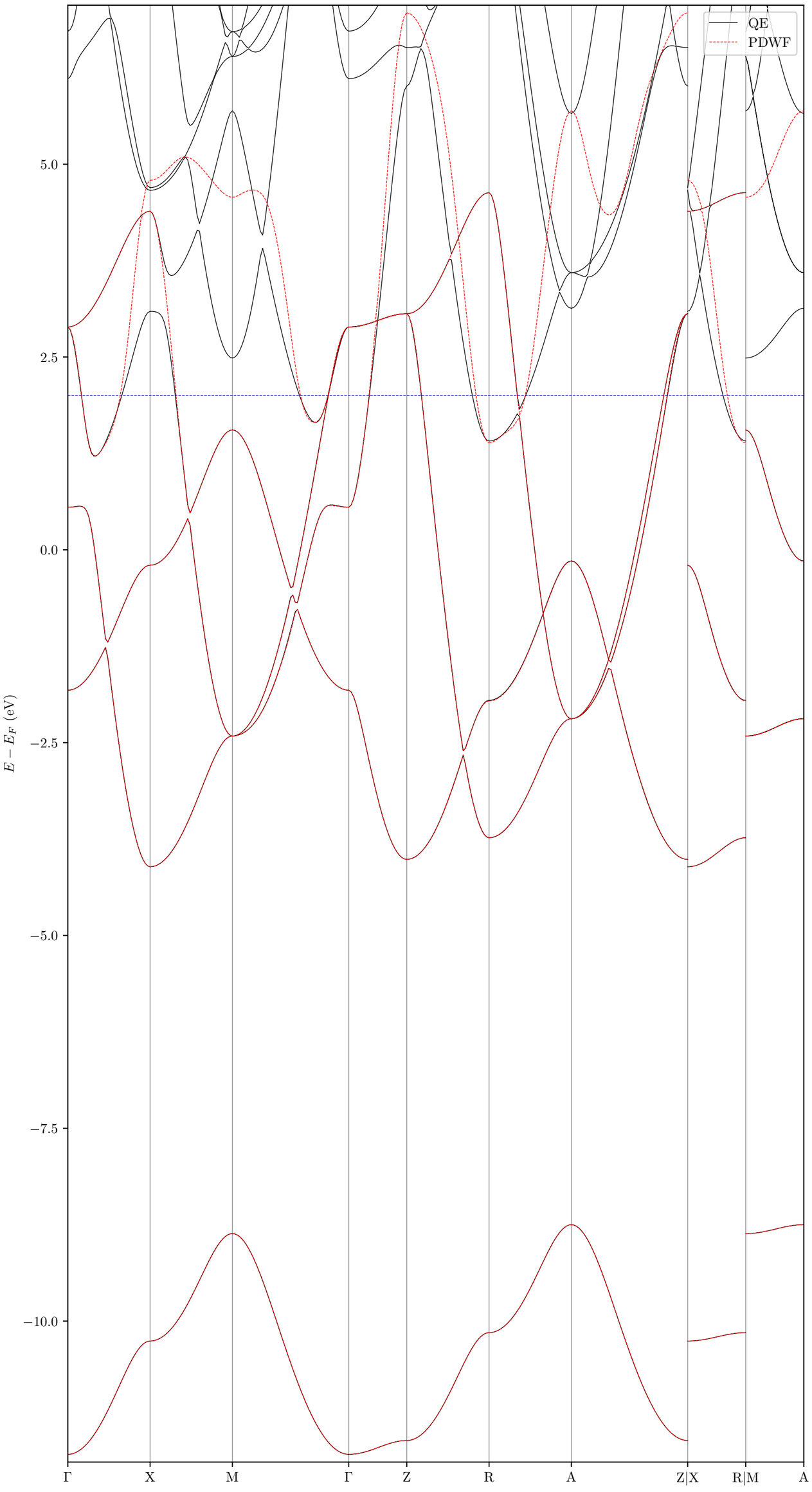
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.1 | 0.6 | 0.5 | 0.5 | 16.3 | 2.151 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

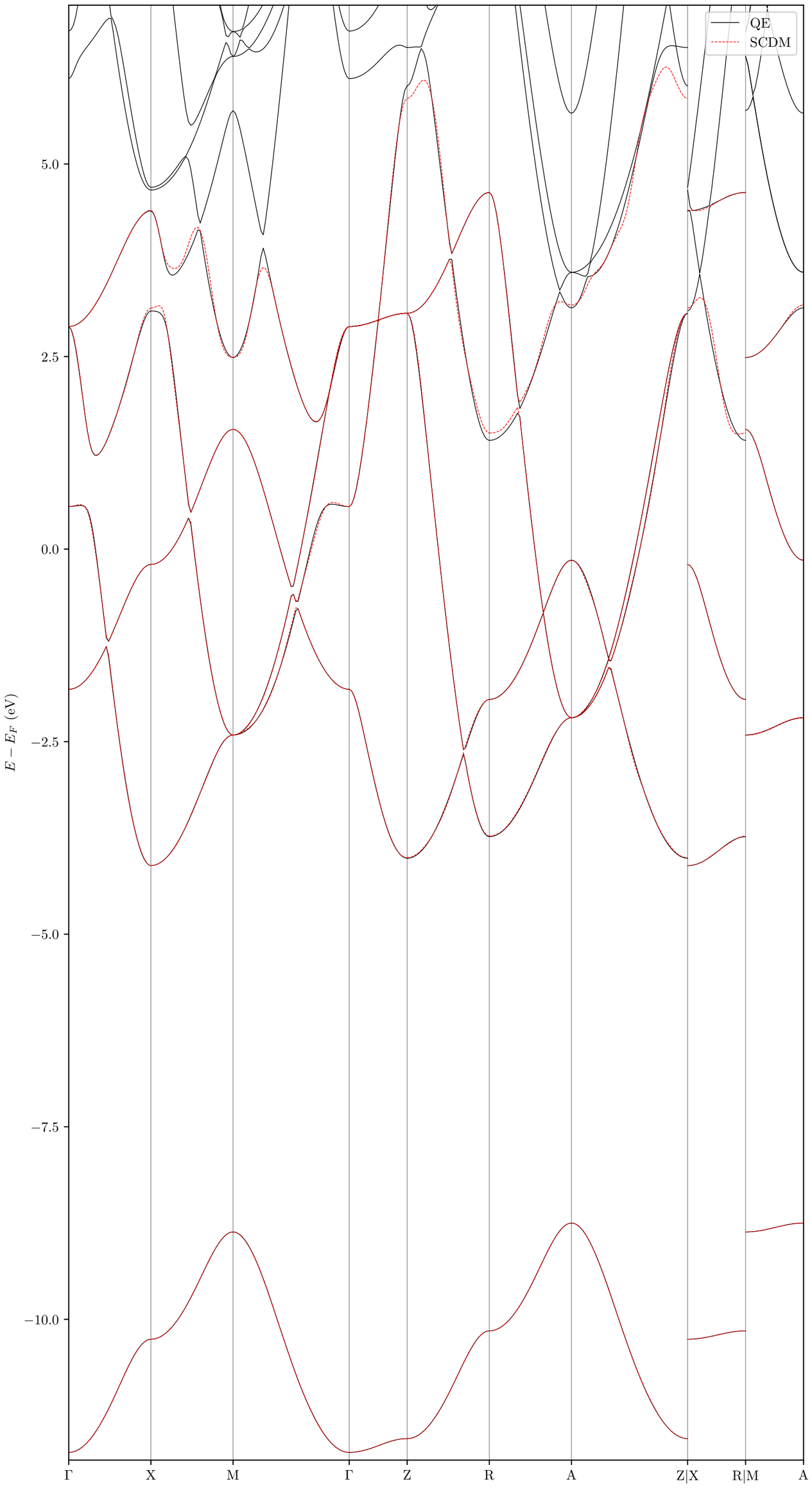
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.1 | 0.1 | 0.5 | 0.5 | 0.7 | 2.127 |





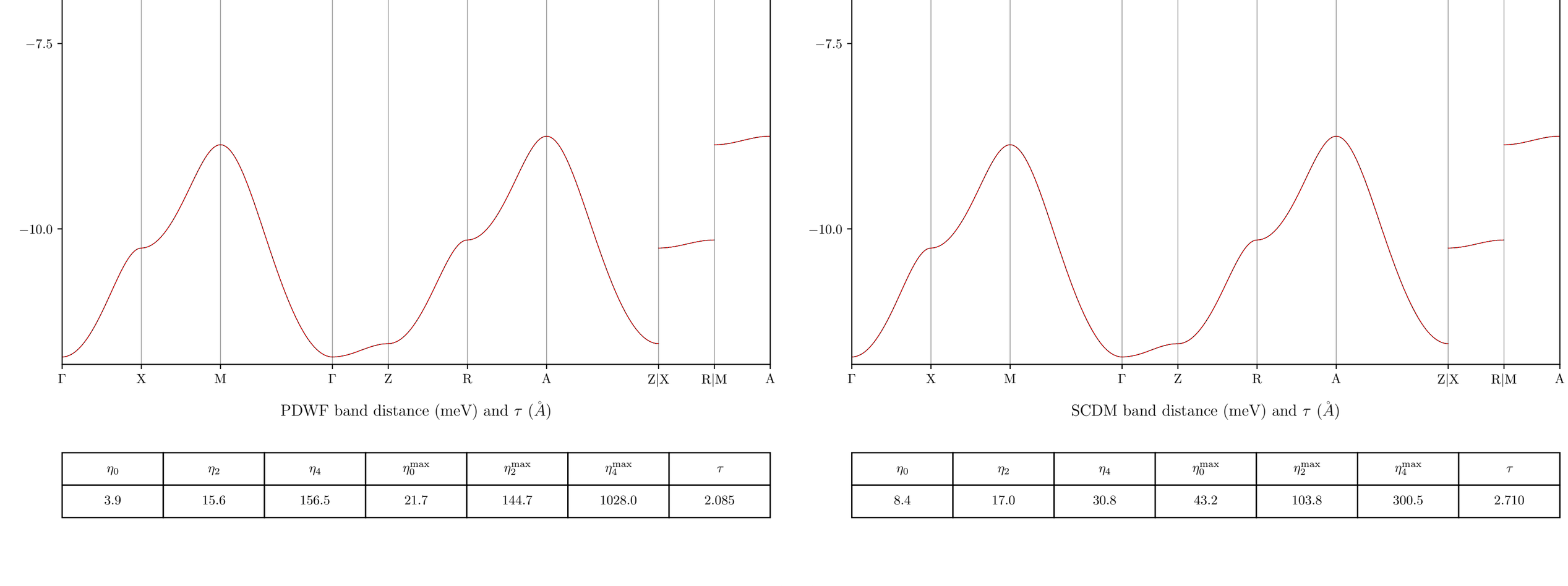

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.9 | 15.6 | 156.5 | 21.7 | 144.7 | 1028.0 | 2.085 |

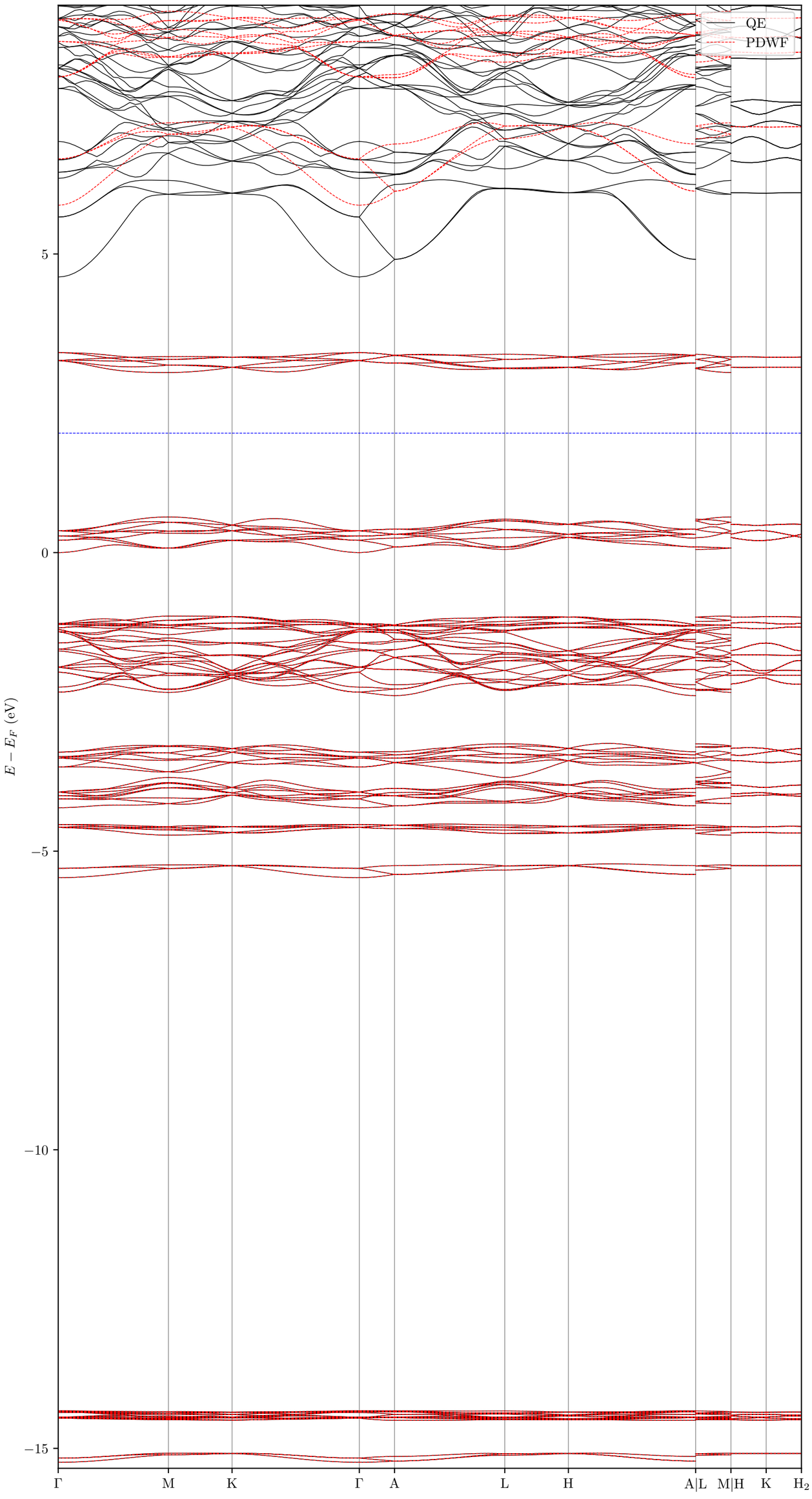



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.4 | 17.0 | 30.8 | 43.2 | 103.8 | 300.5 | 2.710 |



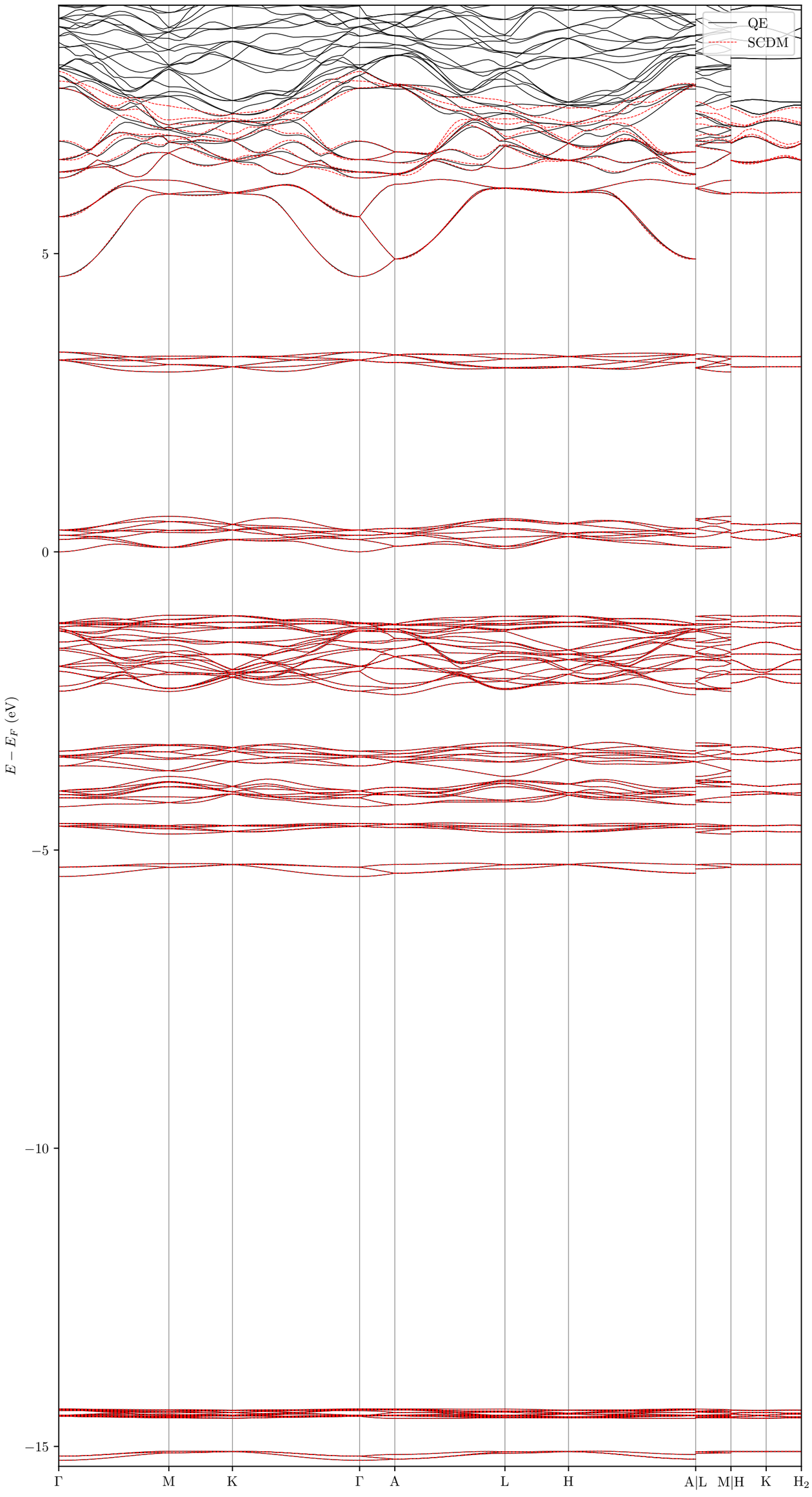
Br18W3 exclude semicore
PW=c923531e-5b97-4143-ba9b-7c2bd1c46a90
W90=bed155b7-5115-4d5d-b74c-77ca1d3901a5




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.1 | 0.1 | 0.7 | 0.7 | 0.7 | 2.916 |

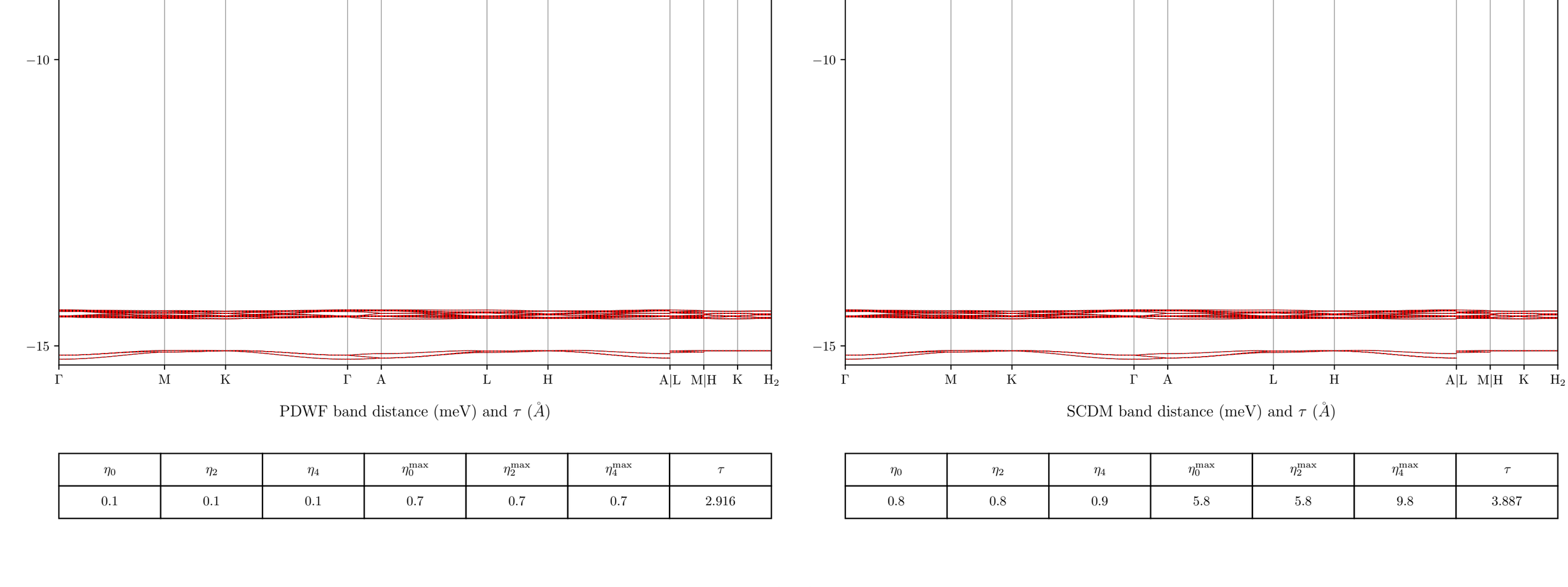
Br18W3 exclude semicore
PW=c923531e-5b97-4143-ba9b-7c2bd1c46a90
W90=6b940209-58a6-4fed-92e4-680e6a2dc632

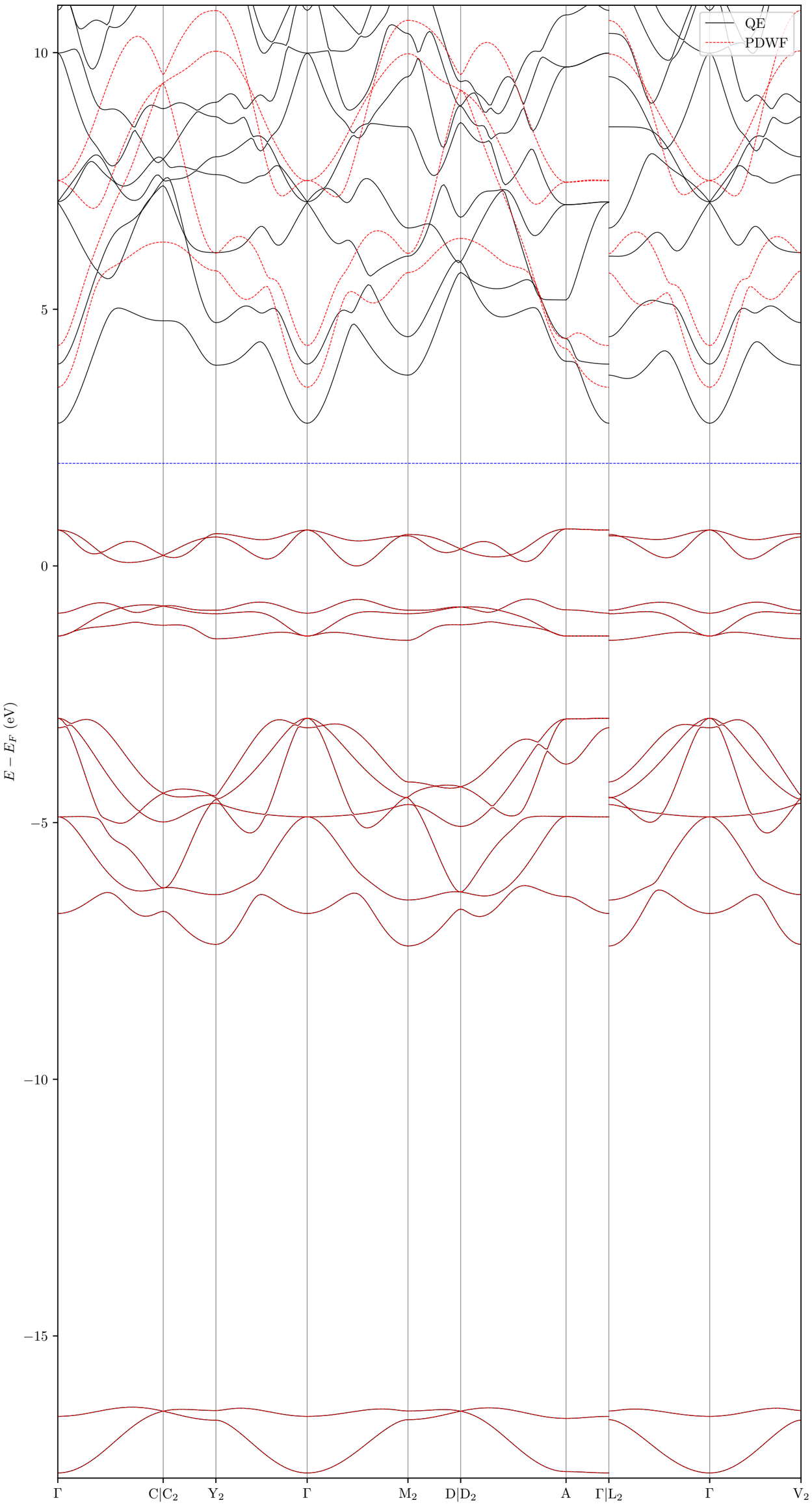



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.8 | 0.8 | 0.9 | 5.8 | 5.8 | 9.8 | 3.887 |

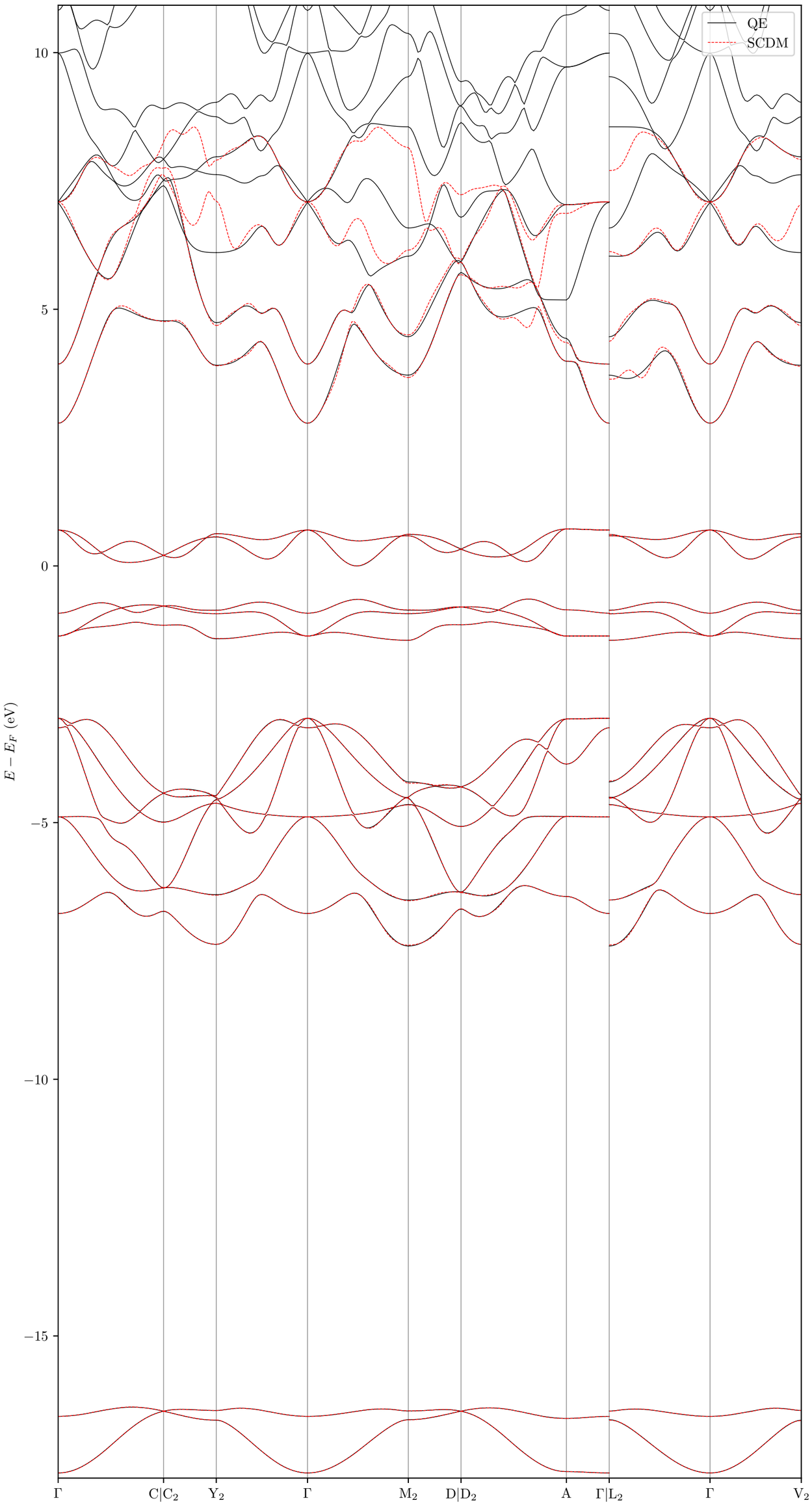
Hamiltonian decay





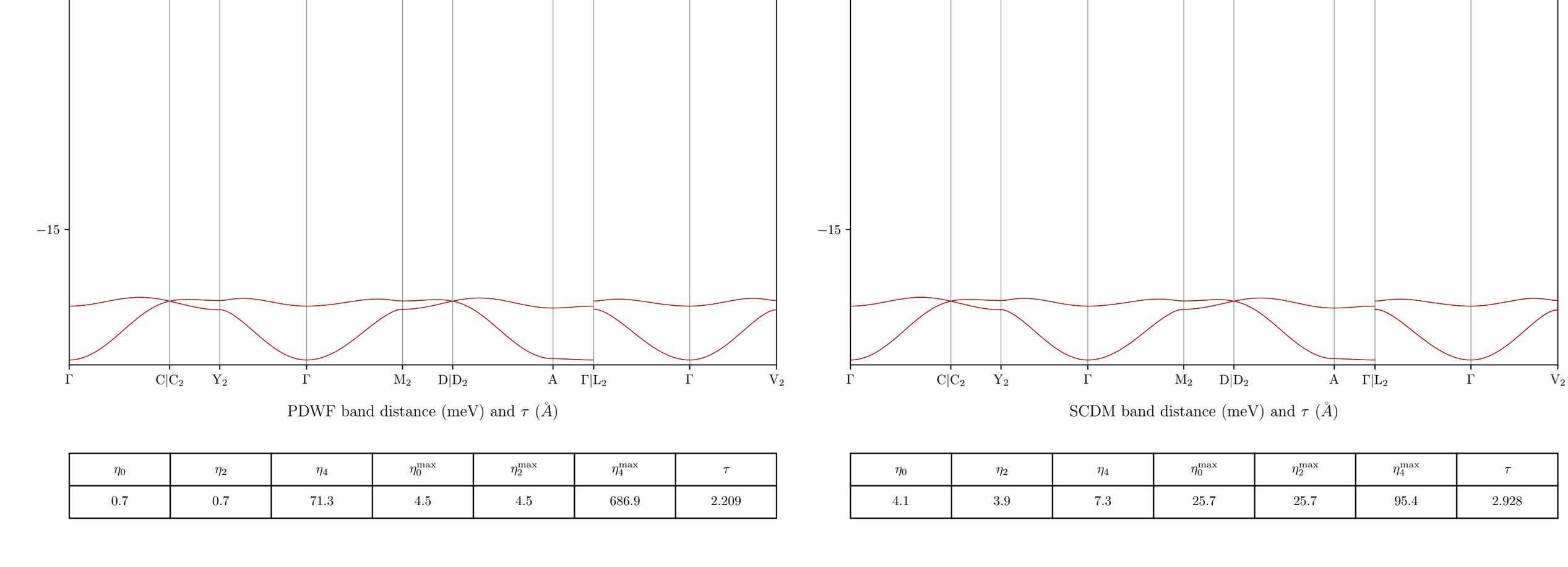

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 0.7 | 71.3 | 4.5 | 4.5 | 686.9 | 2.209 |

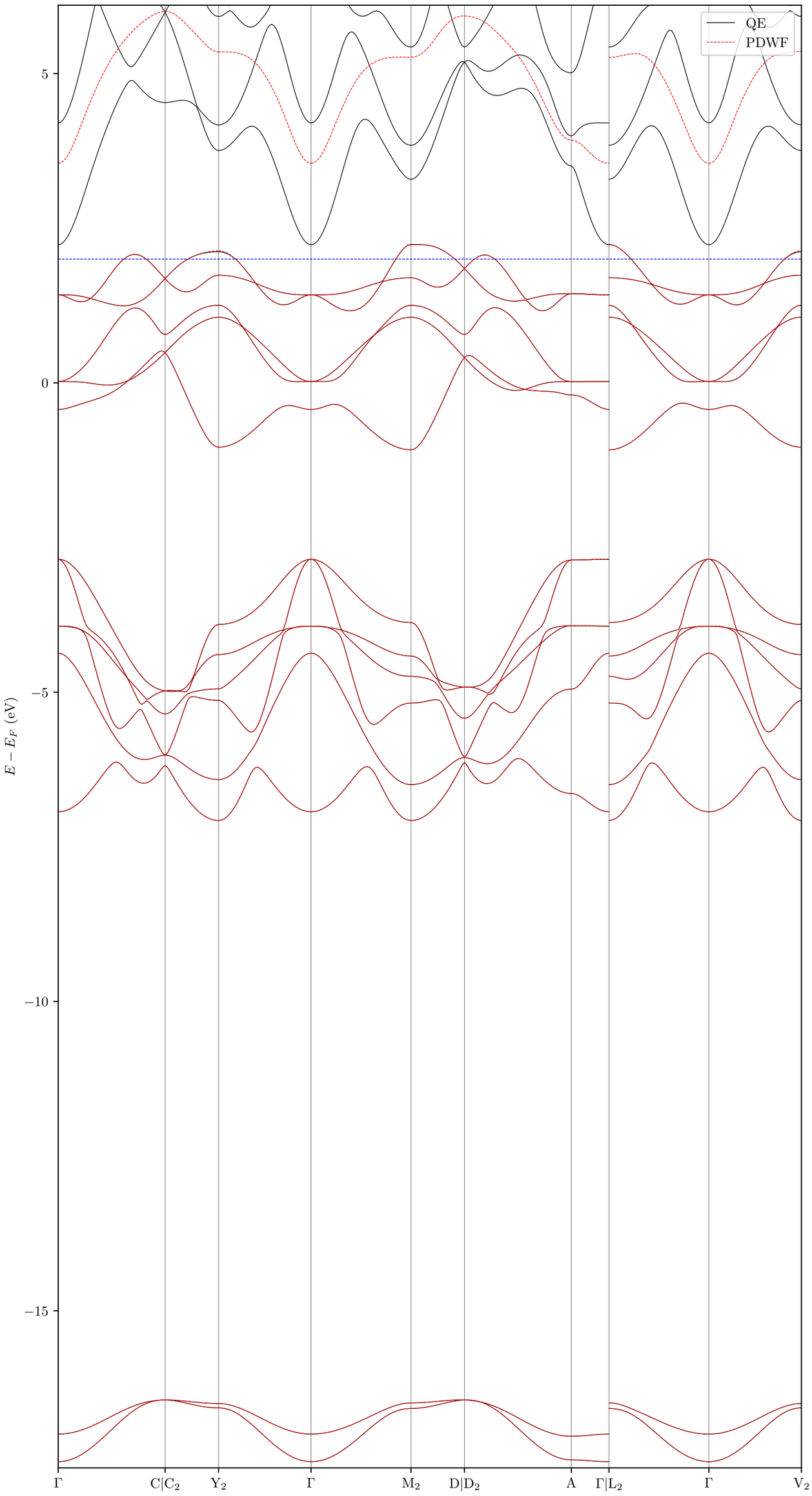



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.1 | 3.9 | 7.3 | 25.7 | 25.7 | 95.4 | 2.928 |



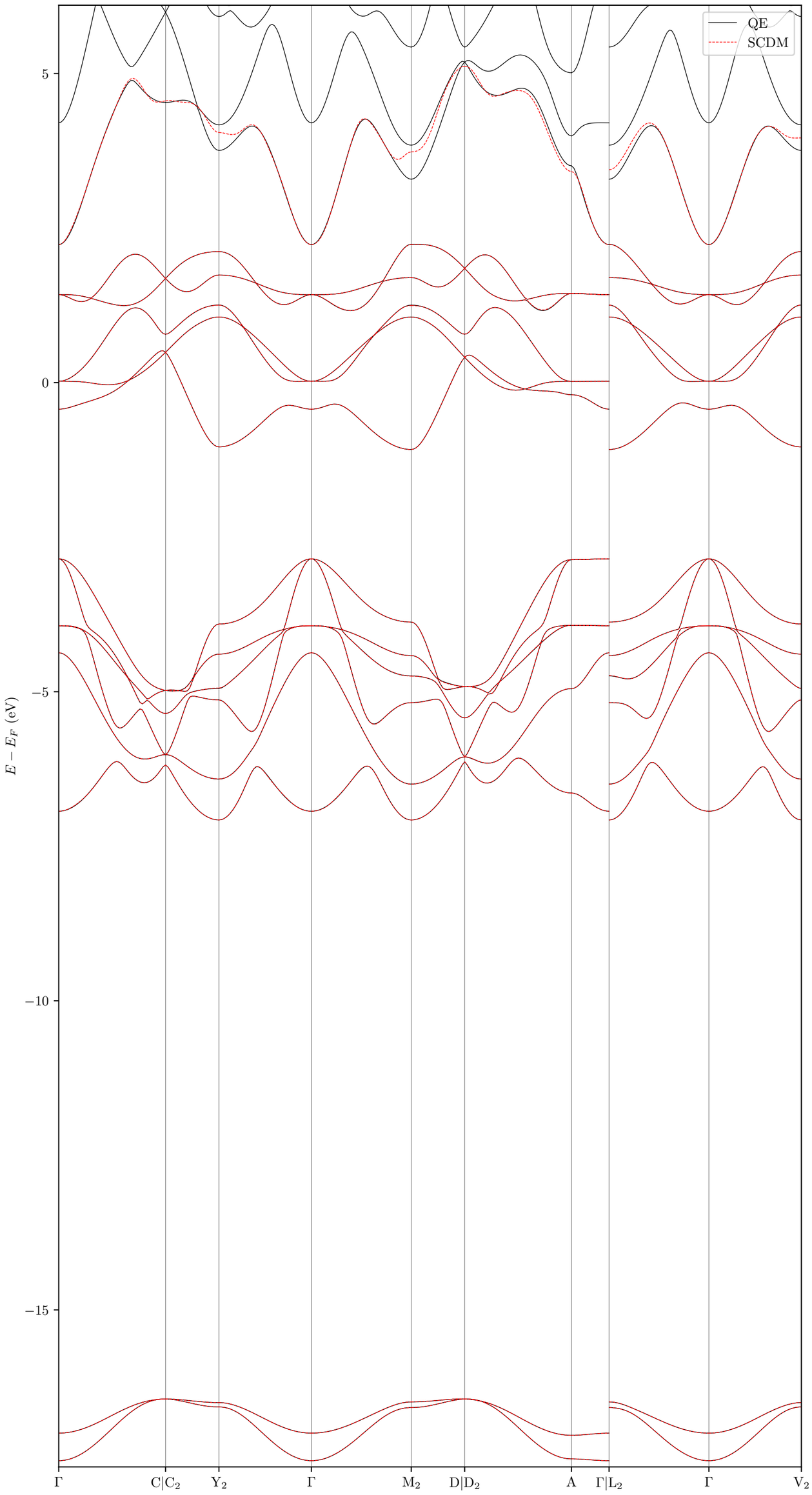
Br2Ti exclude semicore
PW=470a429d-7cfa-40b2-9c29-807a61fa2b69
W90=8856bd3e-e08a-4ff3-a83f-e2c3f1a39173




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 1.2 | 152.2 | 1.5 | 3.6 | 1308.5 | 2.176 |

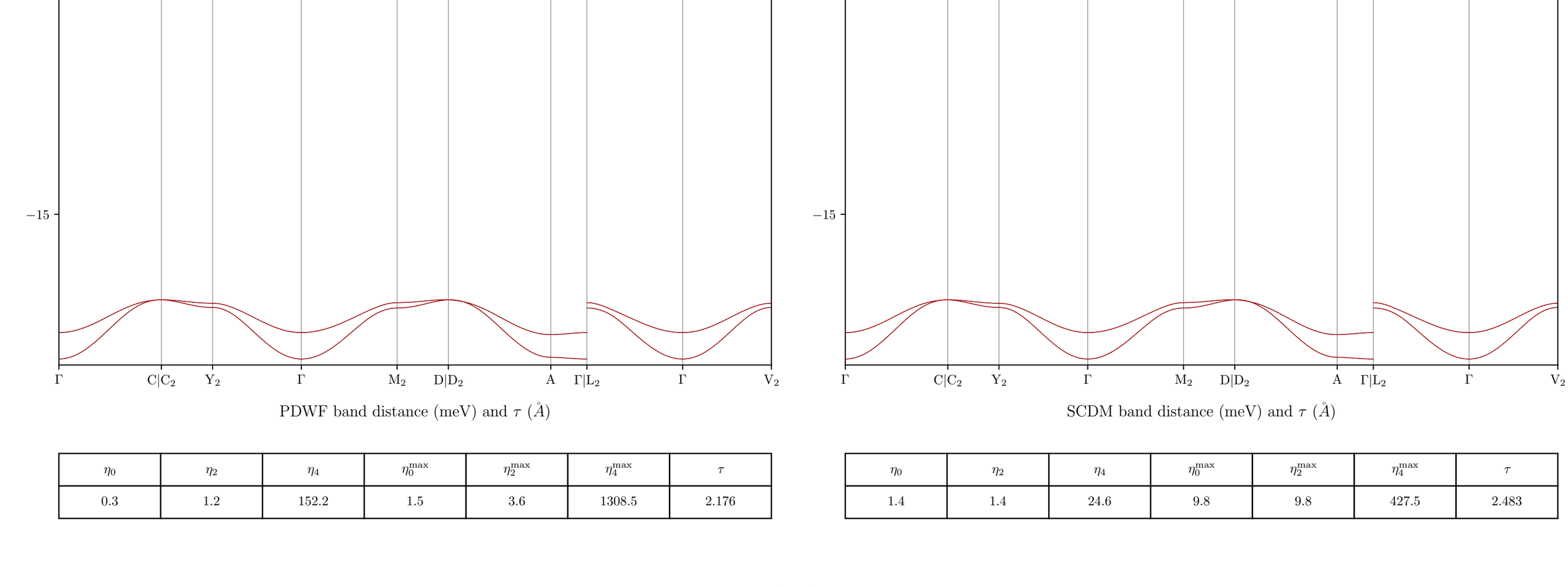
Br2Ti exclude semicore
PW=470a429d-7cfa-40b2-9c29-807a61fa2b69
W90=ee8462f0-5acd-48fd-84f0-3cd66d6014cd



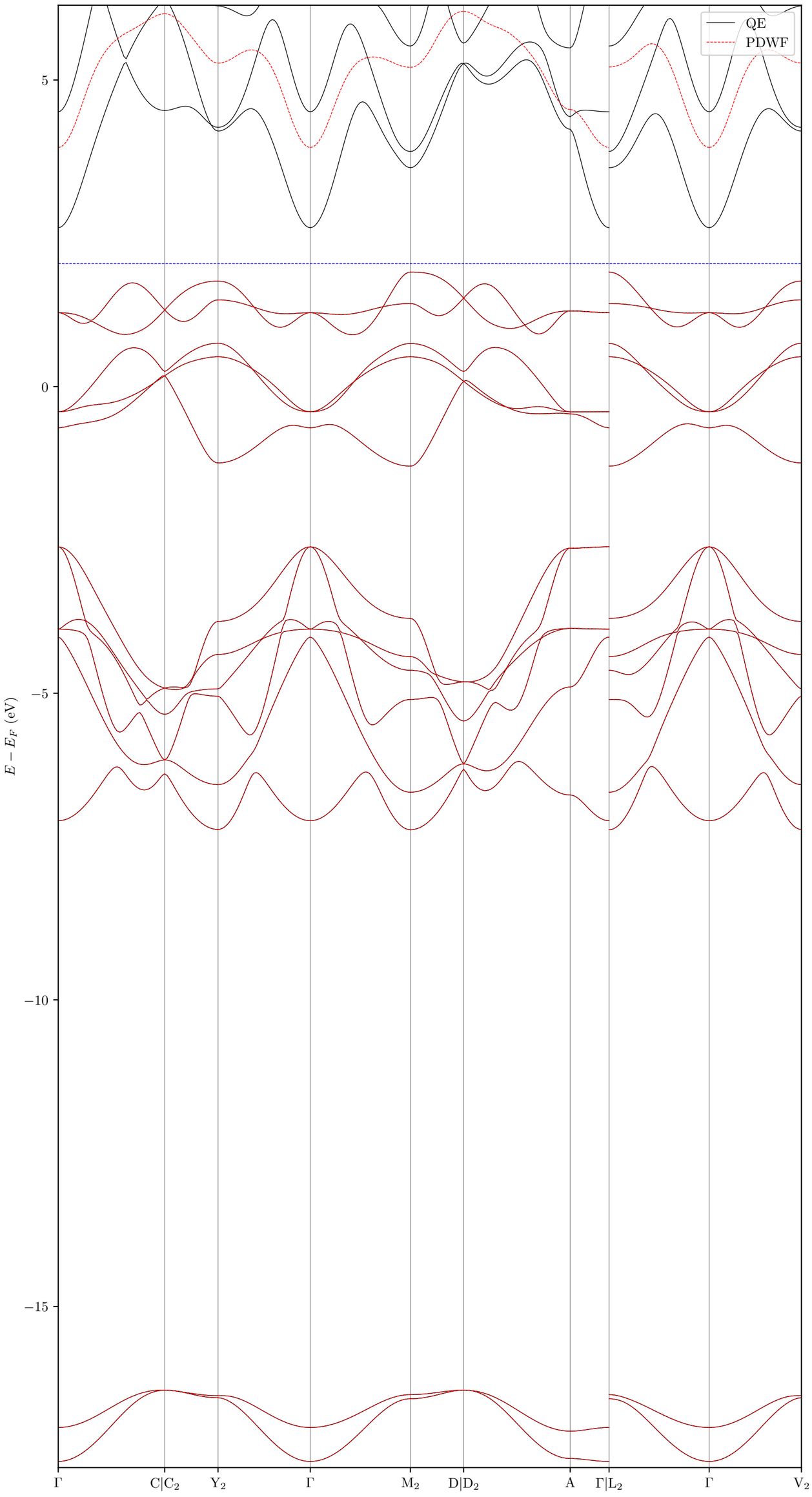

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.4 | 1.4 | 24.6 | 9.8 | 9.8 | 427.5 | 2.483 |

Hamiltonian decay



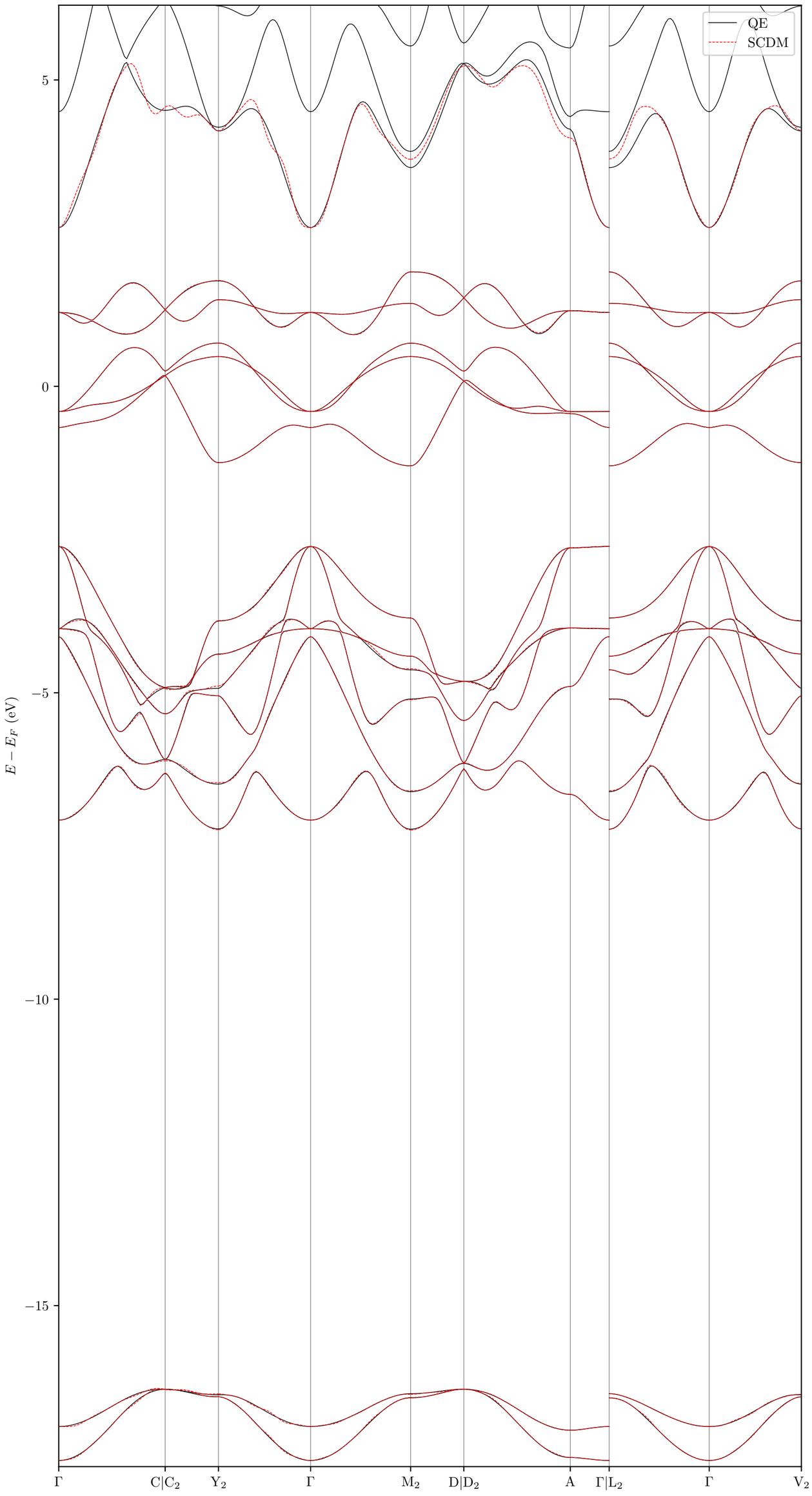
Br2V exclude semicore
PW=2908f5ff-2bd1-4532-bd93-cbaf947db417
W90=4eb8e7ac-5dc0-4021-96fc-0980a9f02214




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.4 | 113.2 | 1.3 | 2.3 | 1119.6 | 1.787 |

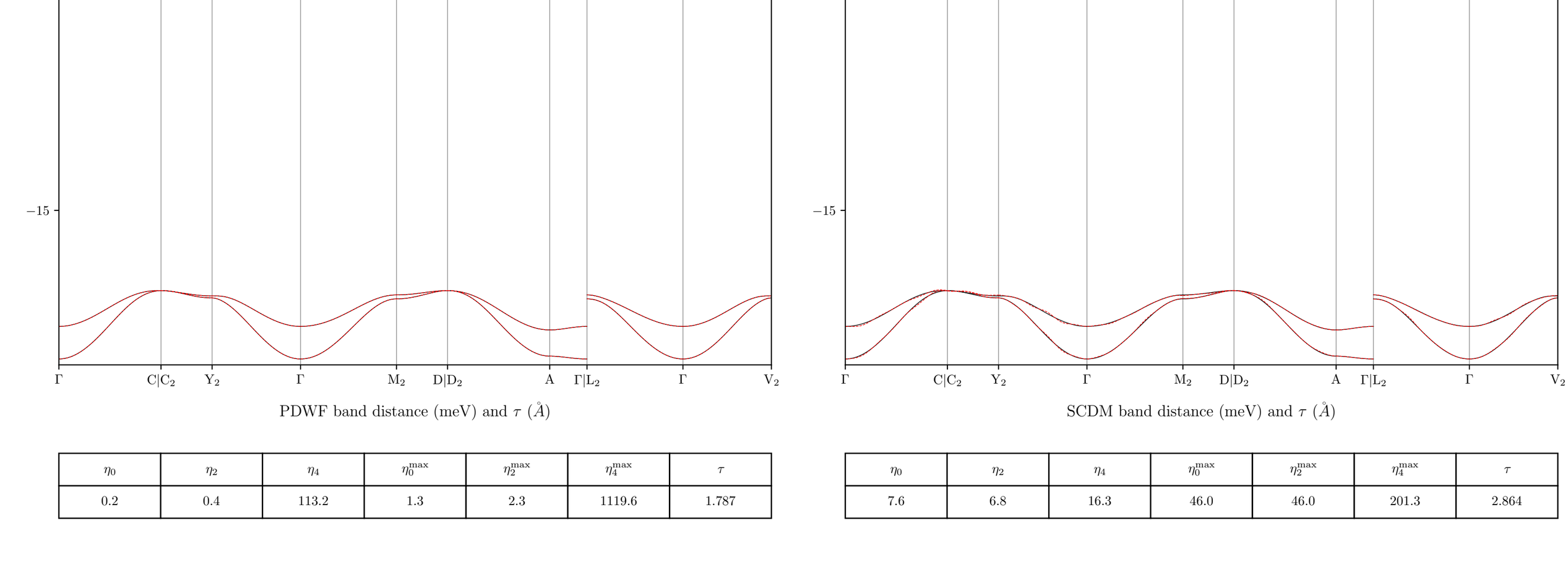
Br2V exclude semicore
PW=2908f5ff-2bd1-4532-bd93-cbaf947db417
W90=ad46df48-c10c-4358-896d-6f28b3eb21f4



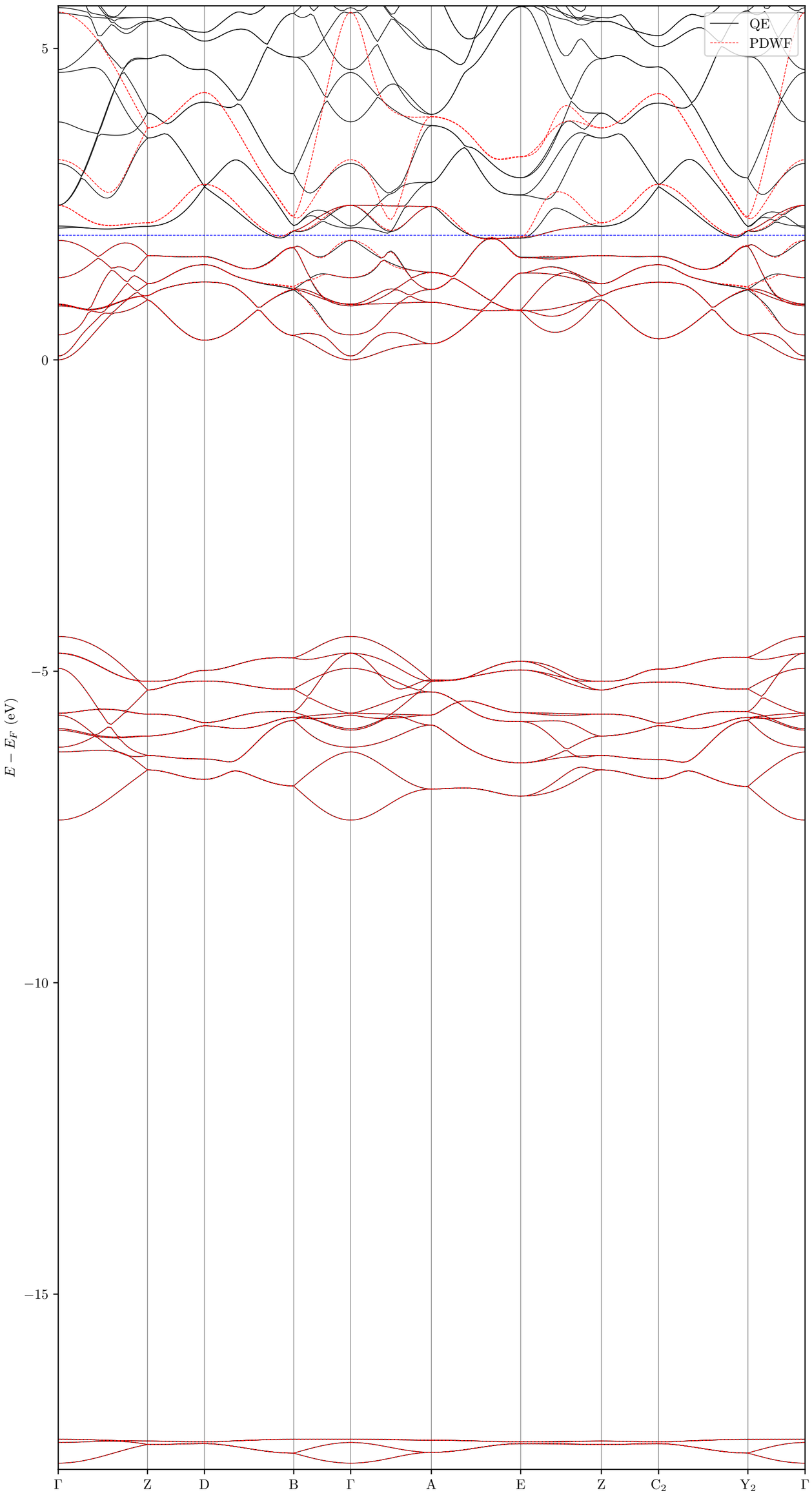

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.6 | 6.8 | 16.3 | 46.0 | 46.0 | 201.3 | 2.864 |

Hamiltonian decay



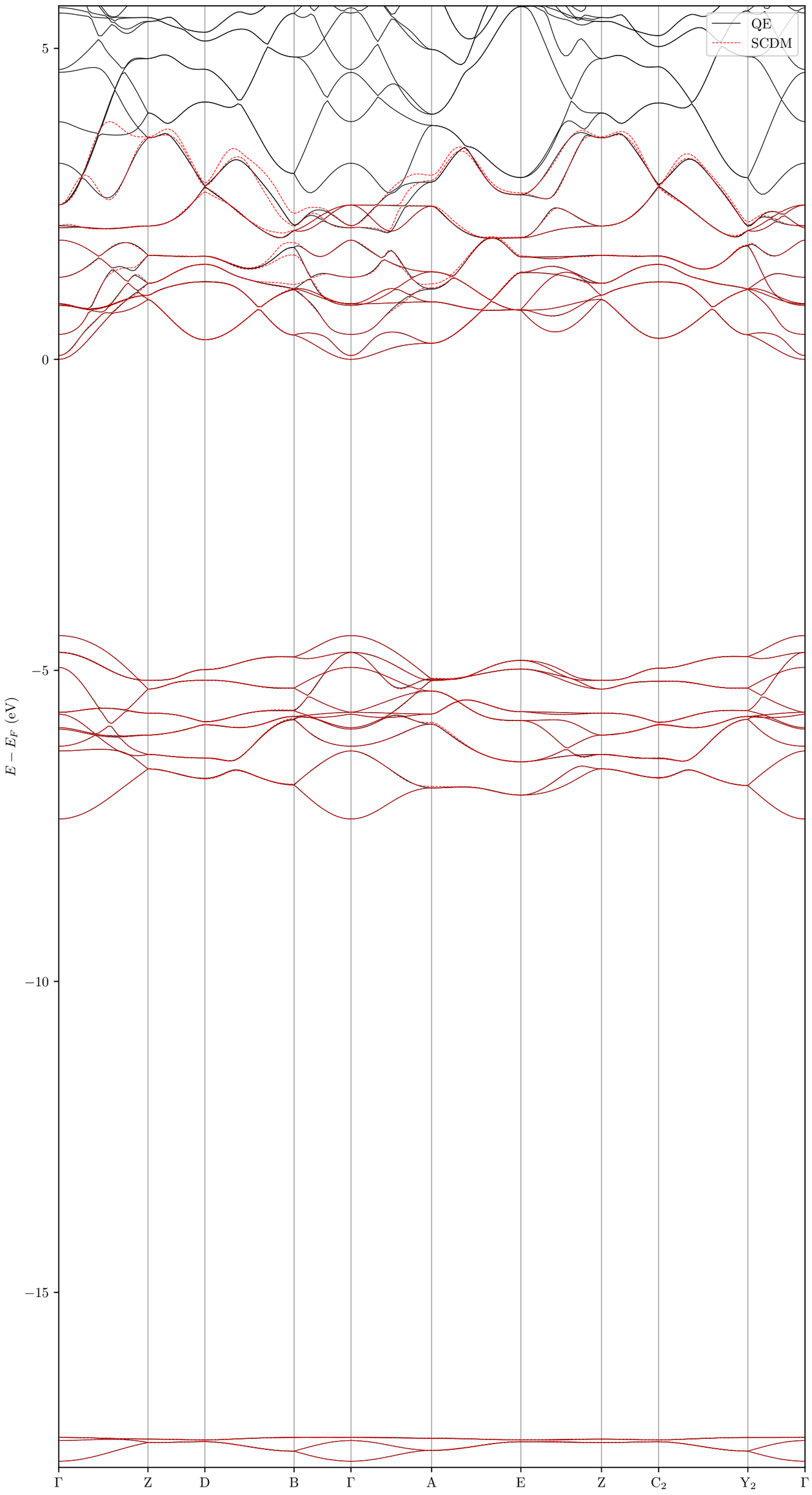
Br4Ca2 exclude semicore
PW=e47ca9ad-81d6-4b86-aa85-174c7ceb1e03
W90=aa8df544-c324-4b2d-b749-a966c01bb1ff




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.8 | 0.8 | 1.7 | 4.9 | 4.9 | 30.4 | 2.500 |

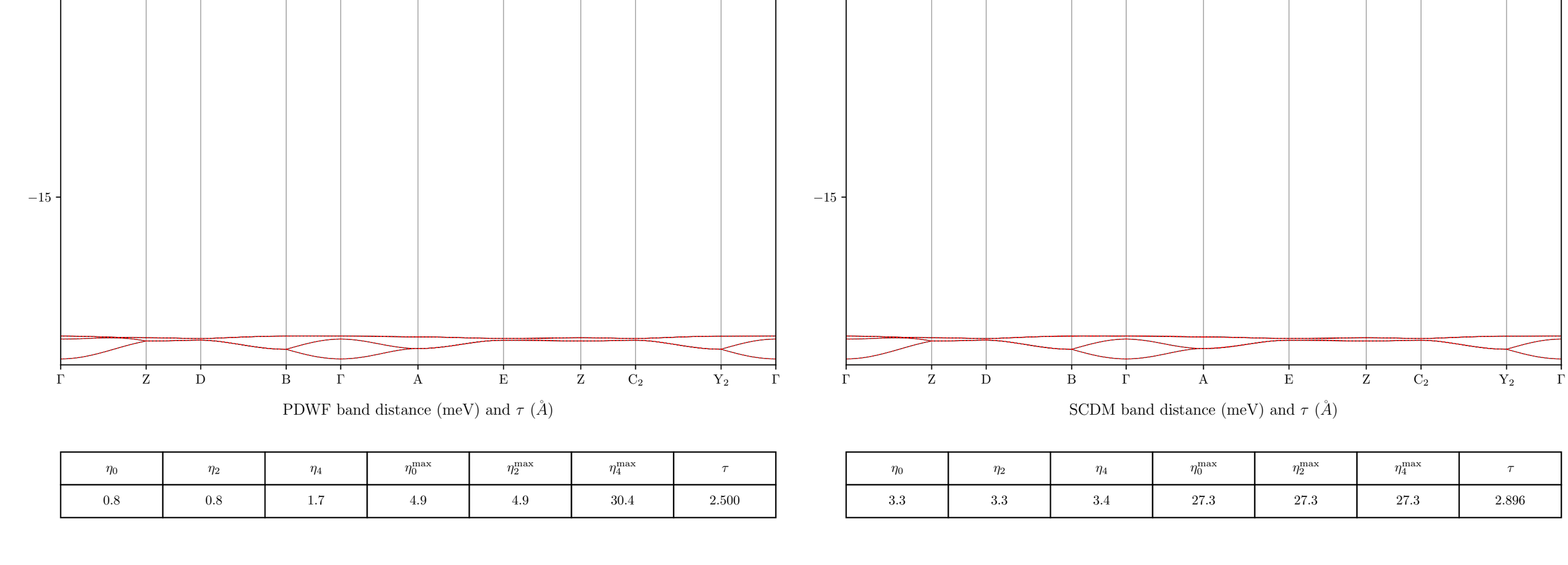
Br4Ca2 exclude semicore
PW=e47ca9ad-81d6-4b86-aa85-174c7ceb1e03
W90=16da7c5d-a87d-4760-b8e6-0eab87dfb55b



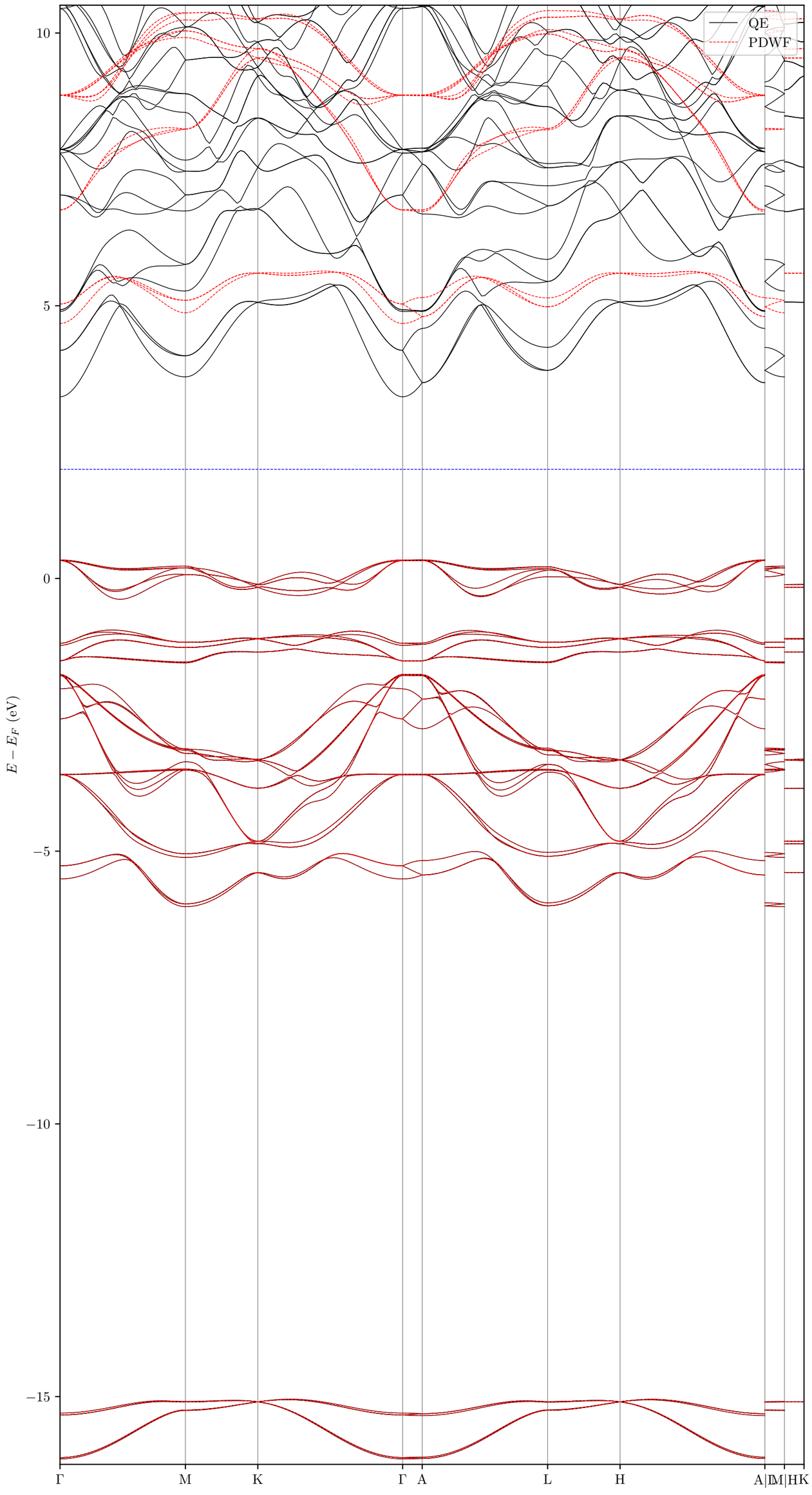

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.3 | 3.3 | 3.4 | 27.3 | 27.3 | 27.3 | 2.896 |

Hamiltonian decay



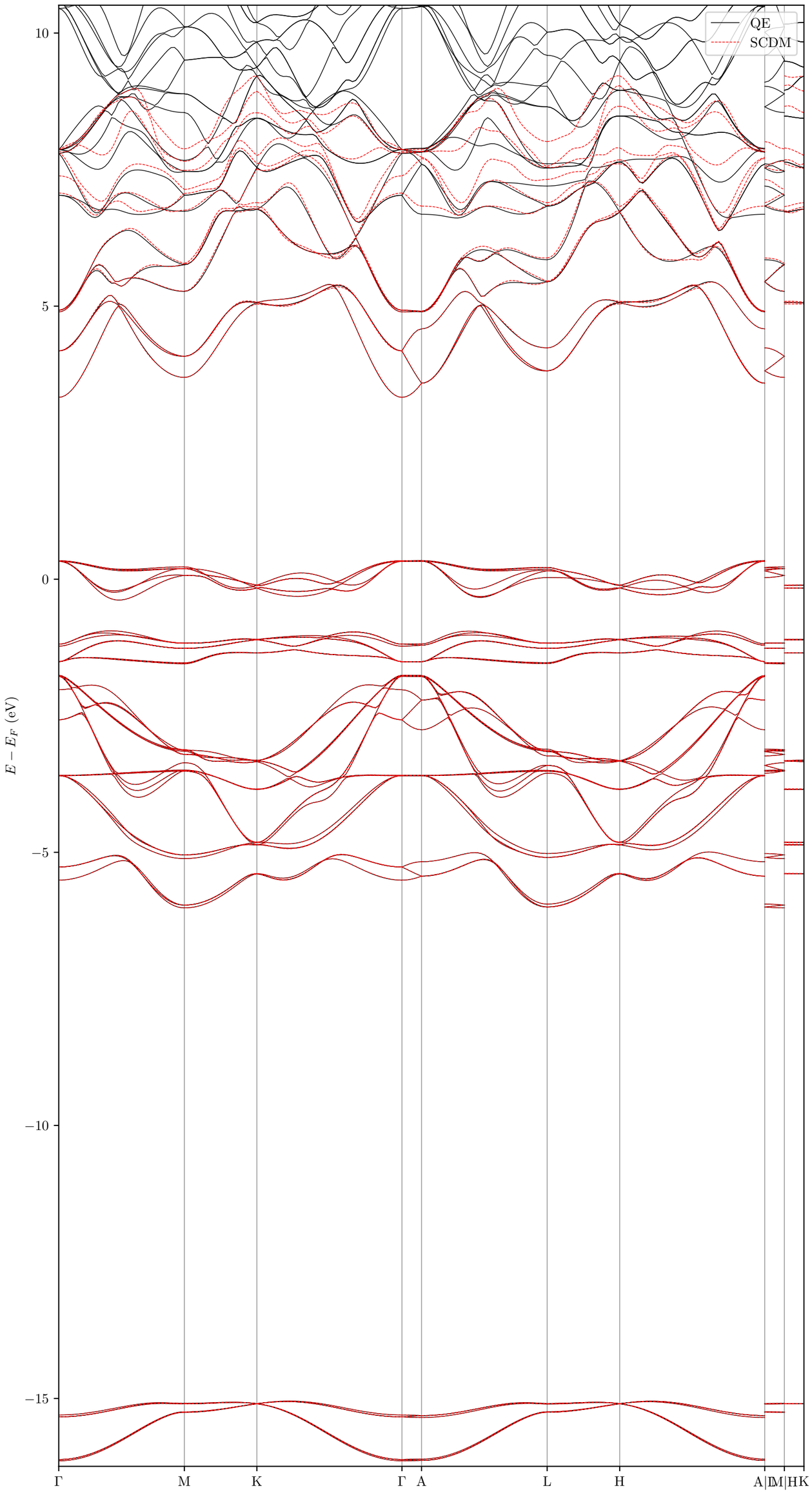
Br6Ni3 exclude semicore
PW=f5421f3c-68b9-4419-a721-47acbdd05e06
W90=5424d59a-af1e-4a43-aa17-37e137d4c2d0




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 15.2 | 1.6 | 1.6 | 46.2 | 2.504 |

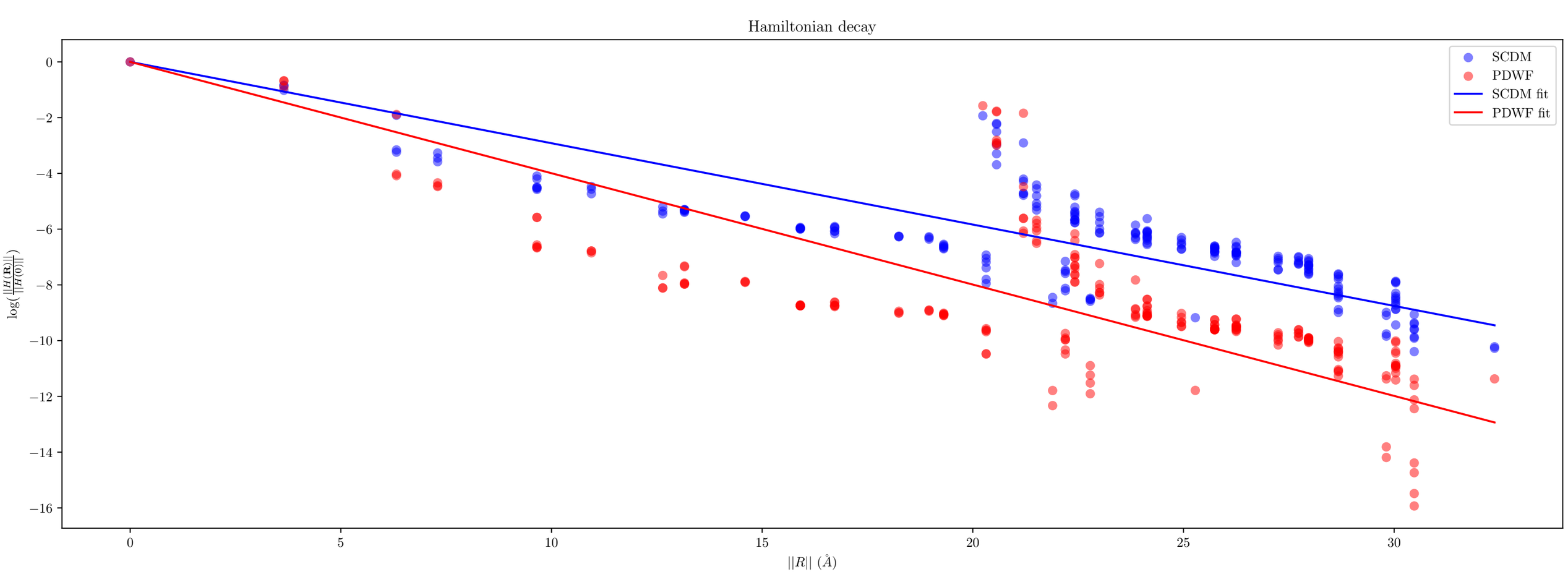
Br6Ni3 exclude semicore
PW=f5421f3c-68b9-4419-a721-47acbdd05e06
W90=a799f609-633e-4d70-a687-6f924e9c1e63




SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.8 | 1.7 | 1.8 | 11.4 | 11.4 | 11.4 | 3.427 |

Hamiltonian decay



Br6Zr2 exclude semicore
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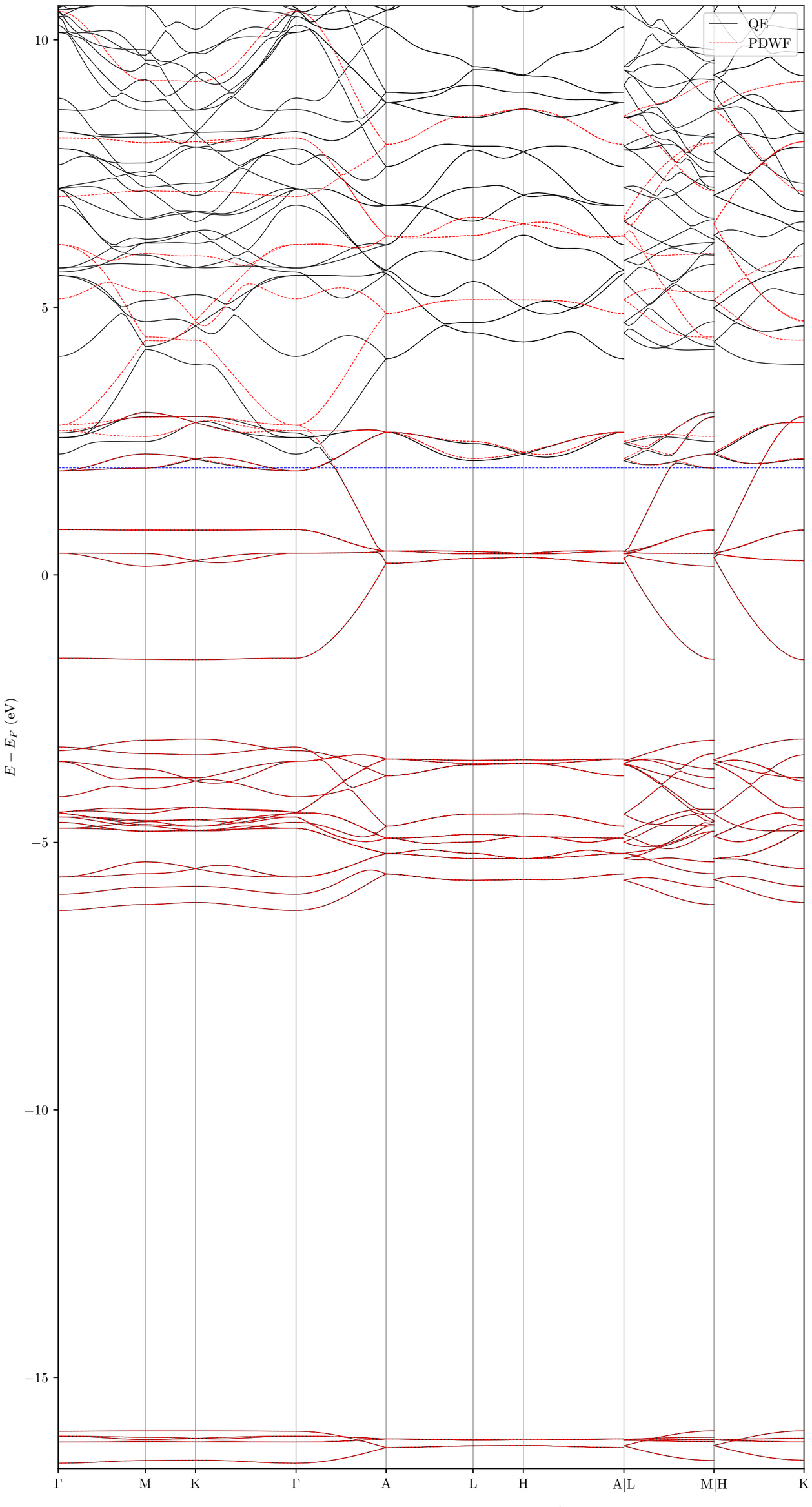
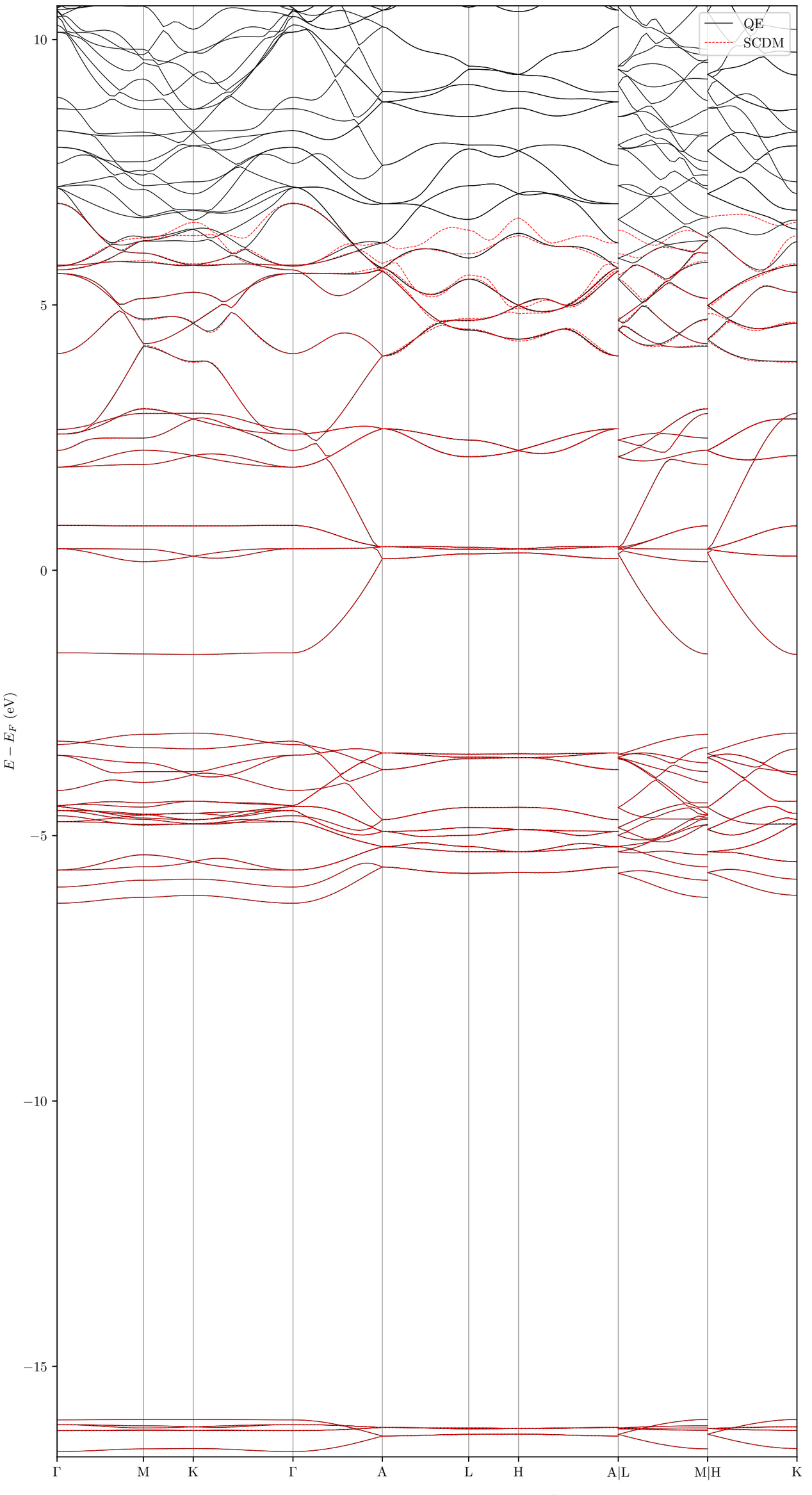
W90=d77f11d3-6e40-46ce-af4f-2da9a0a631f1




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.0 | 3.1 | 47.9 | 5.1 | 14.3 | 739.9 | 2.981 |

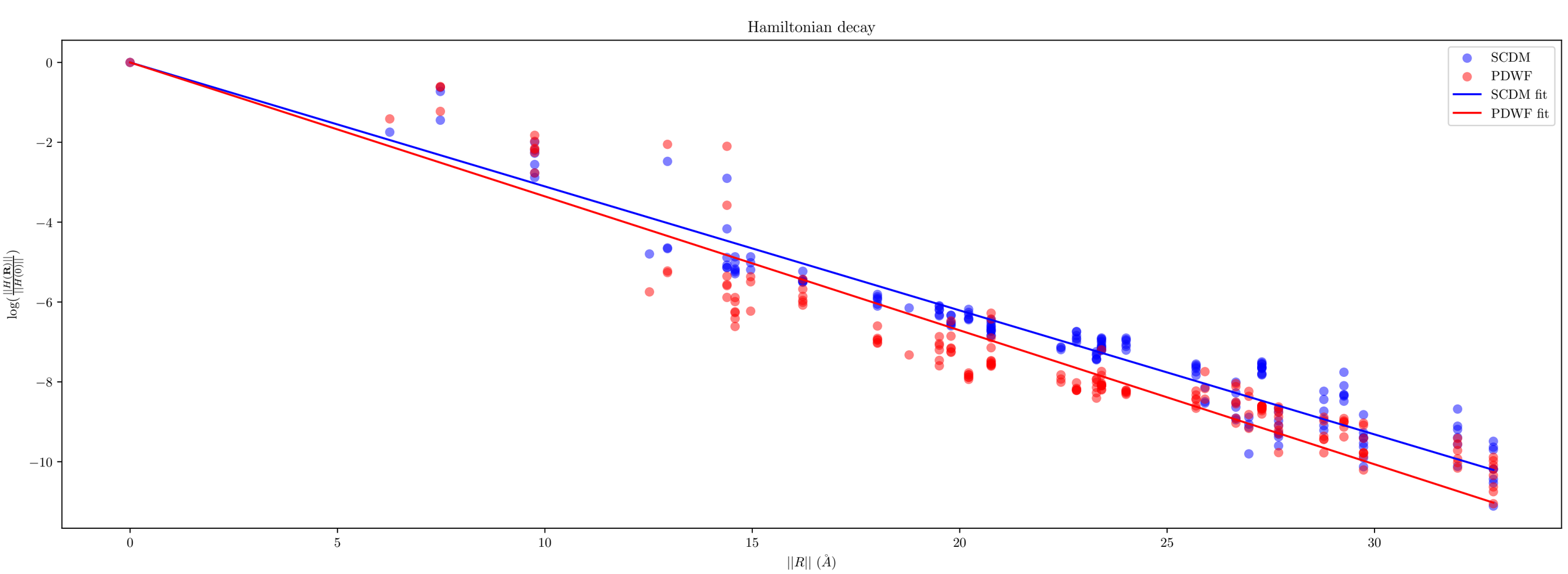
Br6Zr2 exclude semicore
PW=16beb9da-db31-4975-84ac-c0d4097a5f0c
W90=ad0ac761-af46-4e8c-a946-5f069cd6818f

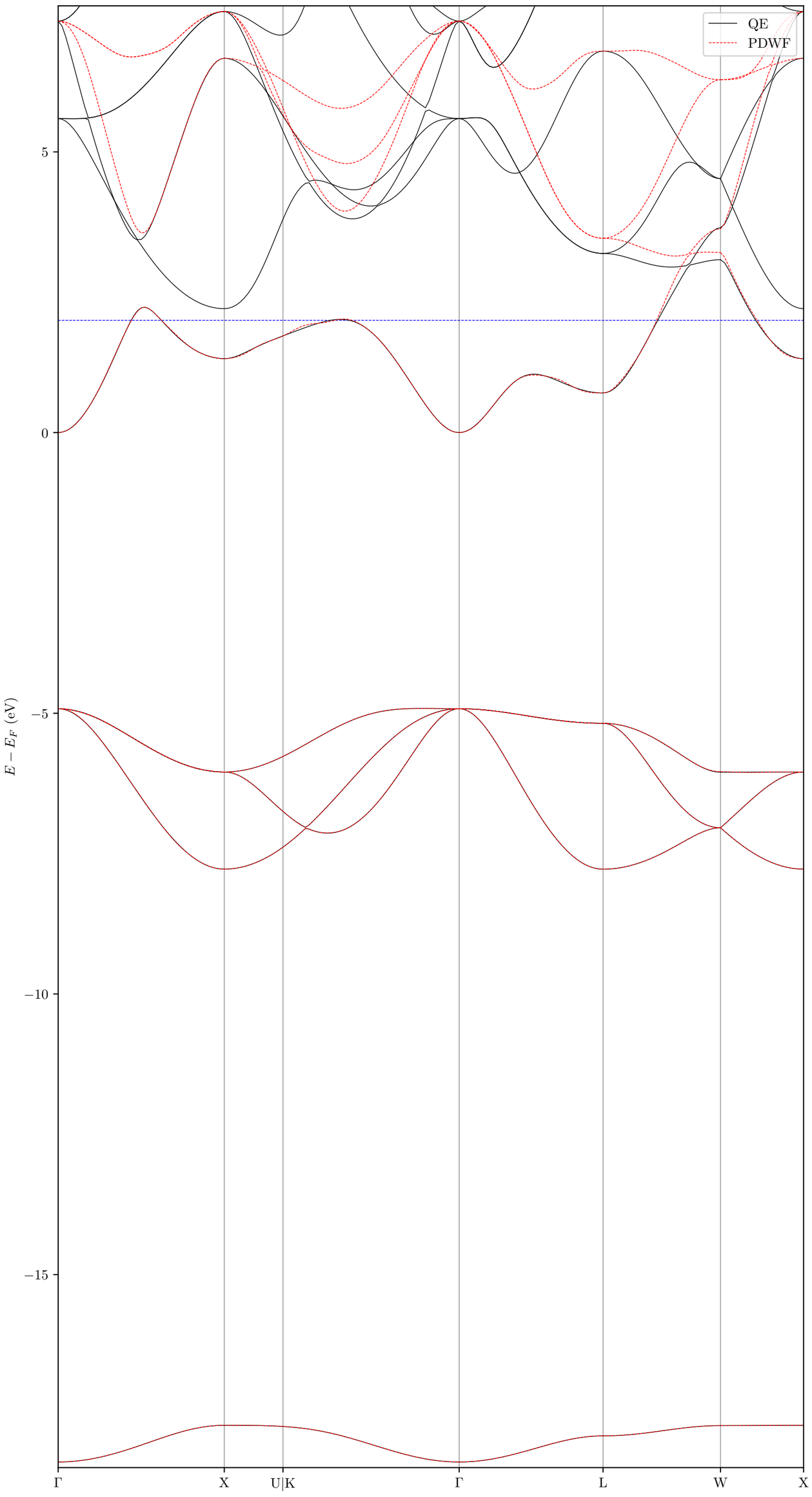



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.7 | 1.7 | 2.4 | 12.4 | 12.4 | 17.1 | 3.220 |

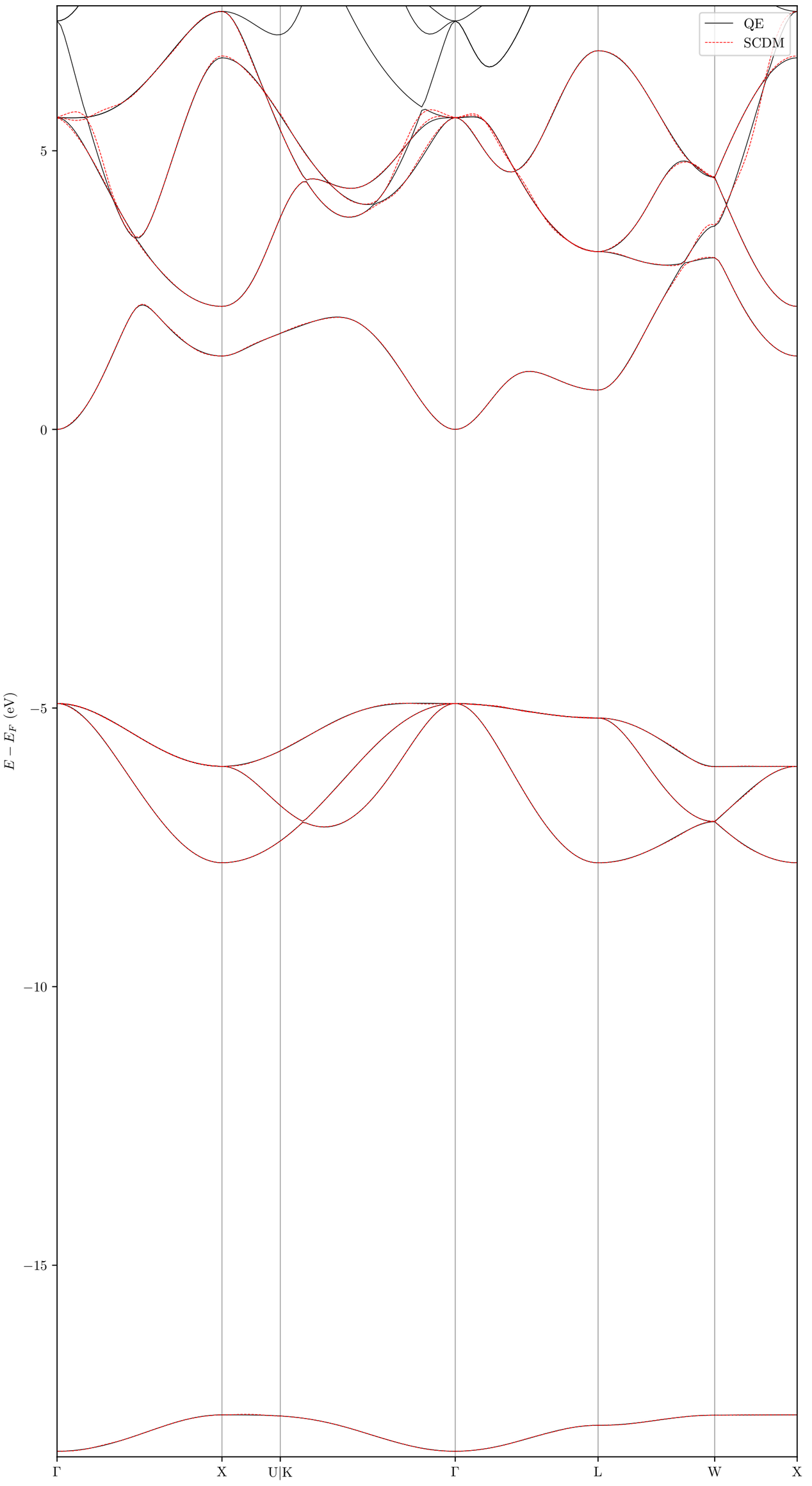
Hamiltonian decay





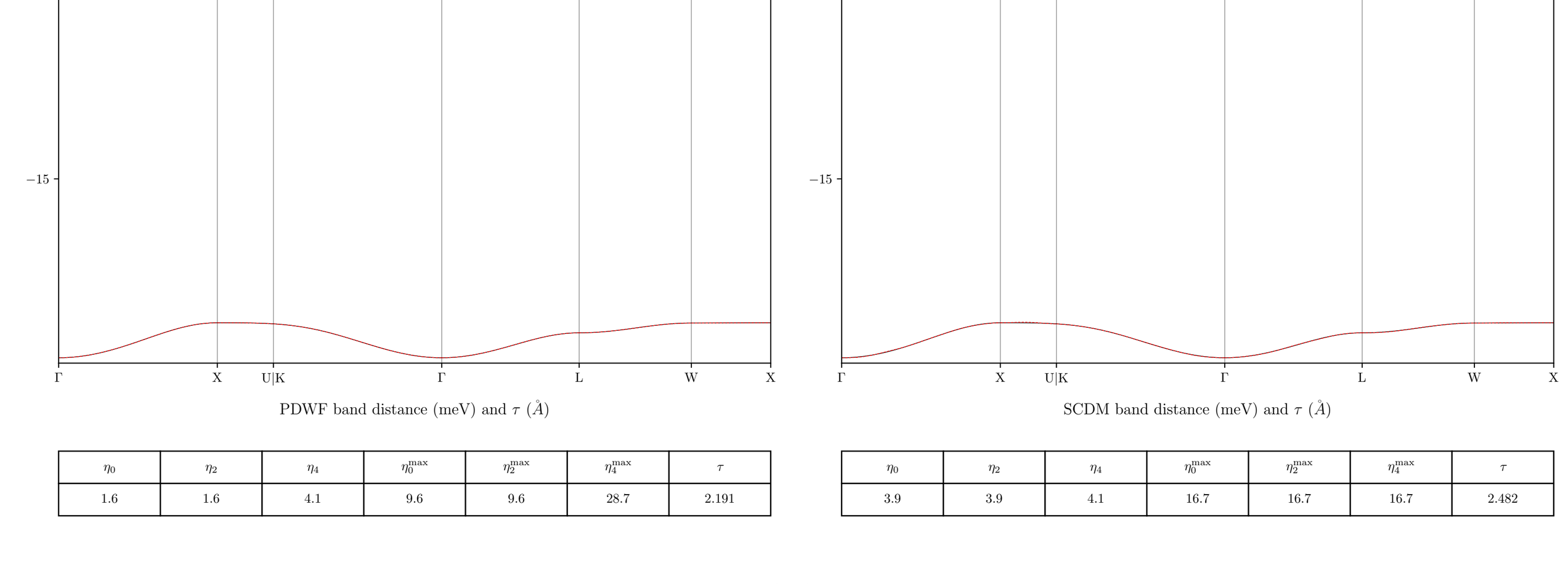

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.6 | 1.6 | 4.1 | 9.6 | 9.6 | 28.7 | 2.191 |

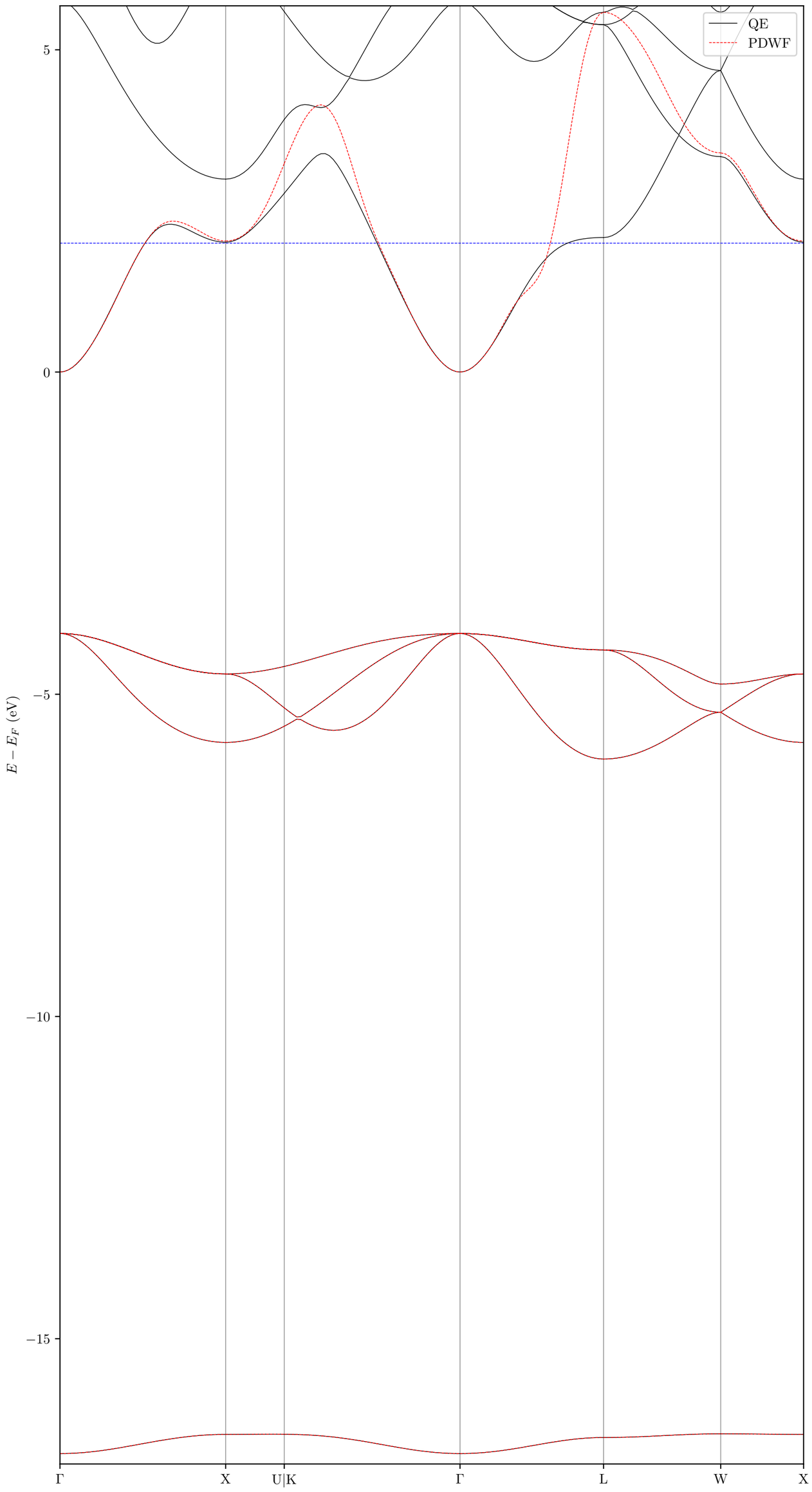



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.9 | 3.9 | 4.1 | 16.7 | 16.7 | 16.7 | 2.482 |



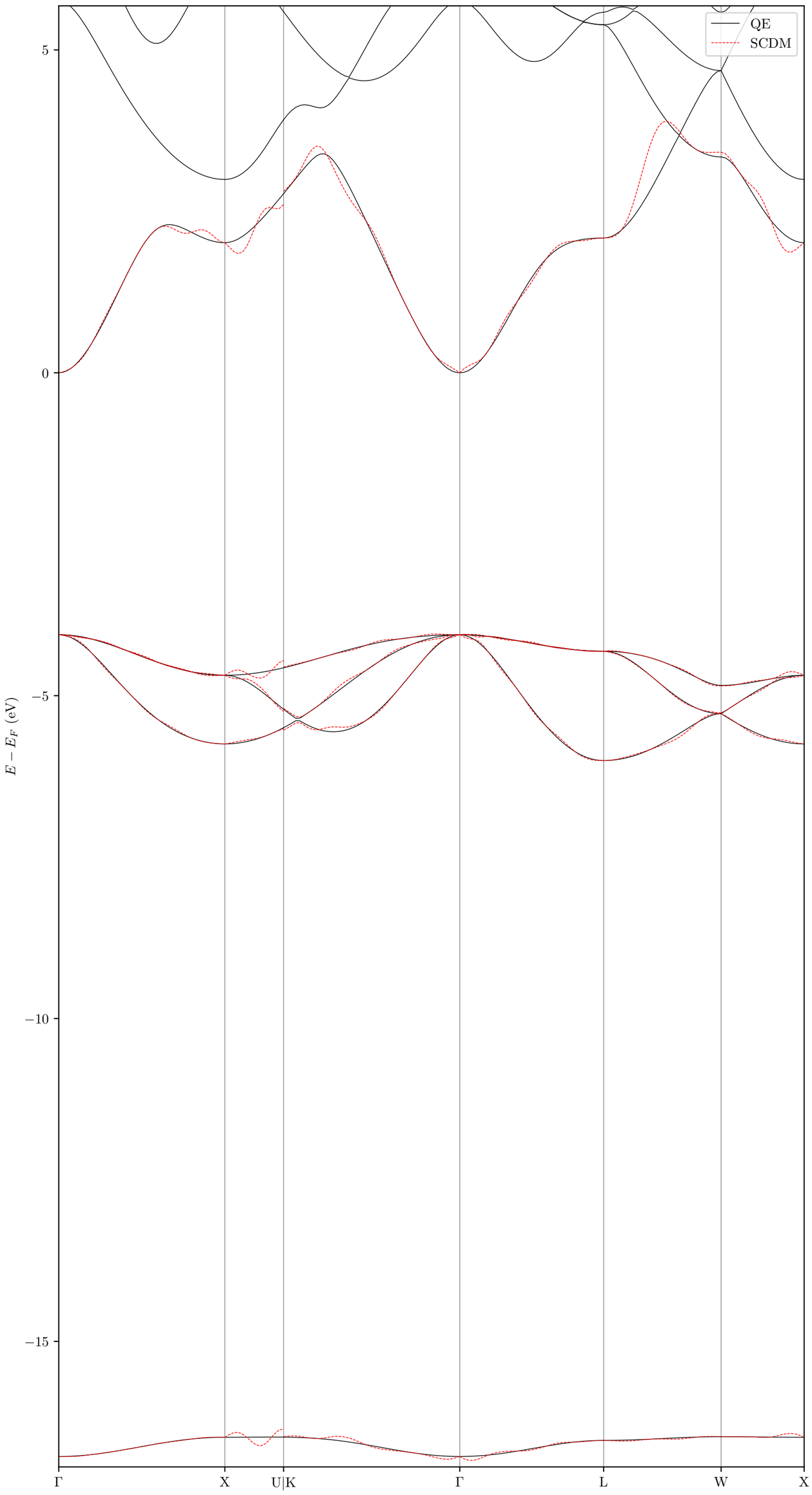
BrNa exclude semicore
PW=82d3ac89-14fd-45a5-855a-7f2a0f931ea0
W90=fe1ee2e5-0074-4623-aee4-6bd398cb7e4b




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 14.4 | 3.3 | 3.3 | 149.6 | 2.077 |

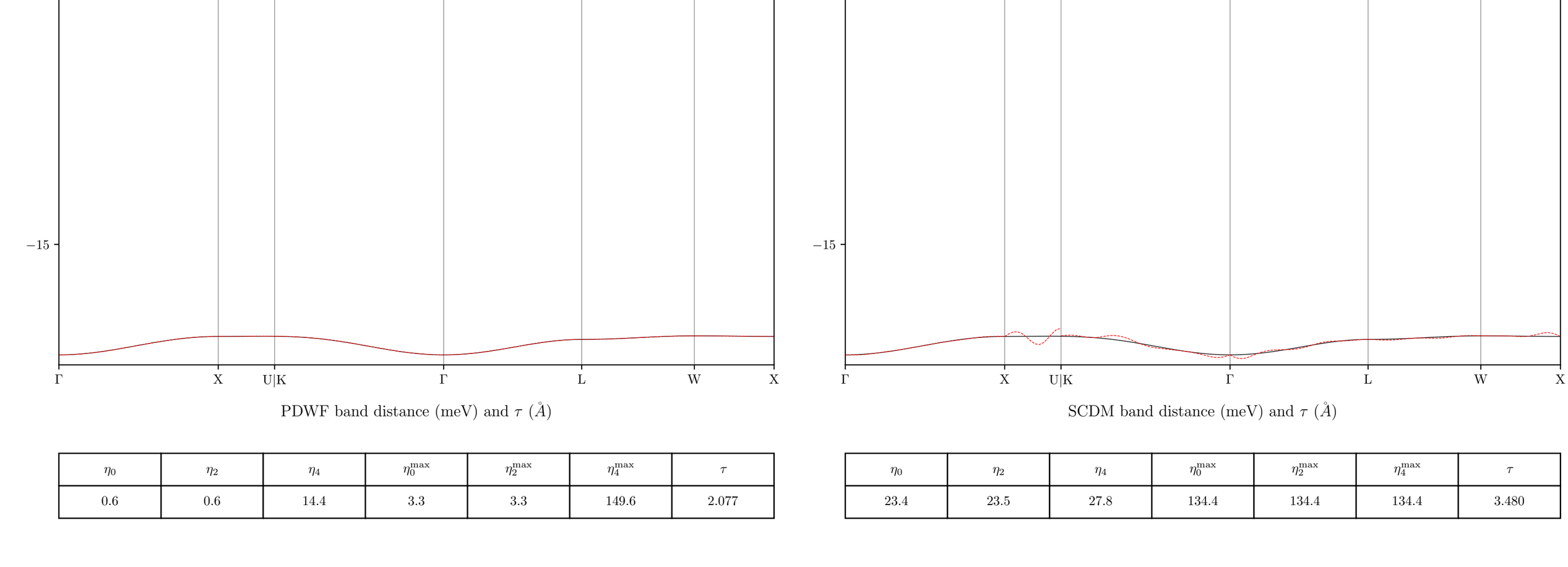
BrNa exclude semicore
PW=82d3ac89-14fd-45a5-855a-7f2a0f931ea0
W90=c28f3748-734f-400a-a37f-5e65e2a01b14



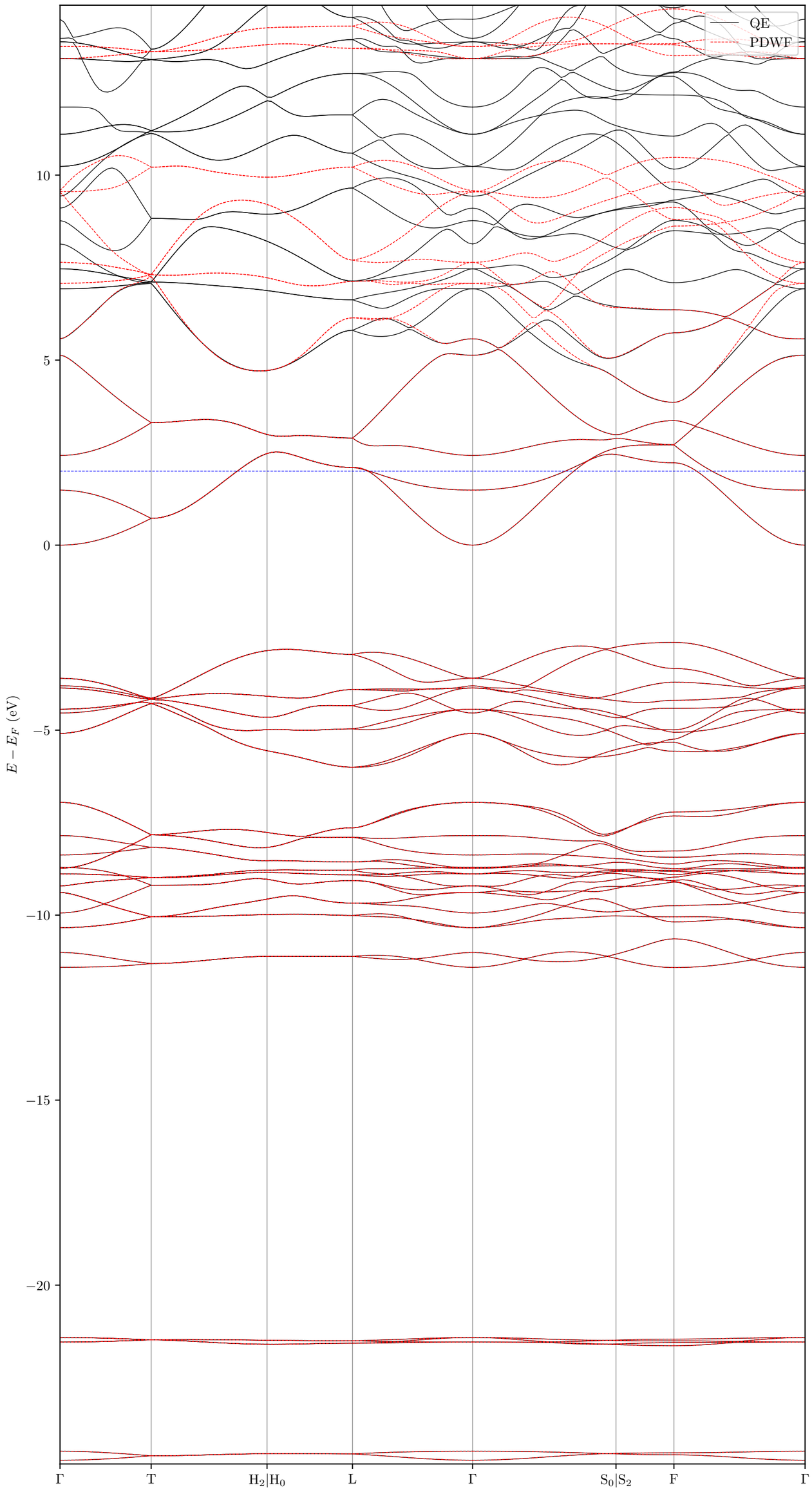

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 23.4 | 23.5 | 27.8 | 134.4 | 134.4 | 134.4 | 3.480 |

Hamiltonian decay



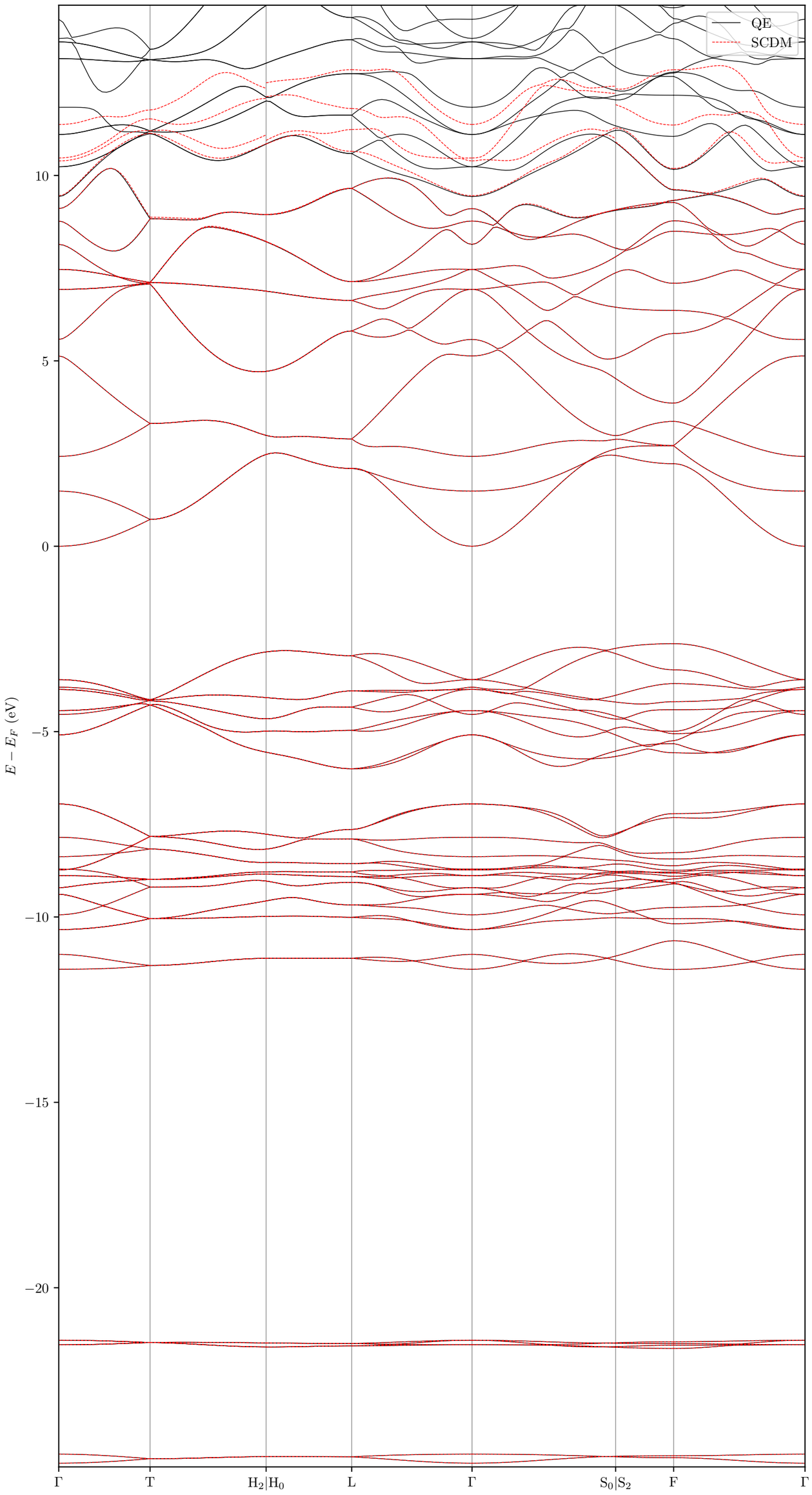
C2Cd2O6 exclude semicore
PW=bab43eee-e044-4cbe-959a-9103b7244454
W90=0f5d584d-d04f-4aa6-8a6c-552c1a5e0669




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 0.4 | 2.0 | 2.0 | 3.8 | 2.719 |

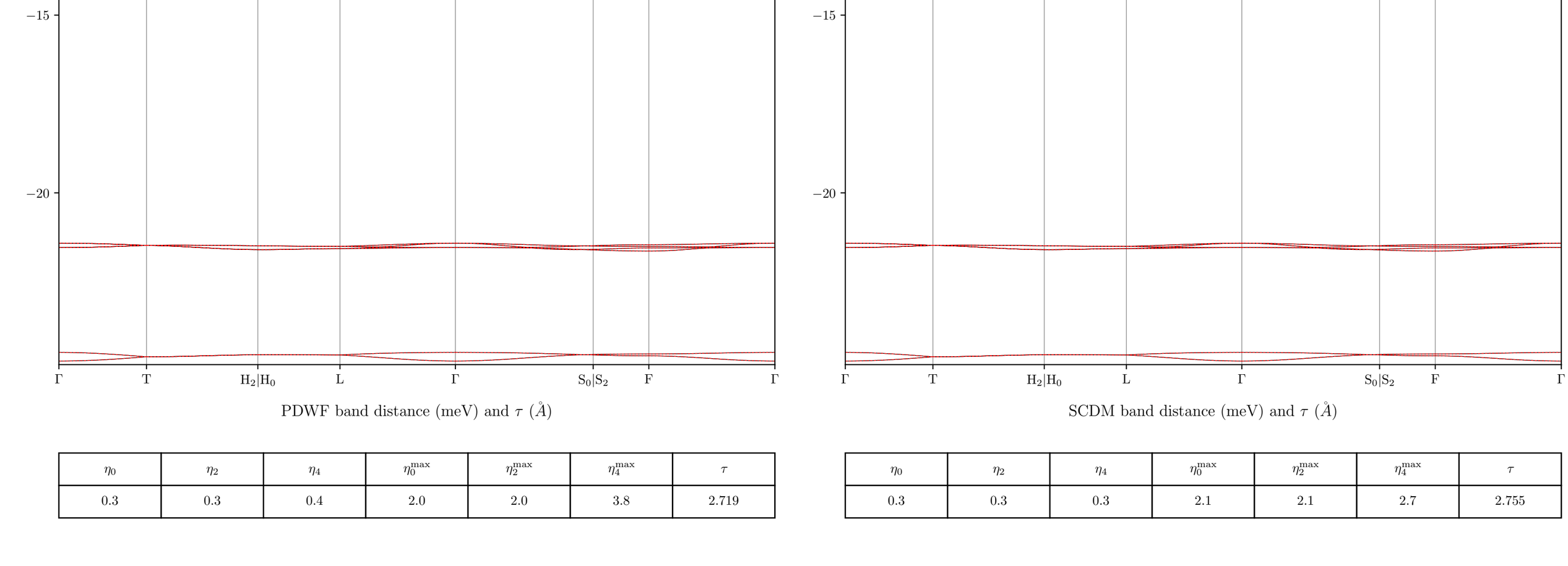
C2Cd2O6 exclude semicore
PW=bab43eee-e044-4cbe-959a-9103b7244454
W90=c15caa3b-c030-42b5-bd3e-4d5d2e6fe538



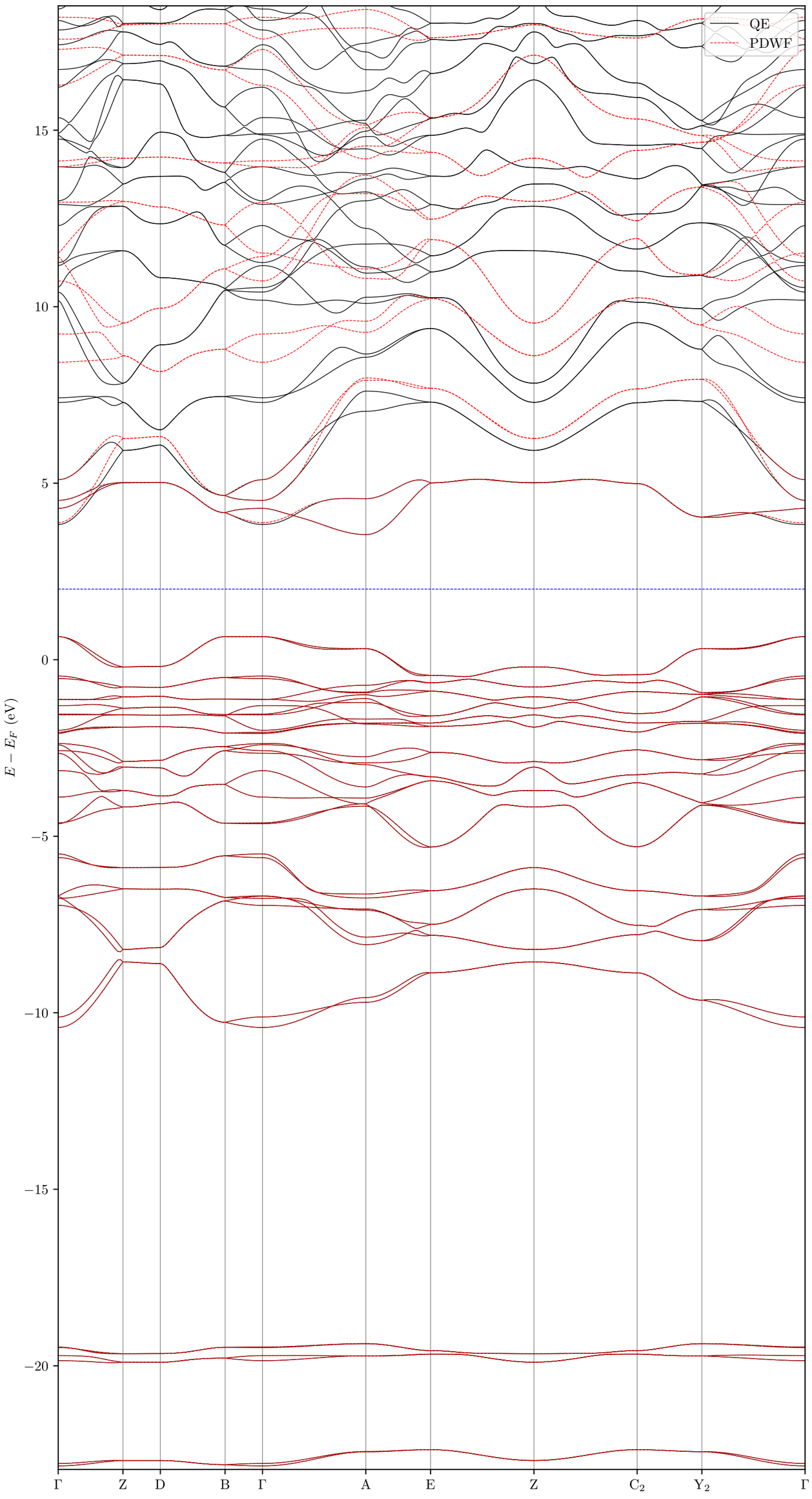

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 0.3 | 2.1 | 2.1 | 2.7 | 2.755 |

Hamiltonian decay



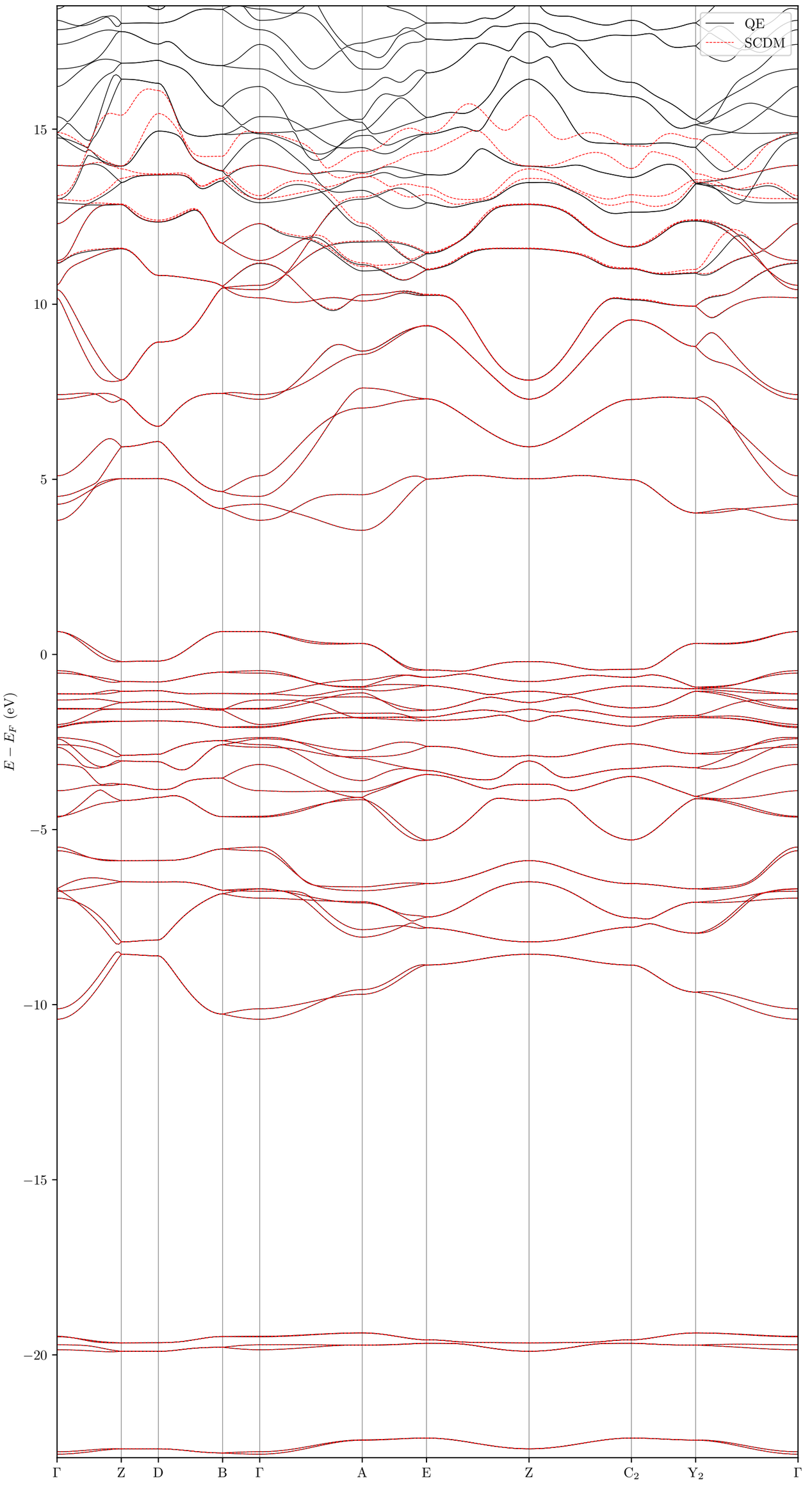
C2Cu2O6 exclude semicore
PW=58e038ac-92c6-4a22-a0c6-e6117830b702
W90=78aa3506-0b21-45ed-a989-98de38f36cda




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.5 | 3.0 | 4.1 | 4.1 | 44.5 | 2.295 |

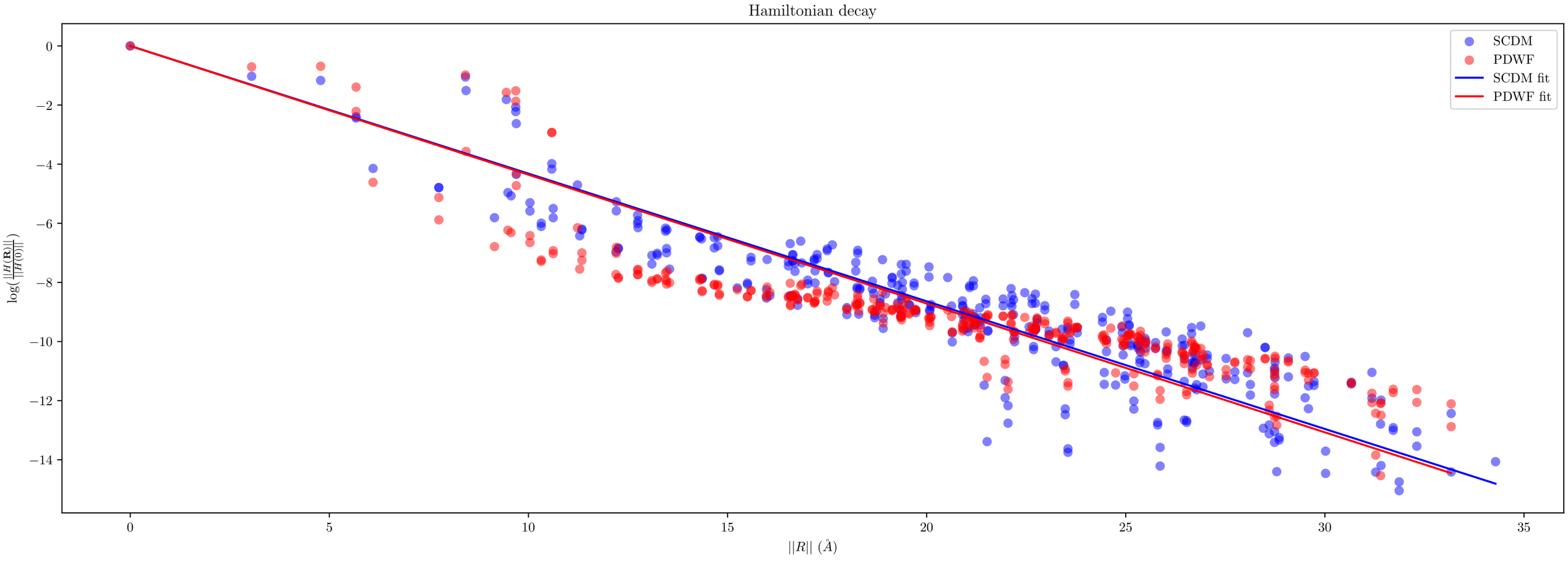
C2Cu2O6 exclude semicore
PW=58e038ac-92c6-4a22-a0c6-e6117830b702
W90=0c2a59f6-0db6-4498-b26a-24c179355ed0



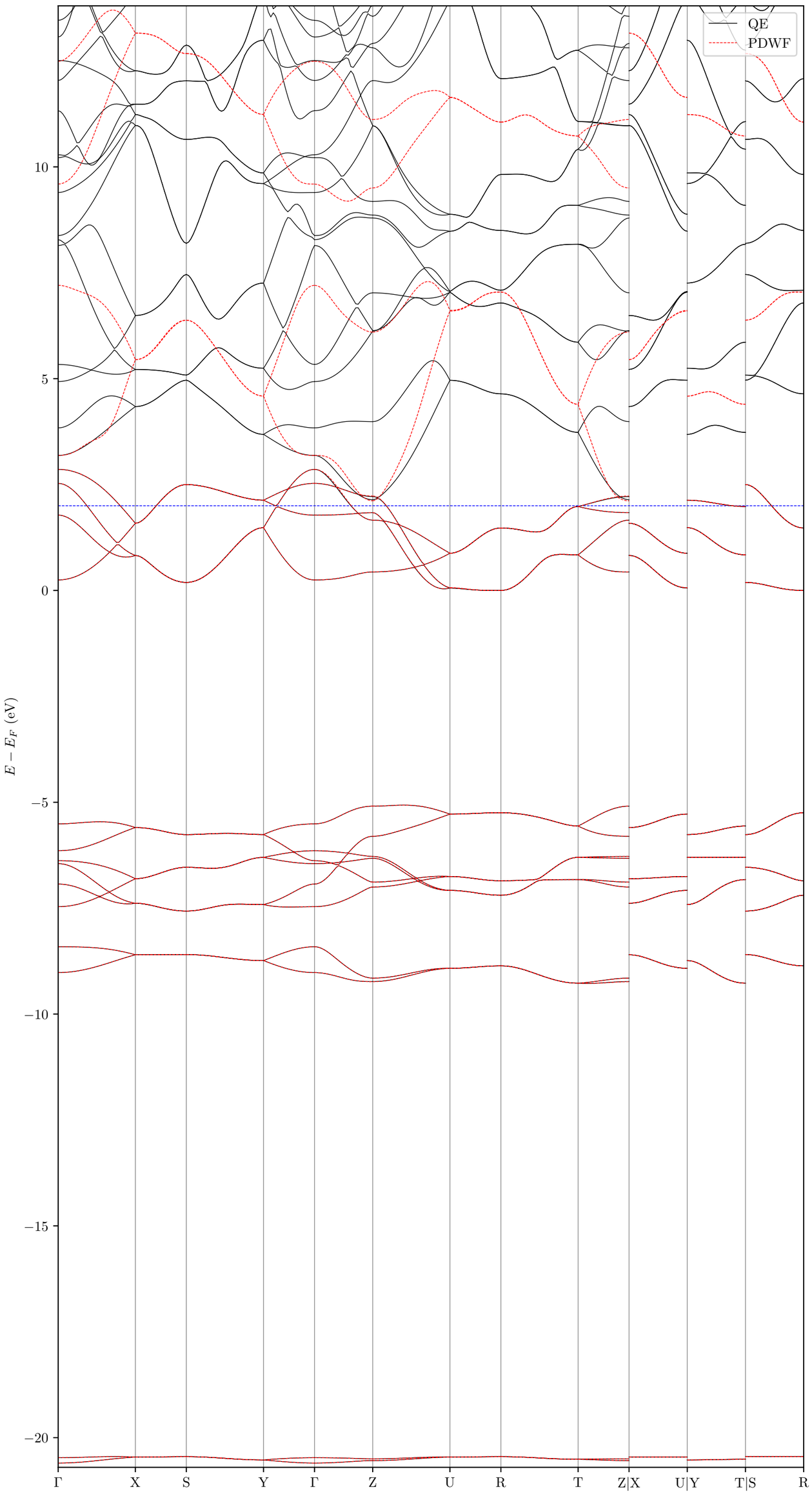

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.5 | 0.5 | 3.3 | 3.3 | 3.7 | 2.315 |

Hamiltonian decay



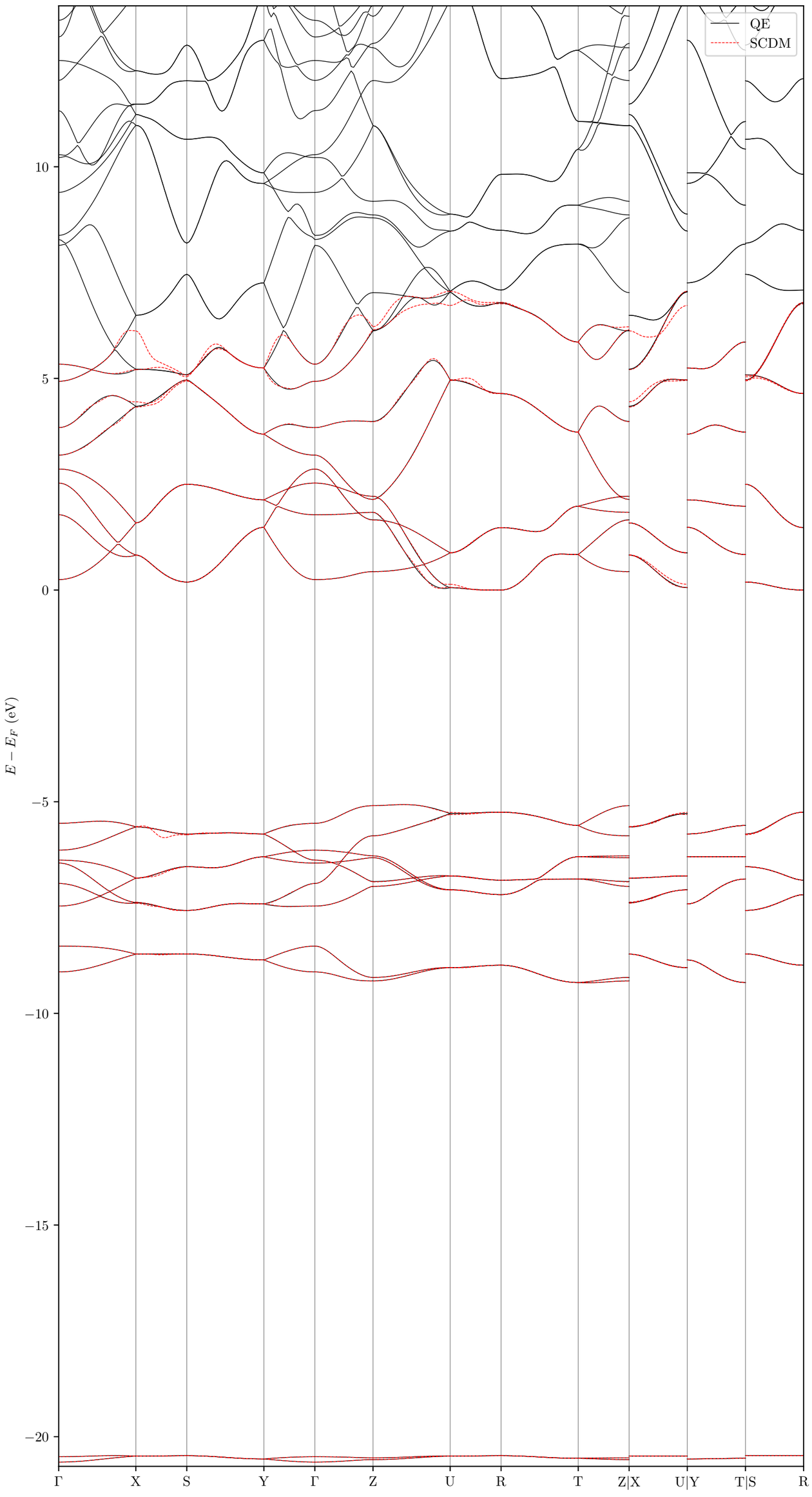
C2N2Na2 exclude semicore
PW=98324d79-57ec-4a90-af5a-60b985b4022b
W90=0ff72702-d00b-4104-8347-4c49a57be768




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.9 | 0.9 | 1.2 | 5.2 | 5.2 | 9.6 | 2.347 |

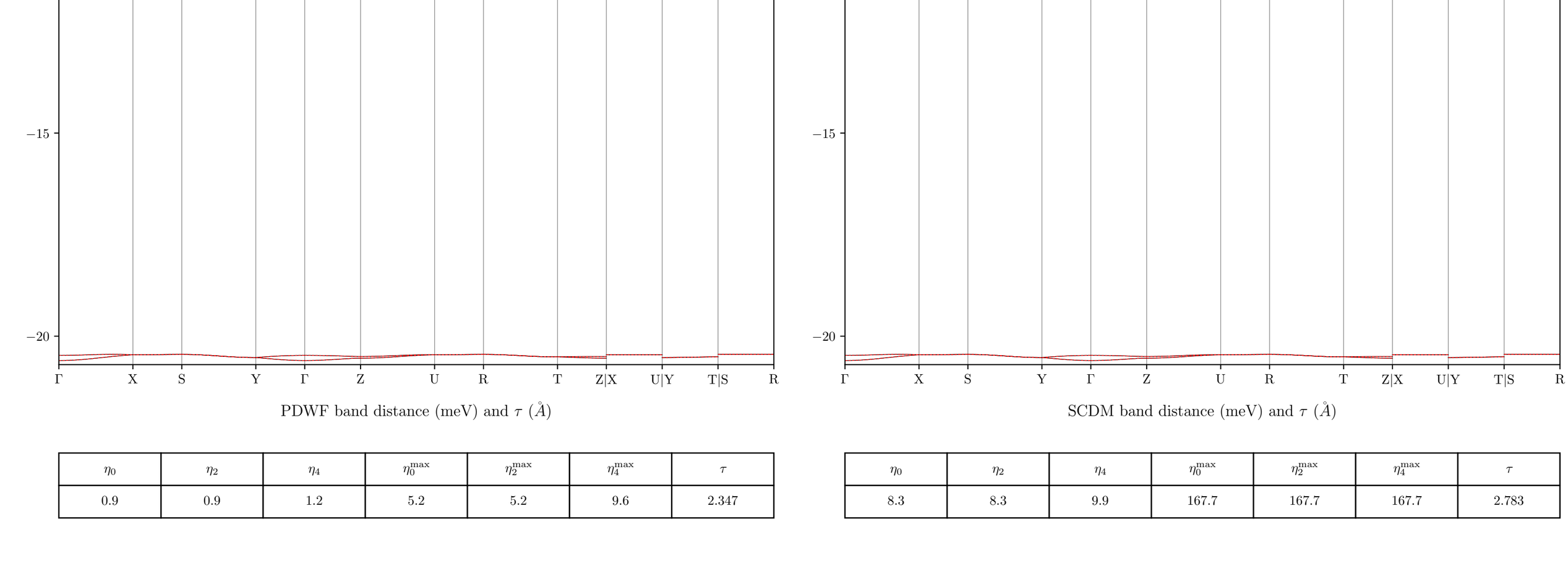
C2N2Na2 exclude semicore
PW=98324d79-57ec-4a90-af5a-60b985b4022b
W90=872f9755-b8a1-46be-9056-04e9dc17f637



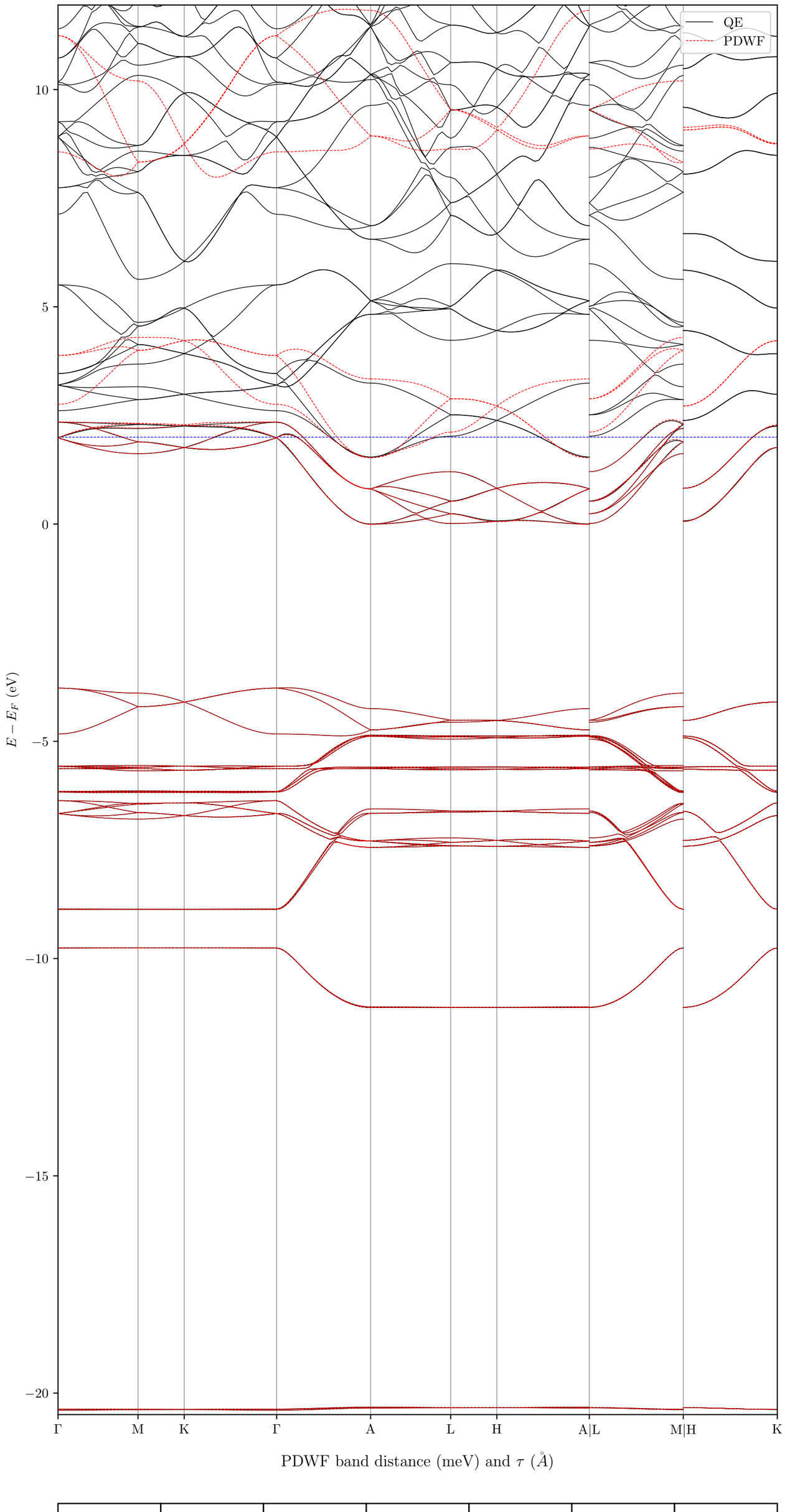

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.3 | 8.3 | 9.9 | 167.7 | 167.7 | 167.7 | 2.783 |

Hamiltonian decay



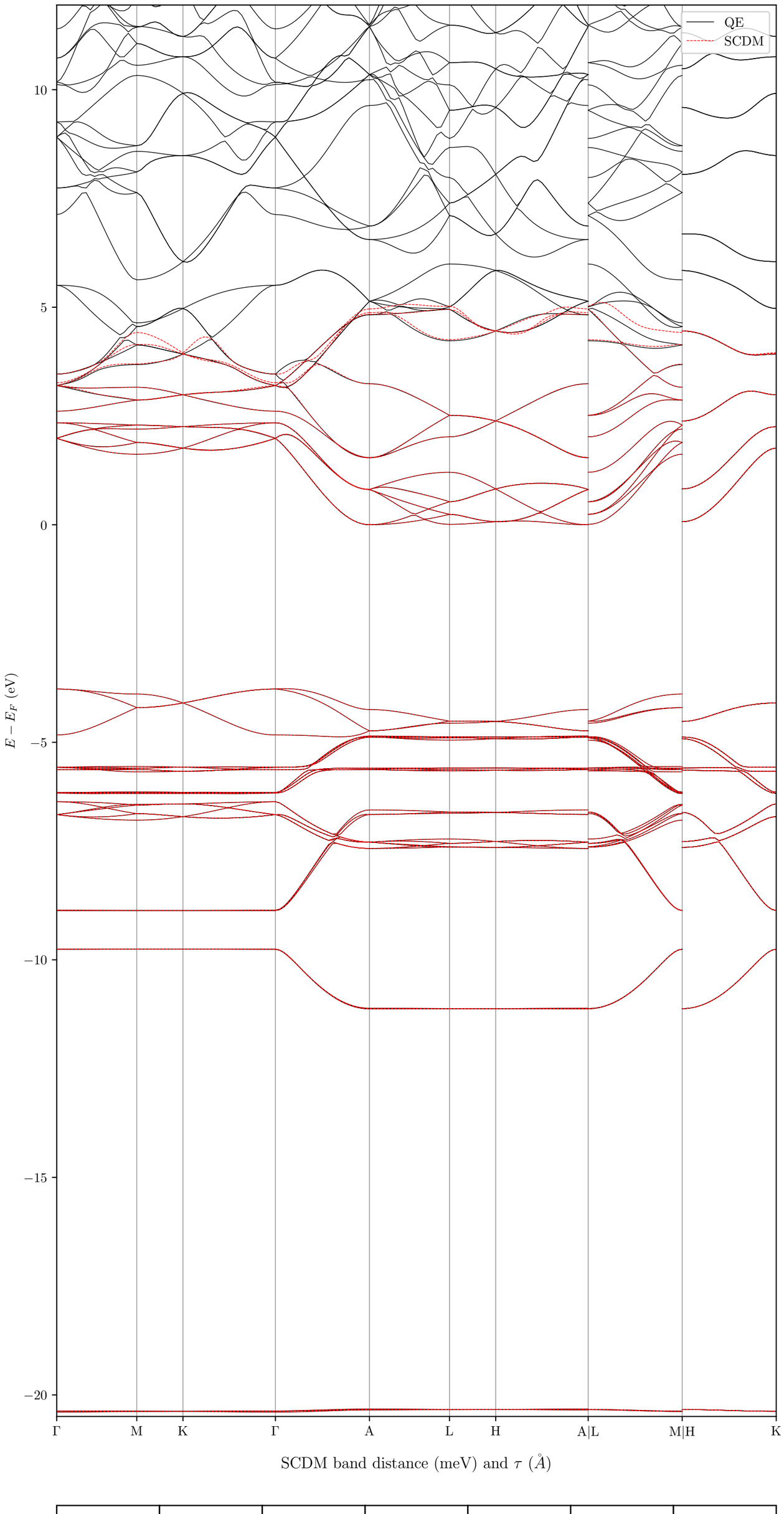
C3Ag3N3 exclude semicore
PW=a0872376-08e7-4f99-a7f0-14395344e330
W90=dd6753ea-a194-422b-8bb3-8d161b1b5f93




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.9 | 1.7 | 16.0 | 5.2 | 12.6 | 157.9 | 2.839 |

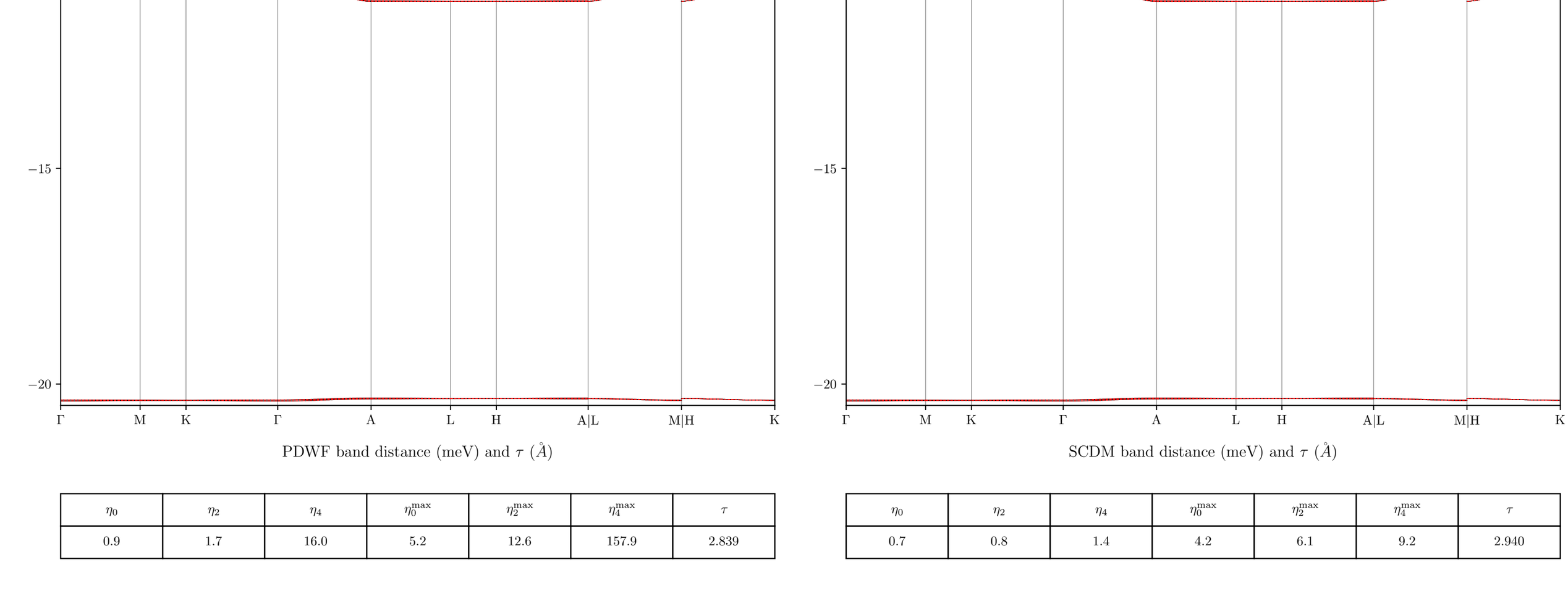
C3Ag3N3 exclude semicore
PW=a0872376-08e7-4f99-a7f0-14395344e330
W90=a7c49eed-0171-4d2e-867b-ff34d91f5ac5



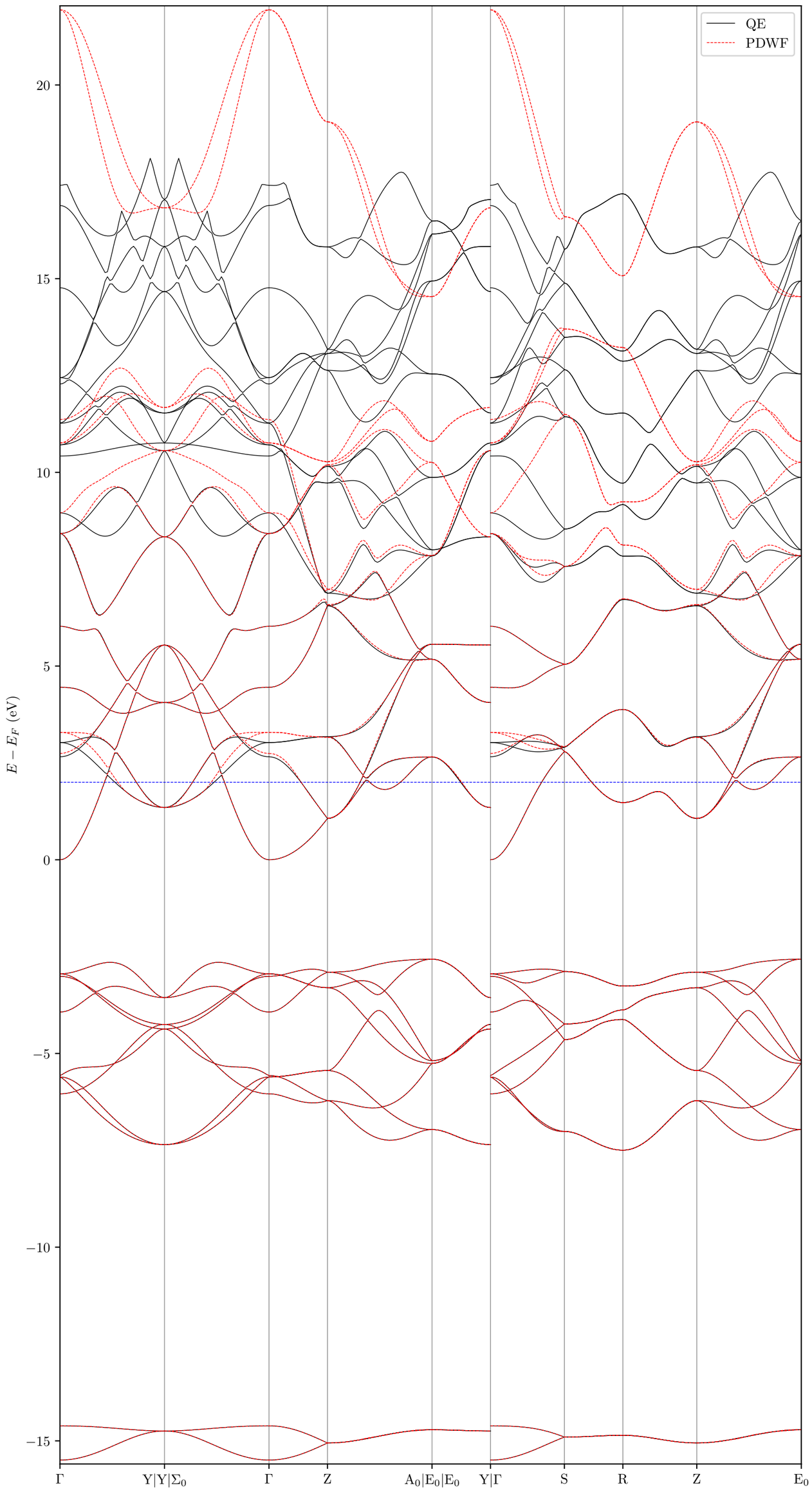

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 0.8 | 1.4 | 4.2 | 6.1 | 9.2 | 2.940 |

Hamiltonian decay



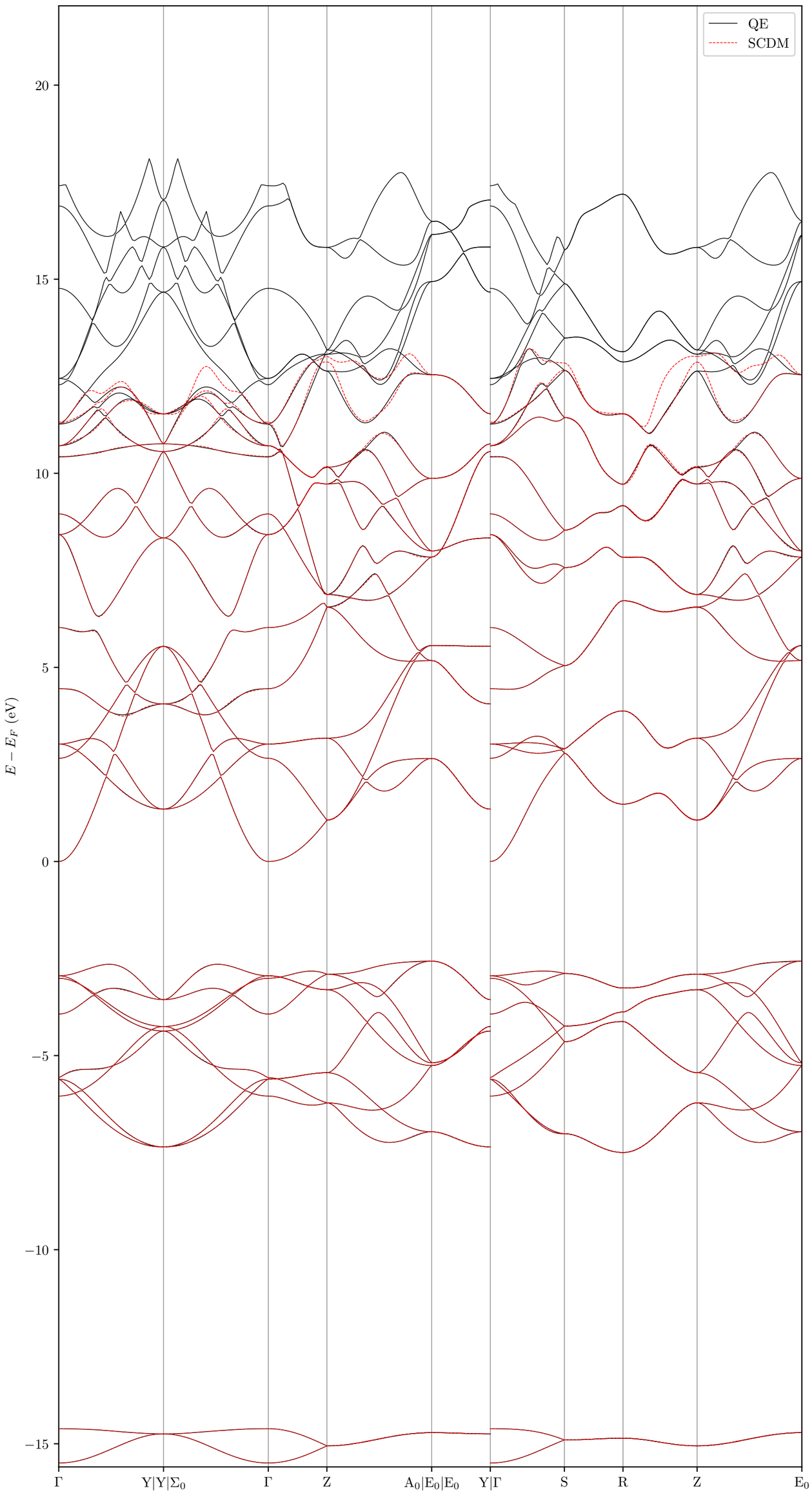
C4Mg2 exclude semicore
PW=5e0a0be1-f706-4fa0-a8e5-791856288039
W90=9bc2e7d5-9423-489e-a55c-0c10d939efce




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.7 | 2.0 | 42.0 | 10.7 | 11.4 | 308.6 | 2.314 |

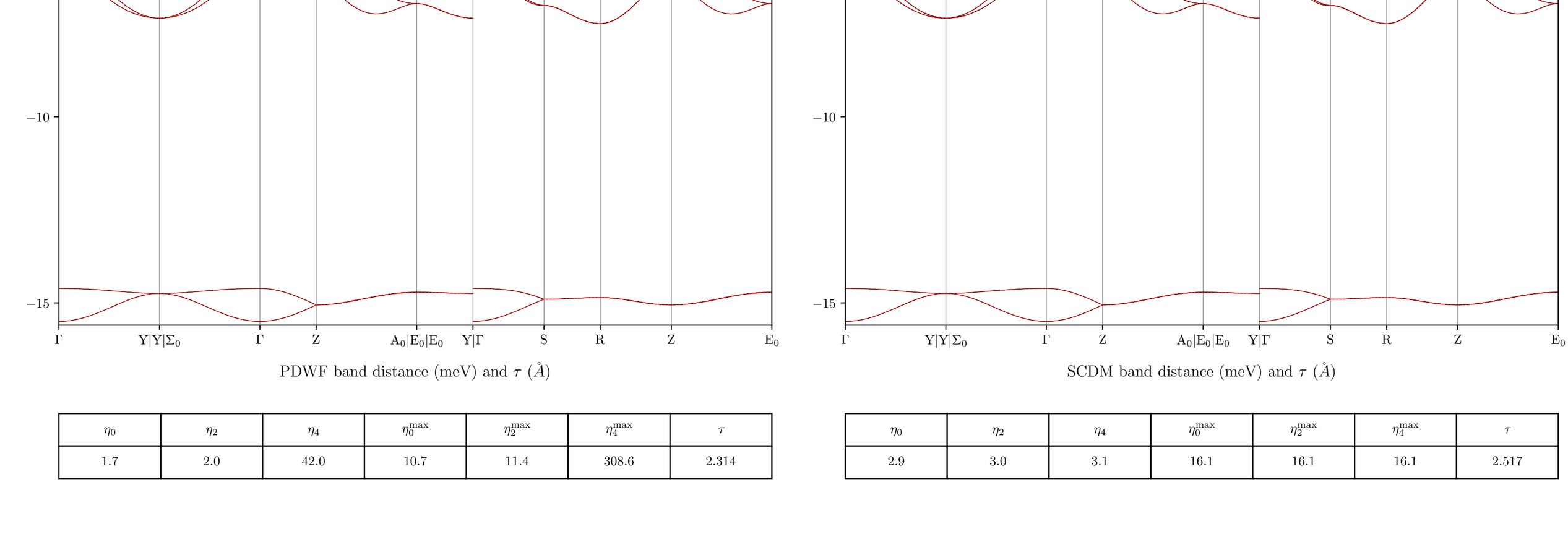
C4Mg2 exclude semicore
PW=5e0a0be1-f706-4fa0-a8e5-791856288039
W90=aa594d30-9817-49f9-954b-5eaed63570b8



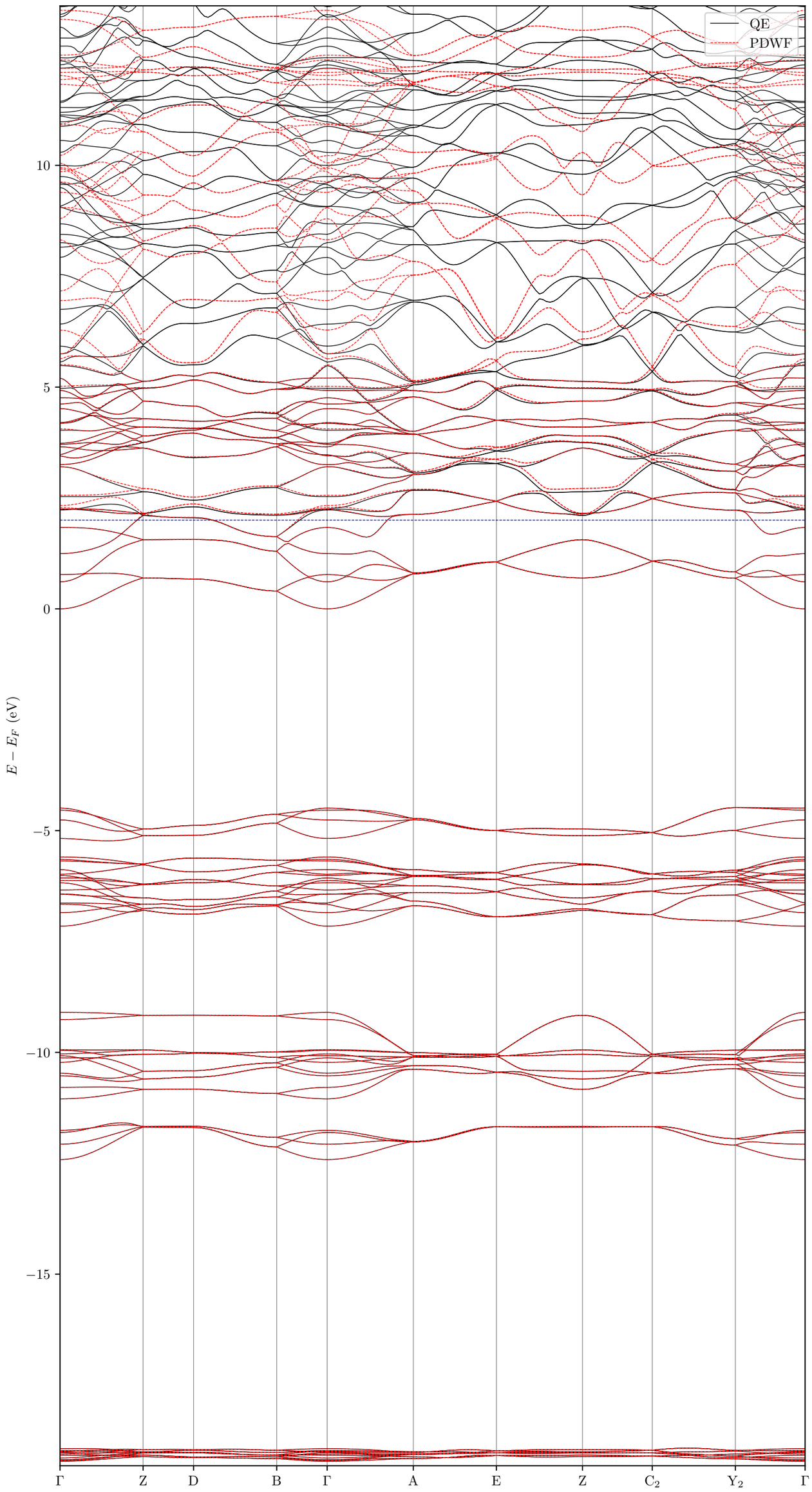

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.9 | 3.0 | 3.1 | 16.1 | 16.1 | 16.1 | 2.517 |

Hamiltonian decay



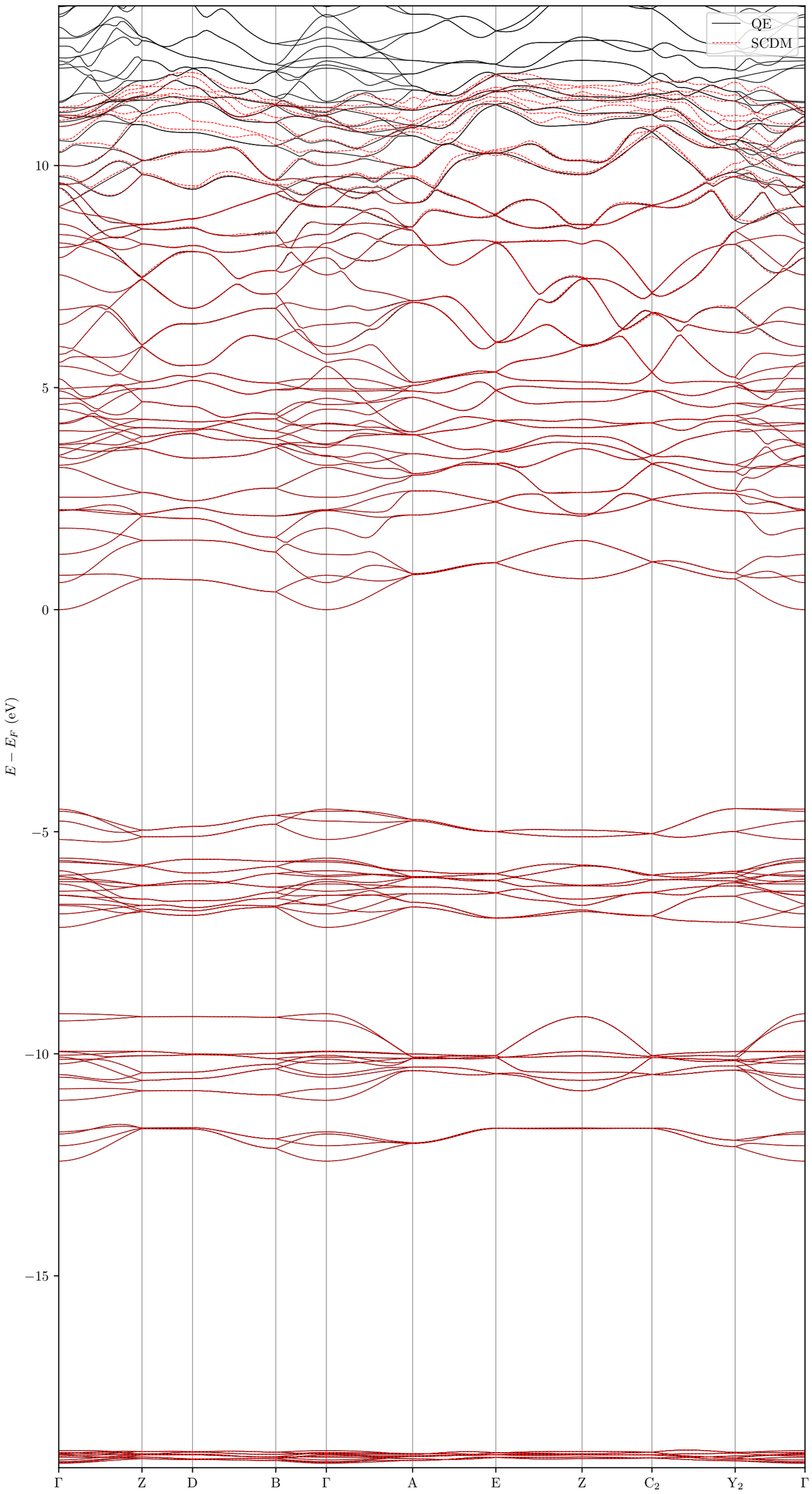
C4O12Sr4 exclude semicore
PW=ca067651-9d37-4d44-a0a0-238959ae1ce6
W90=ba33ad46-233b-4d48-b905-45459dd5213e




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 0.3 | 1.9 | 1.9 | 1.9 | 2.481 |

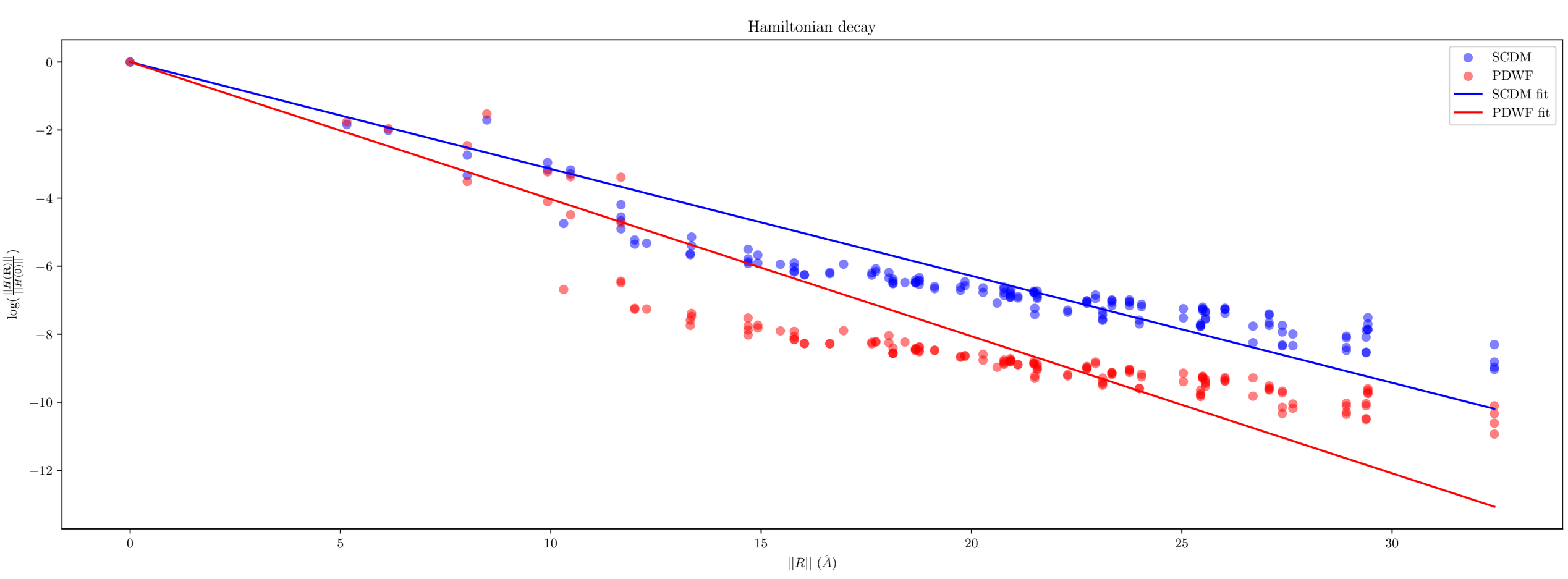
C4O12Sr4 exclude semicore
PW=ca067651-9d37-4d44-a0a0-238959ae1ce6
W90=585d24e8-48e6-4024-8327-0c1b910b2a62

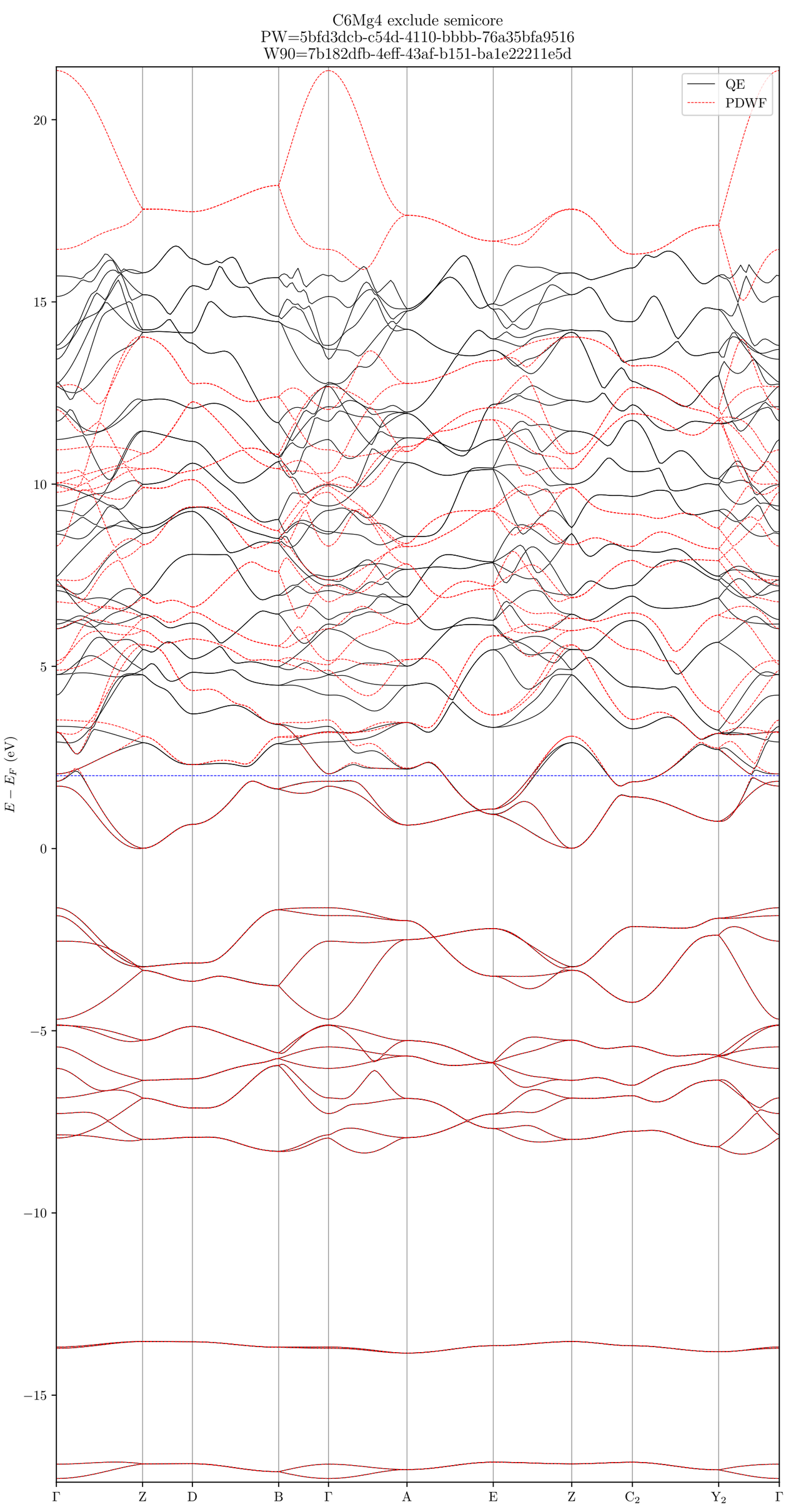



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.2 | 1.2 | 7.9 | 7.9 | 7.9 | 3.182 |

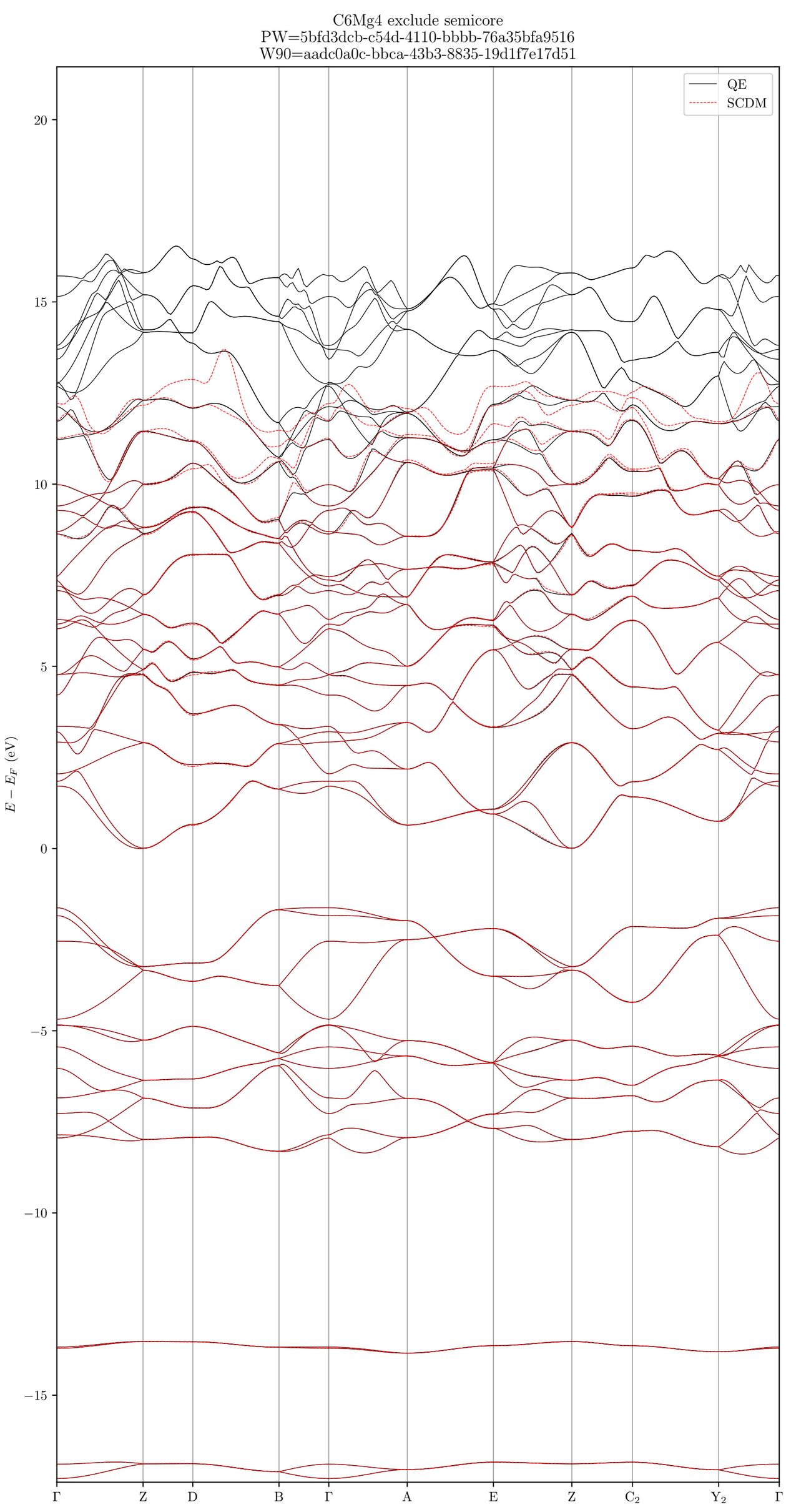
Hamiltonian decay





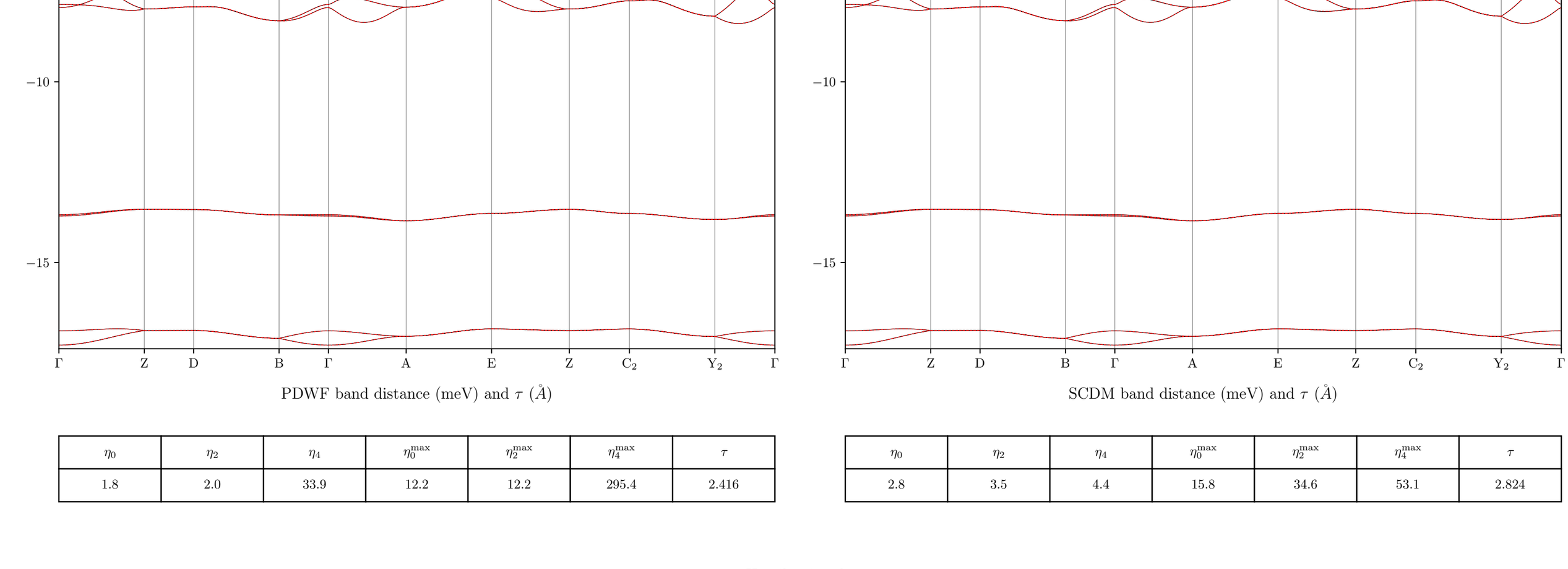

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.8 | 2.0 | 33.9 | 12.2 | 12.2 | 295.4 | 2.416 |

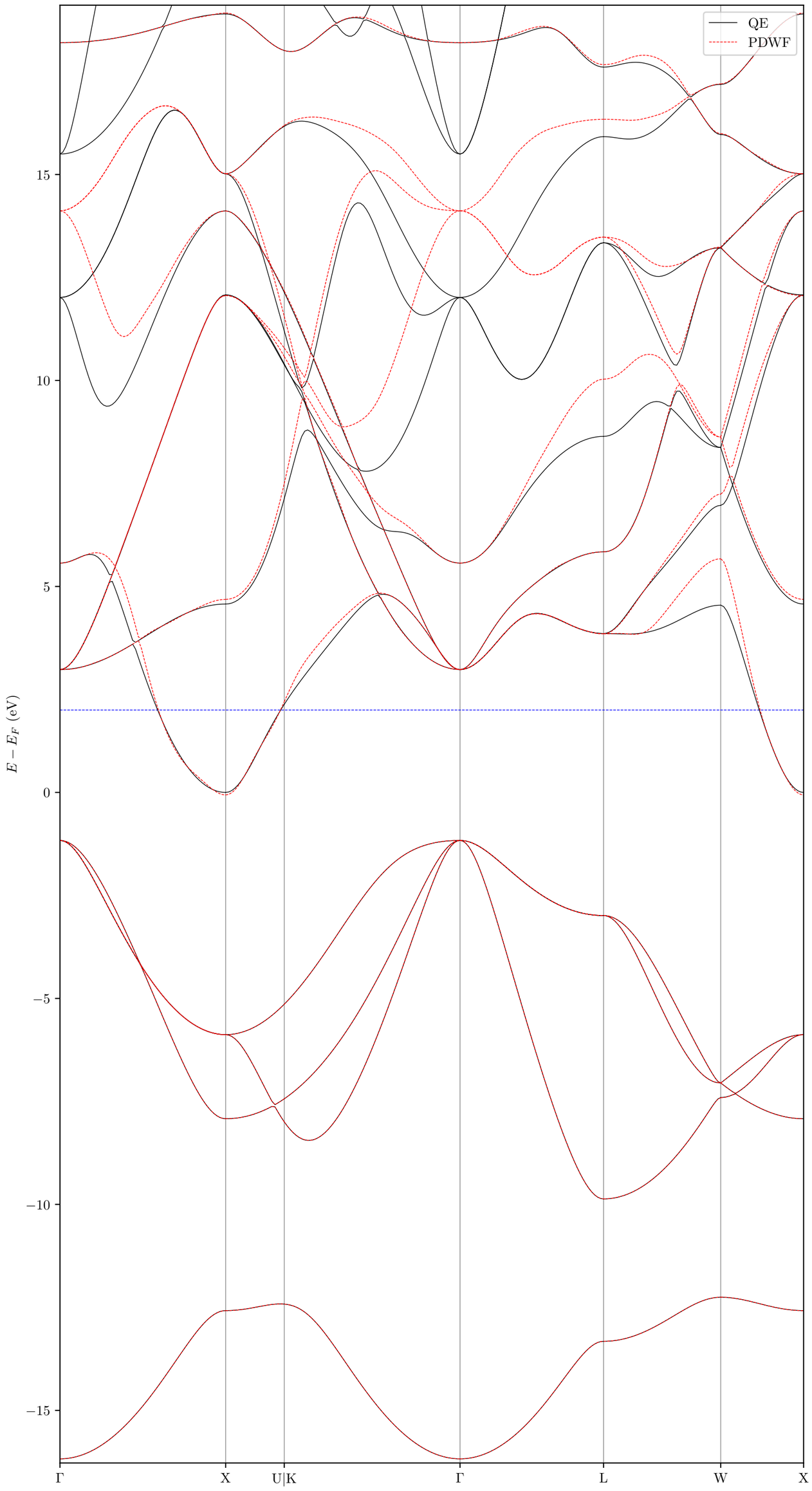



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.8 | 3.5 | 4.4 | 15.8 | 34.6 | 53.1 | 2.824 |



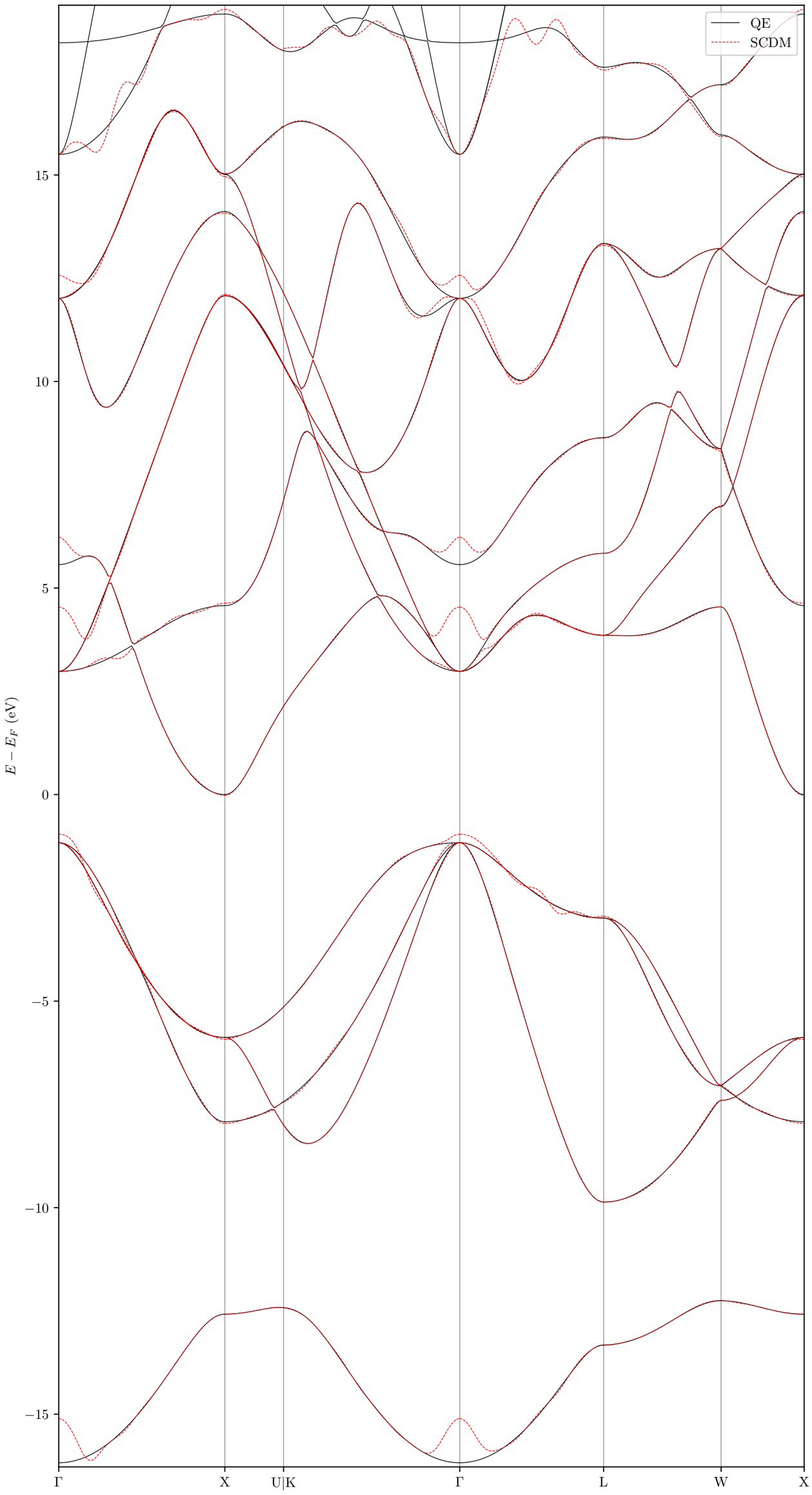
CBe2 exclude semicore
PW=5ea35b82-feb8-49ff-827b-5cf242b975b7
W90=a5717d72-30cb-410f-aa4e-bc10fdcf11fe




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

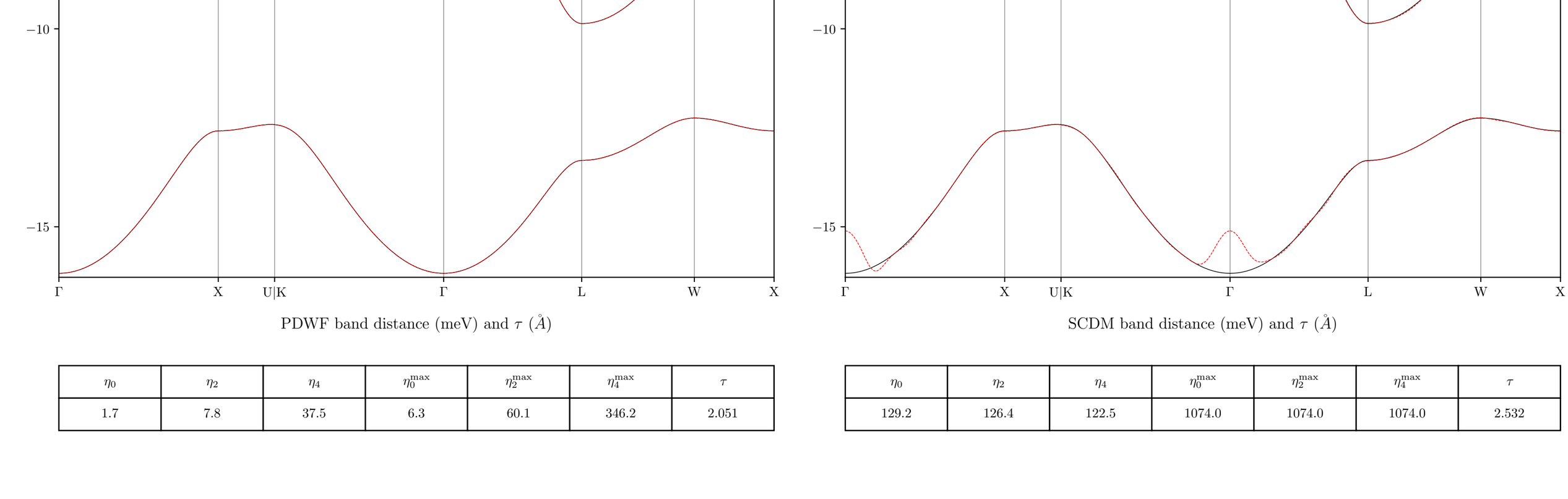
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.7 | 7.8 | 37.5 | 6.3 | 60.1 | 346.2 | 2.051 |

CBe2 exclude semicore
PW=5ea35b82-feb8-49ff-827b-5cf242b975b7
W90=5bd3a5cb-480e-412f-b528-35737e0bca64

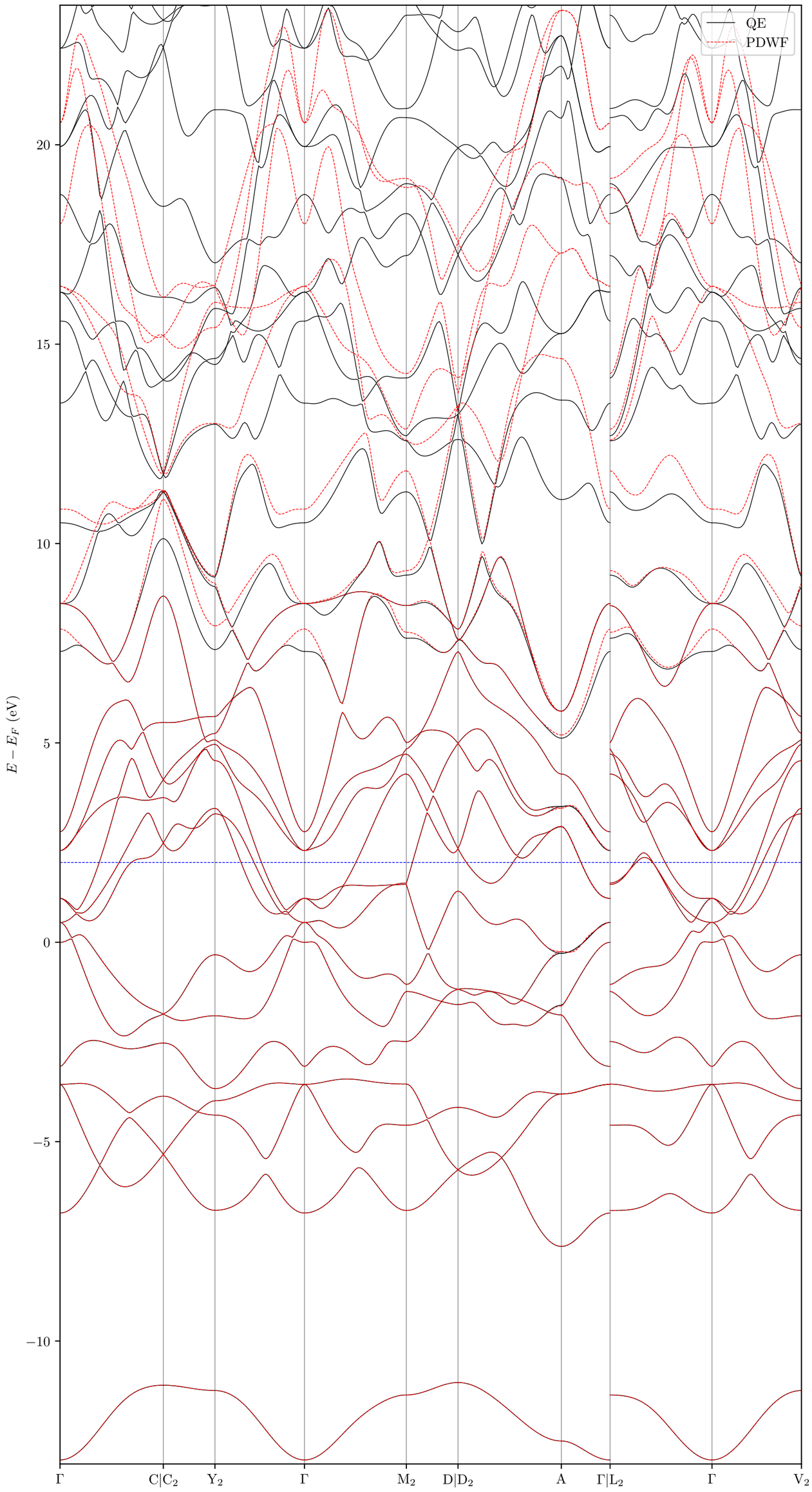



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 129.2 | 126.4 | 122.5 | 1074.0 | 1074.0 | 1074.0 | 2.532 |



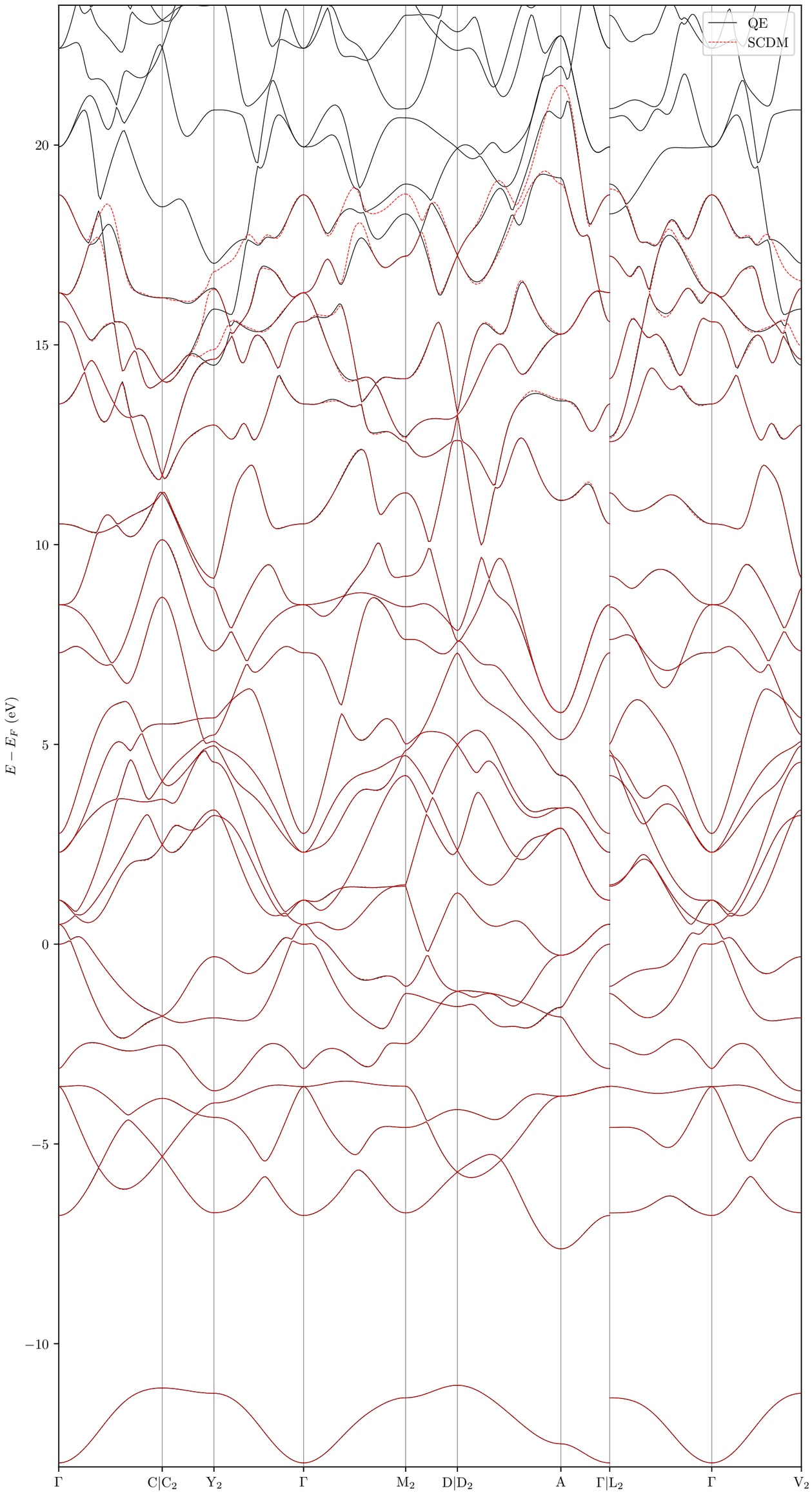
CTa2 exclude semicore
PW=1435f48c-cd25-4993-9c3b-cca0c45fb59d
W90=c042eee4-c3a1-4004-93c3-adddddffd6bf




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.1 | 4.2 | 5.0 | 40.4 | 43.6 | 43.6 | 1.994 |

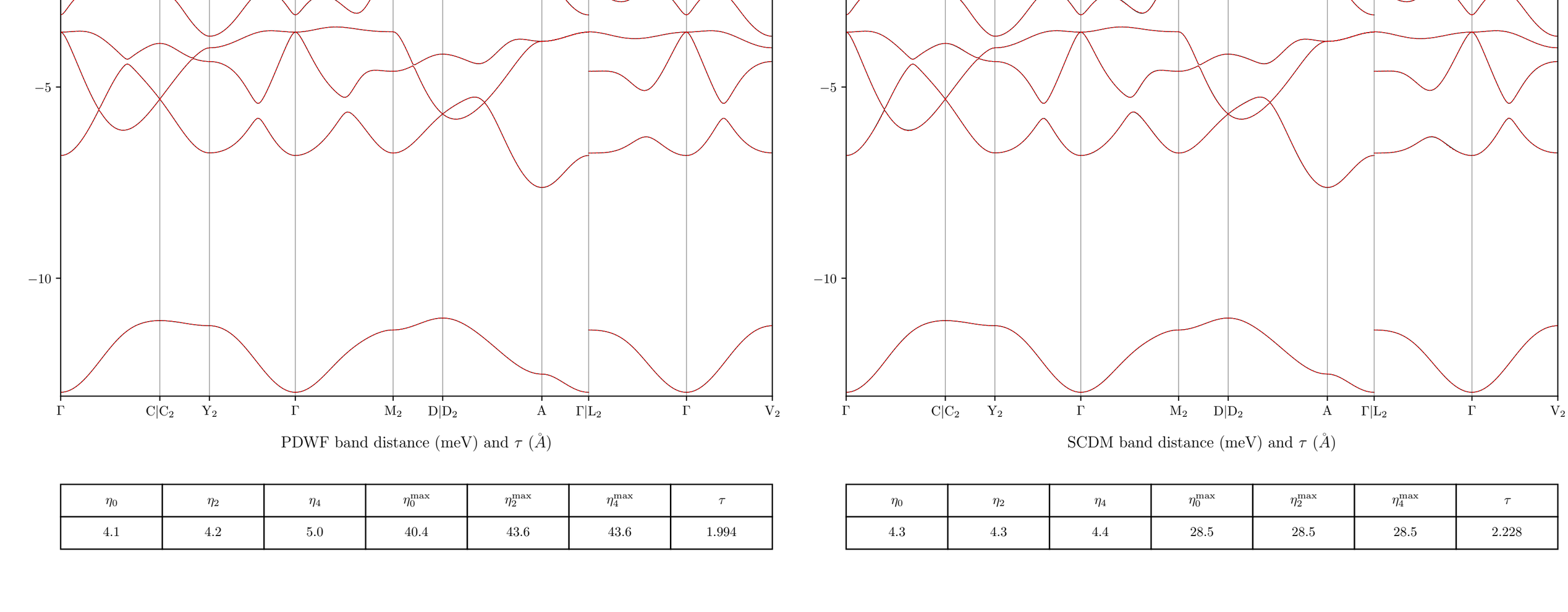
CTa2 exclude semicore
PW=1435f48c-cd25-4993-9c3b-cca0c45fb59d
W90=330f3ea5-73b6-4cfa-a7ea-689487753be1



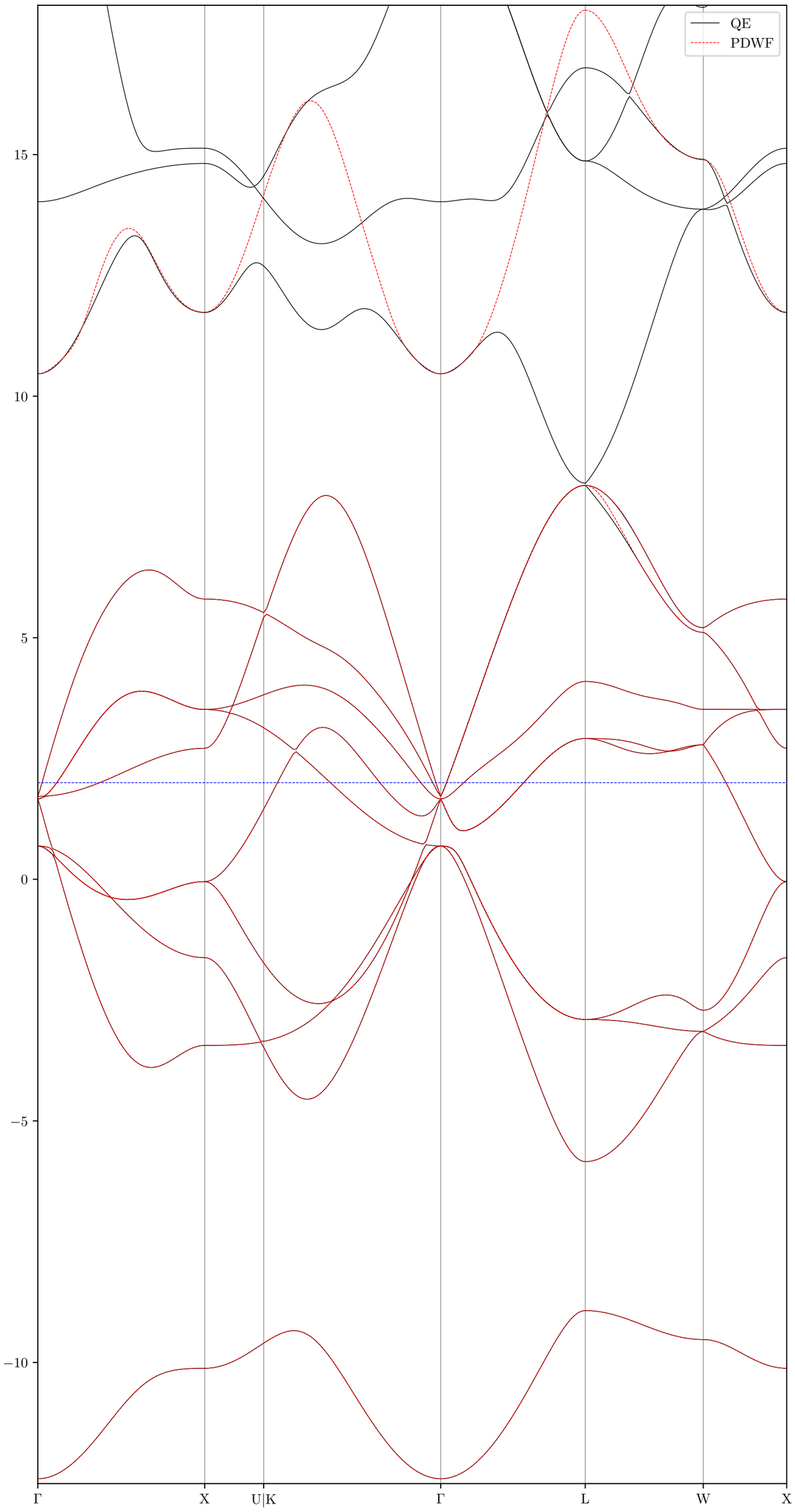

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.3 | 4.3 | 4.4 | 28.5 | 28.5 | 28.5 | 2.228 |

Hamiltonian decay



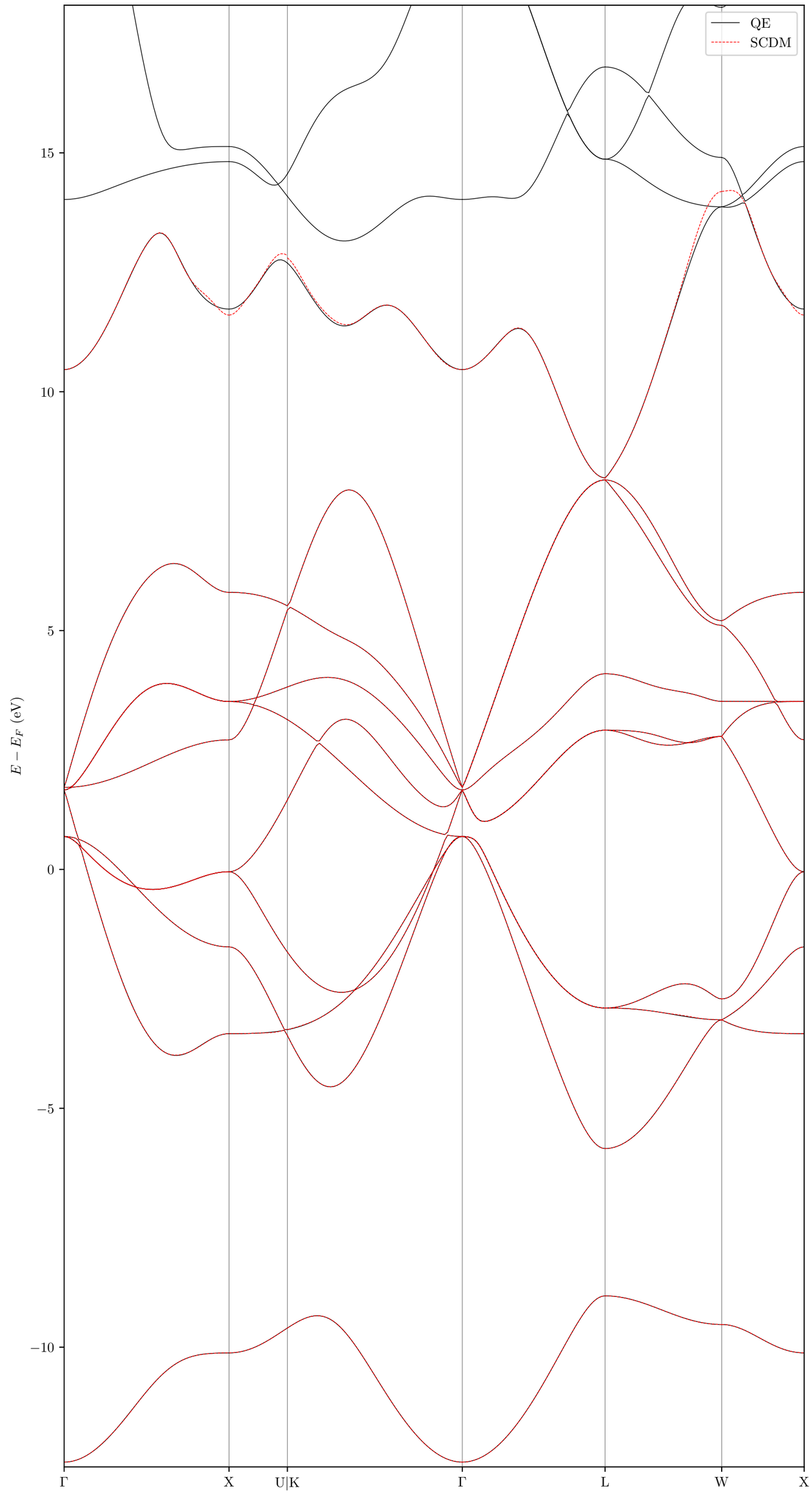
CTi exclude semicore
PW=234b1e48-299e-4a1a-b7f6-b7a3b41ac36b
W90=29d1b844-cf96-4fa1-af43-237dfbf0ffb9




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 0.6 | 0.7 | 2.5 | 2.6 | 5.1 | 1.759 |

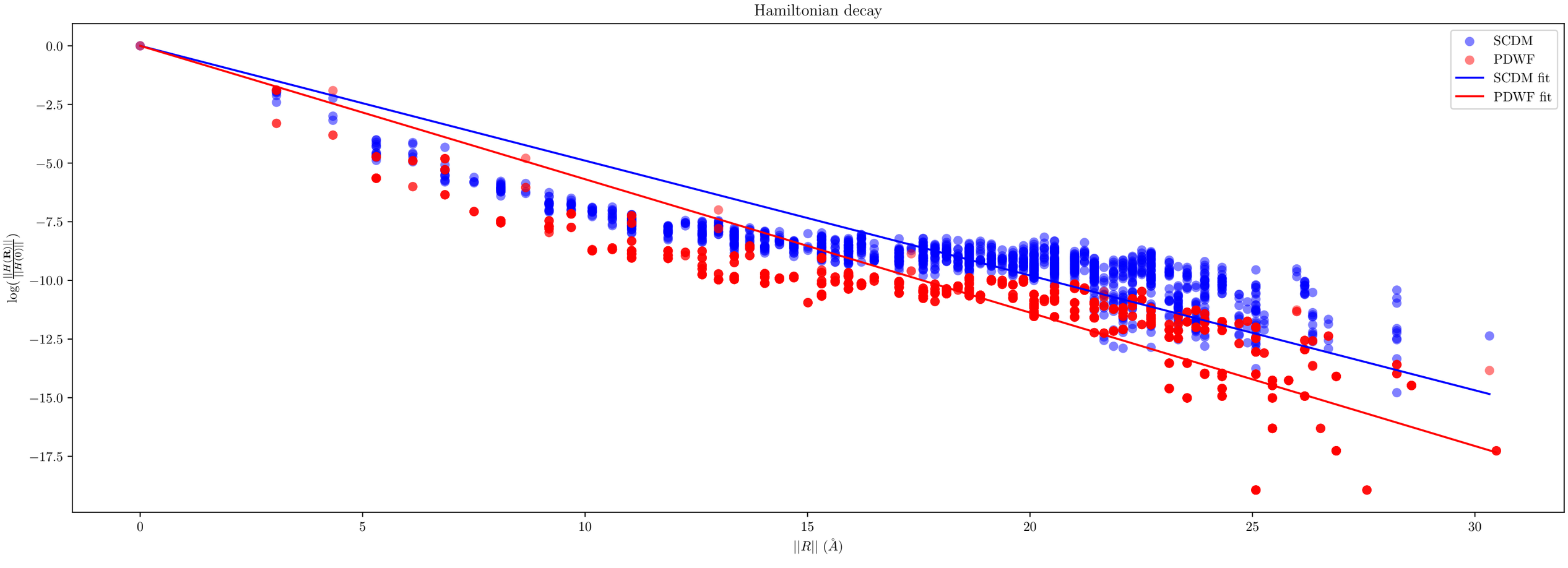
CTi exclude semicore
PW=234b1e48-299e-4a1a-b7f6-b7a3b41ac36b
W90=1384026e-4897-40a4-acca-47af369bd652



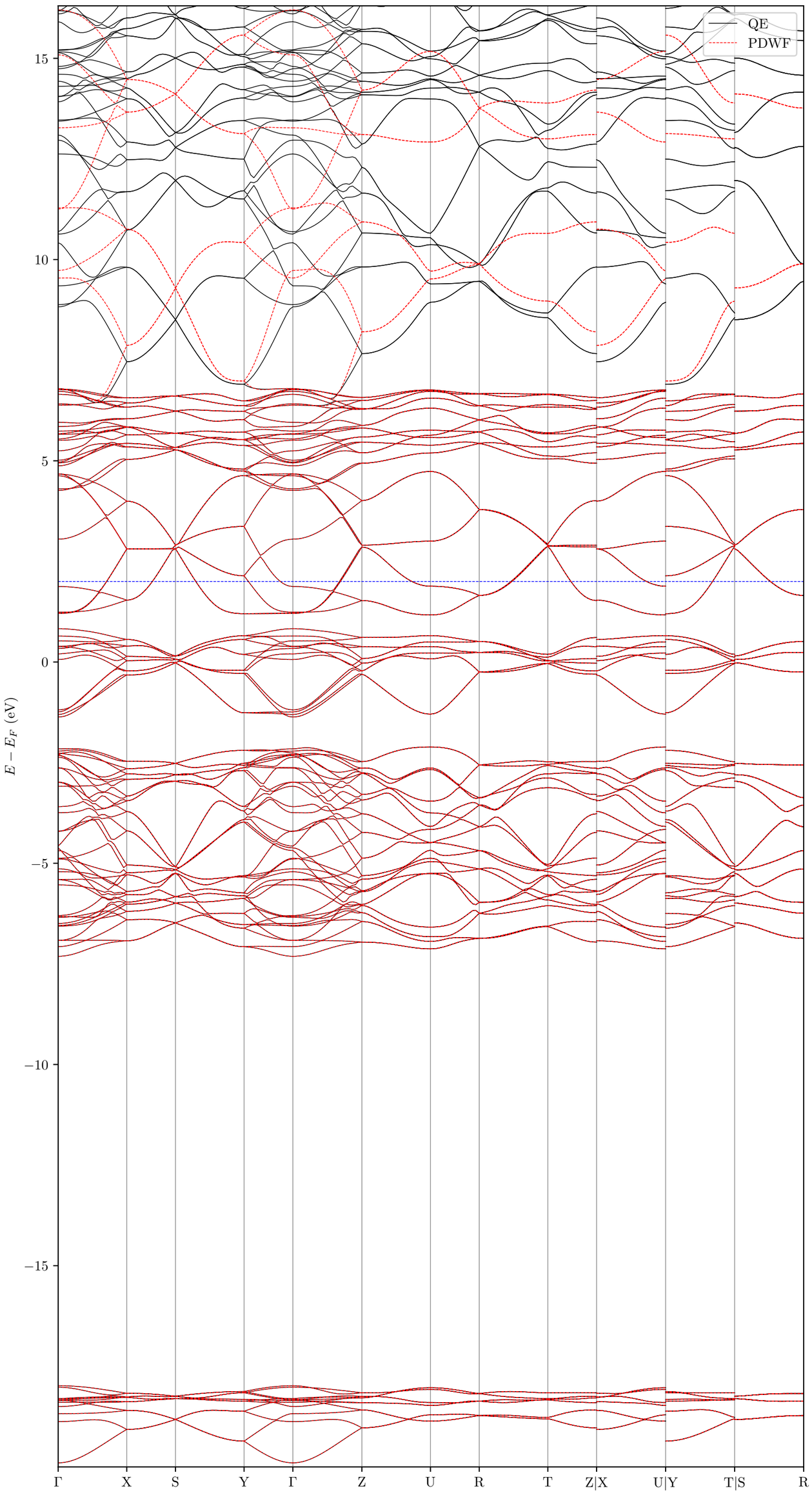

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.3 | 2.0 | 1.7 | 13.0 | 13.0 | 13.0 | 2.043 |

Hamiltonian decay



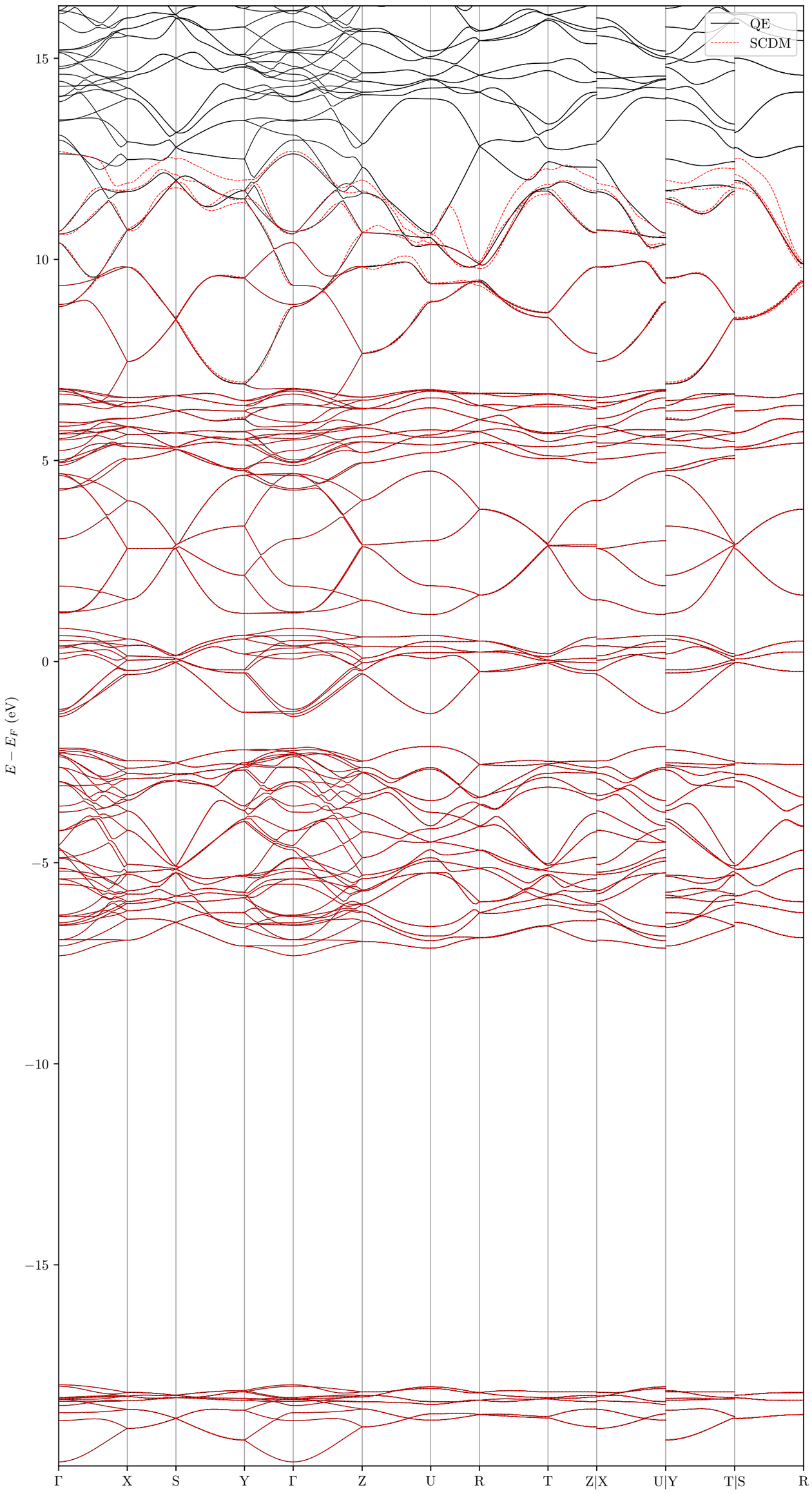
Ca4Cr4O12 exclude semicore
PW=a2527579-7c19-434d-9212-5f3afab4d4b0
W90=6bbf348d-ee67-492b-97af-a8a4a0261e12




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.1 | 0.1 | 0.9 | 0.9 | 0.9 | 1.751 |

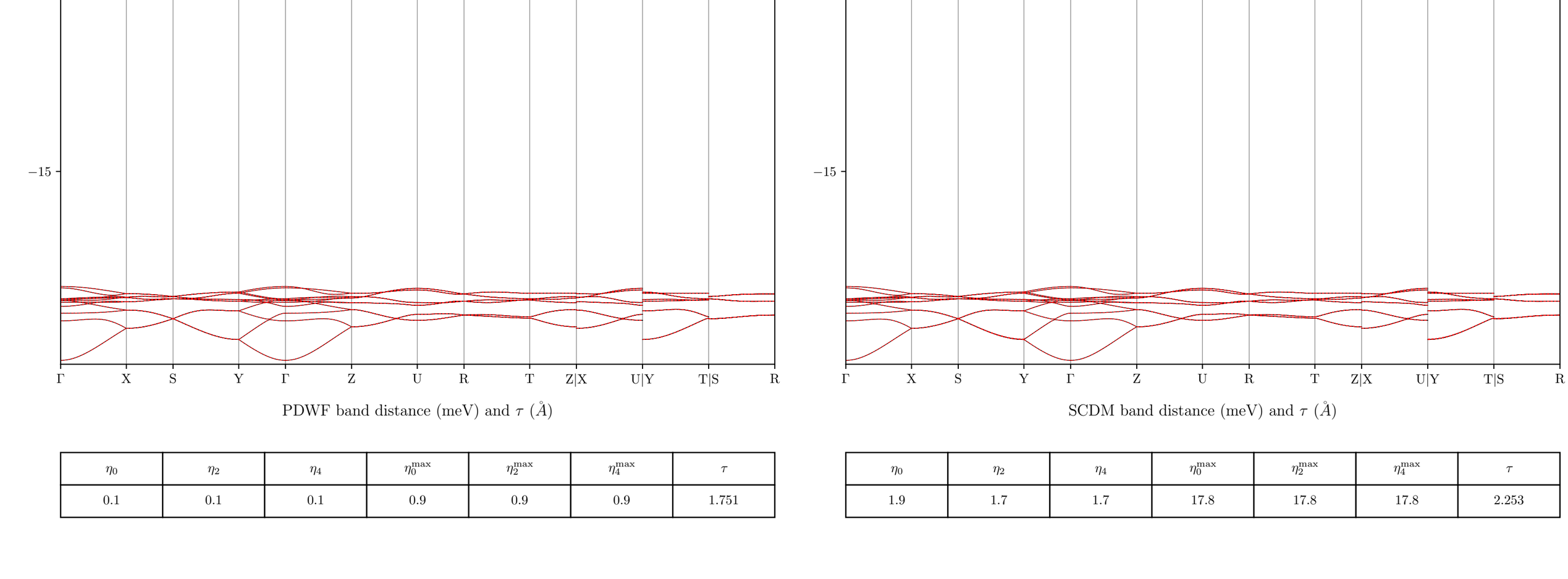
Ca4Cr4O12 exclude semicore
PW=a2527579-7c19-434d-9212-5f3afab4d4b0
W90=609ad657-9052-459d-9796-cd0ec7697d1e



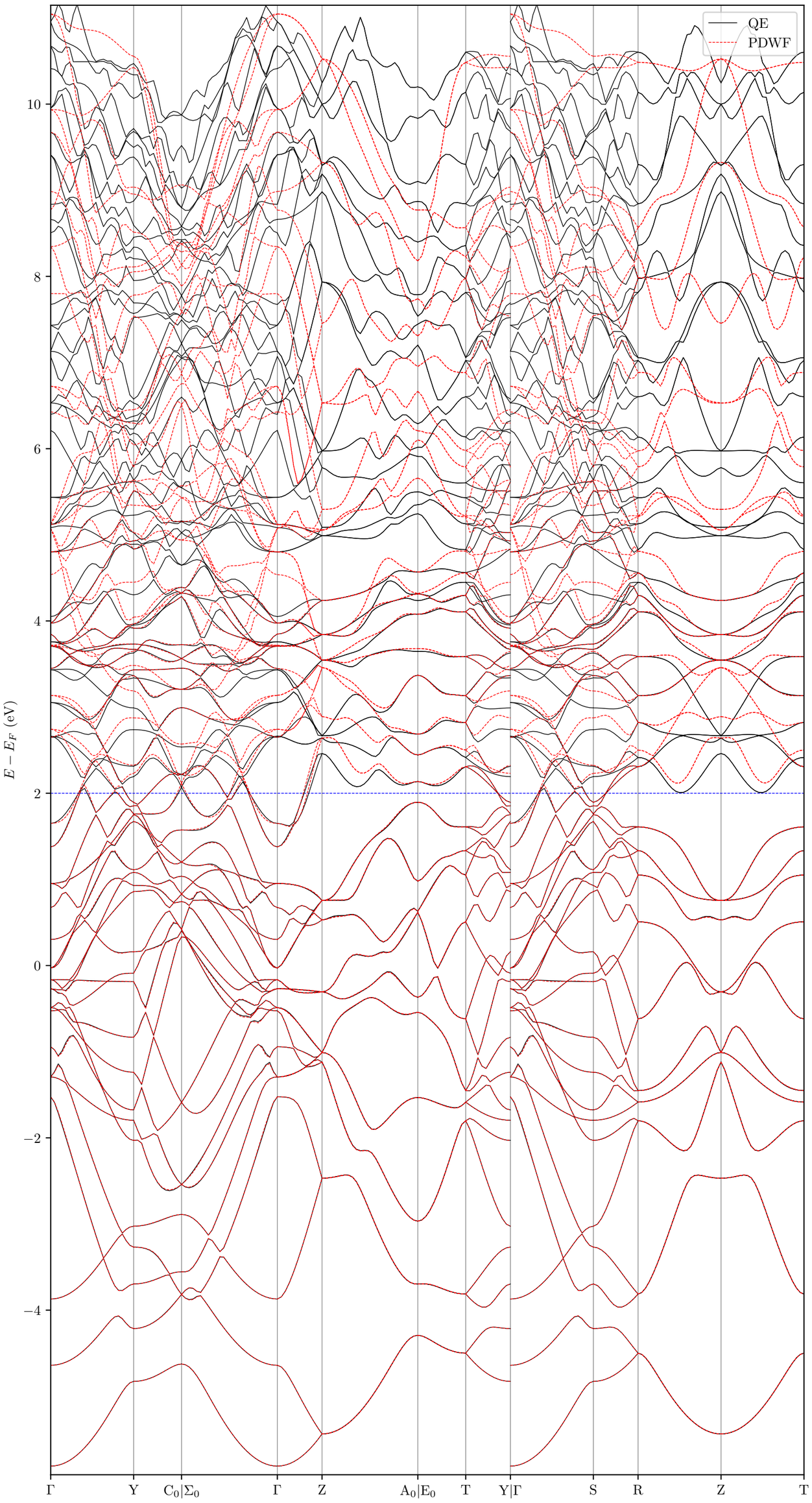

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.9 | 1.7 | 1.7 | 17.8 | 17.8 | 17.8 | 2.253 |

Hamiltonian decay



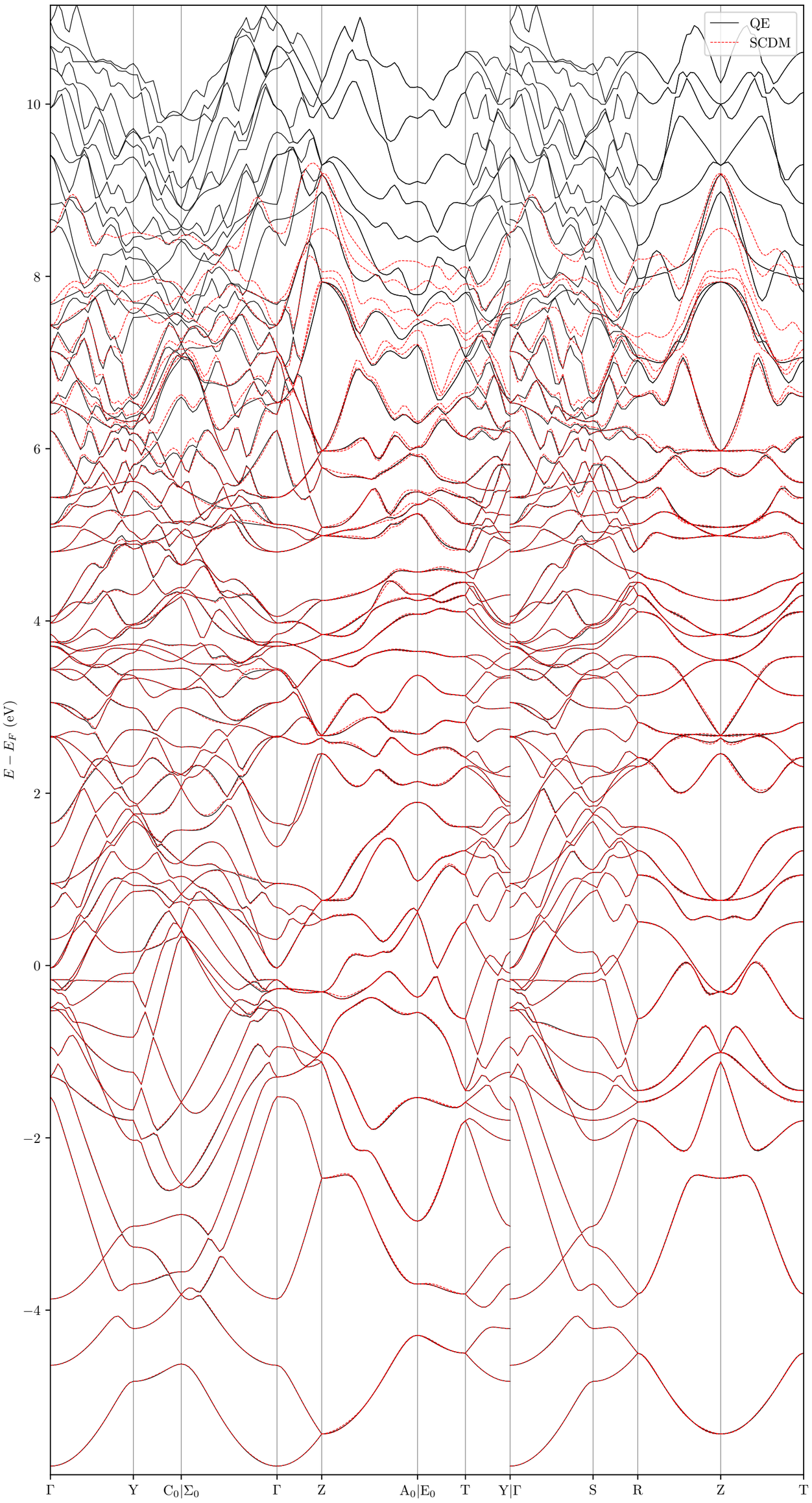
Ca4Mg8 exclude semicore
PW=1d849ab7-4497-46b8-95db-1bd69067ccd4
W90=9f1f2eb9-3e82-4bfe-8a74-553c6979dd2b




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.0 | 9.4 | 102.8 | 21.1 | 41.1 | 789.6 | 3.225 |

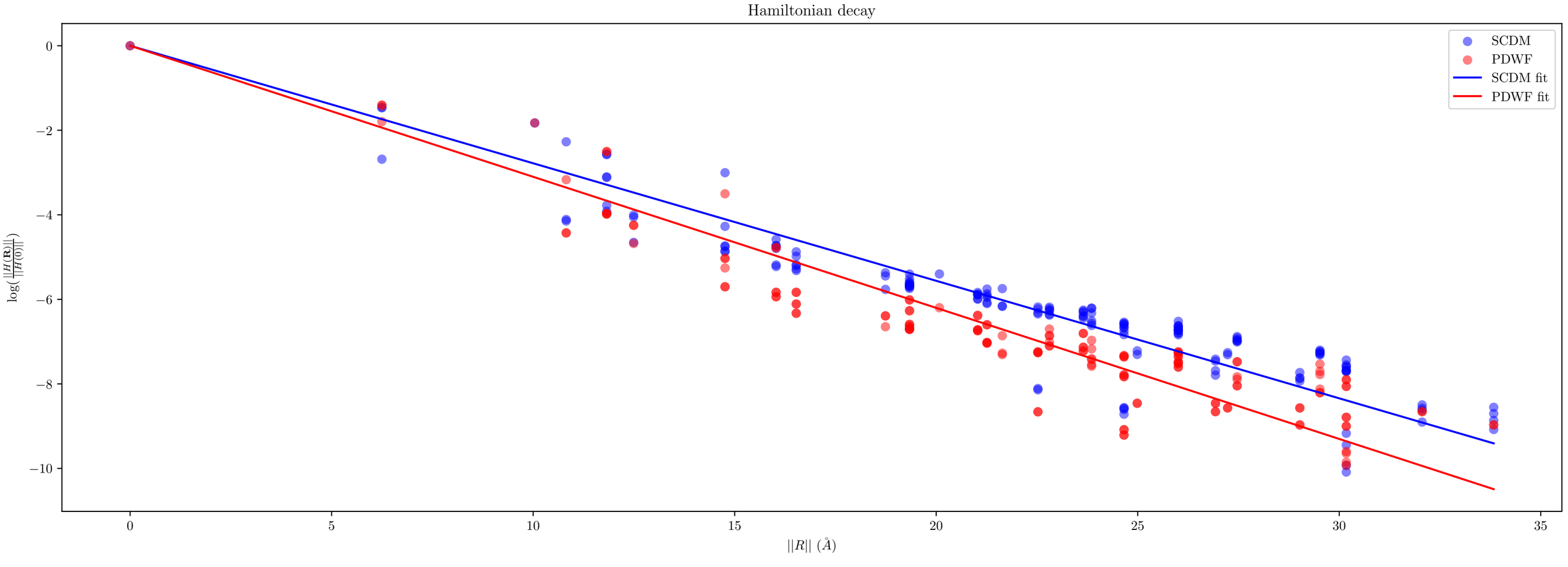
Ca4Mg8 exclude semicore
PW=1d849ab7-4497-46b8-95db-1bd69067ccd4
W90=8dff509f-39d0-49a0-b66a-db6d05e7cc0b

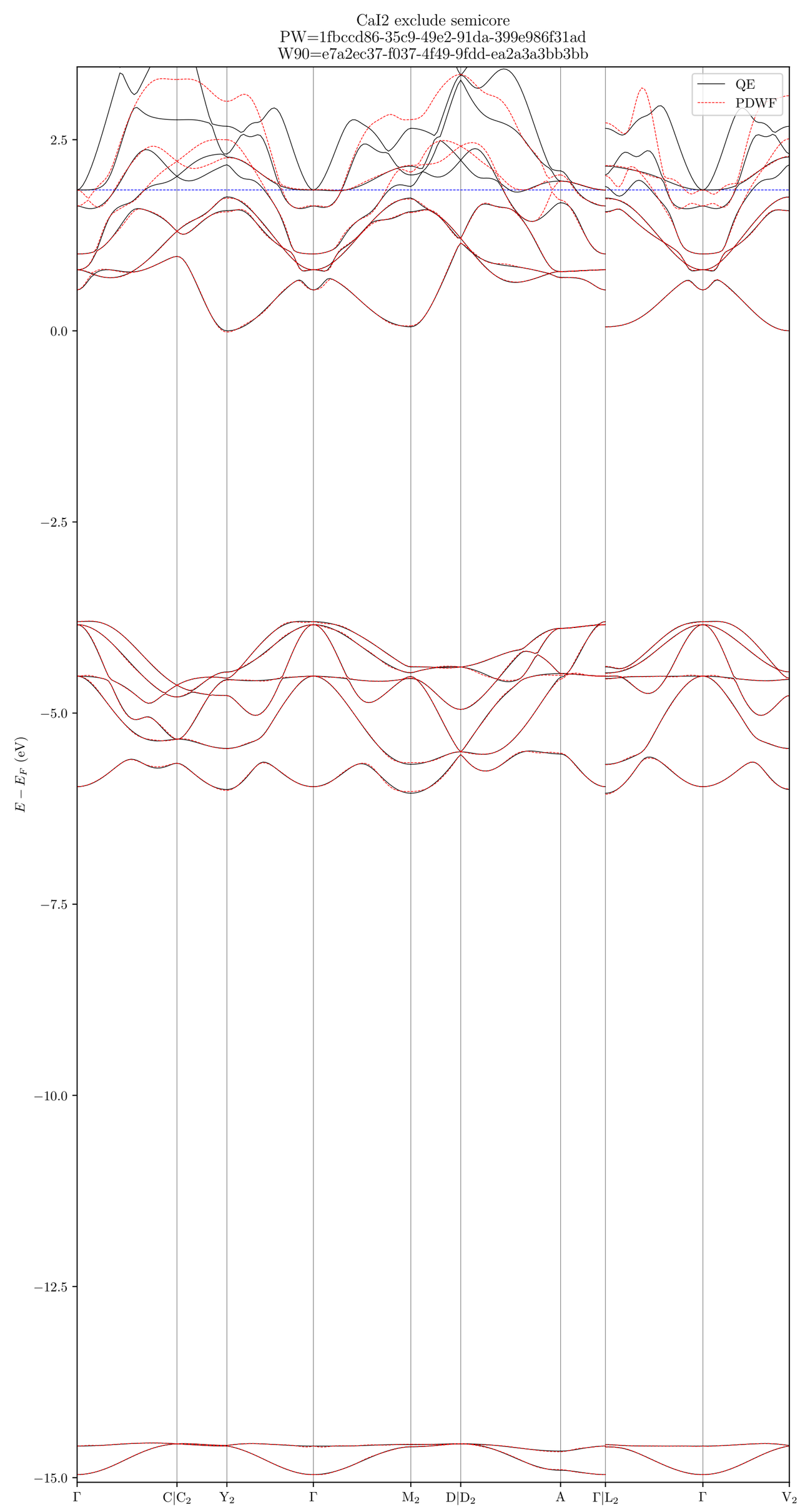



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.6 | 5.7 | 6.1 | 28.0 | 28.8 | 39.4 | 3.597 |

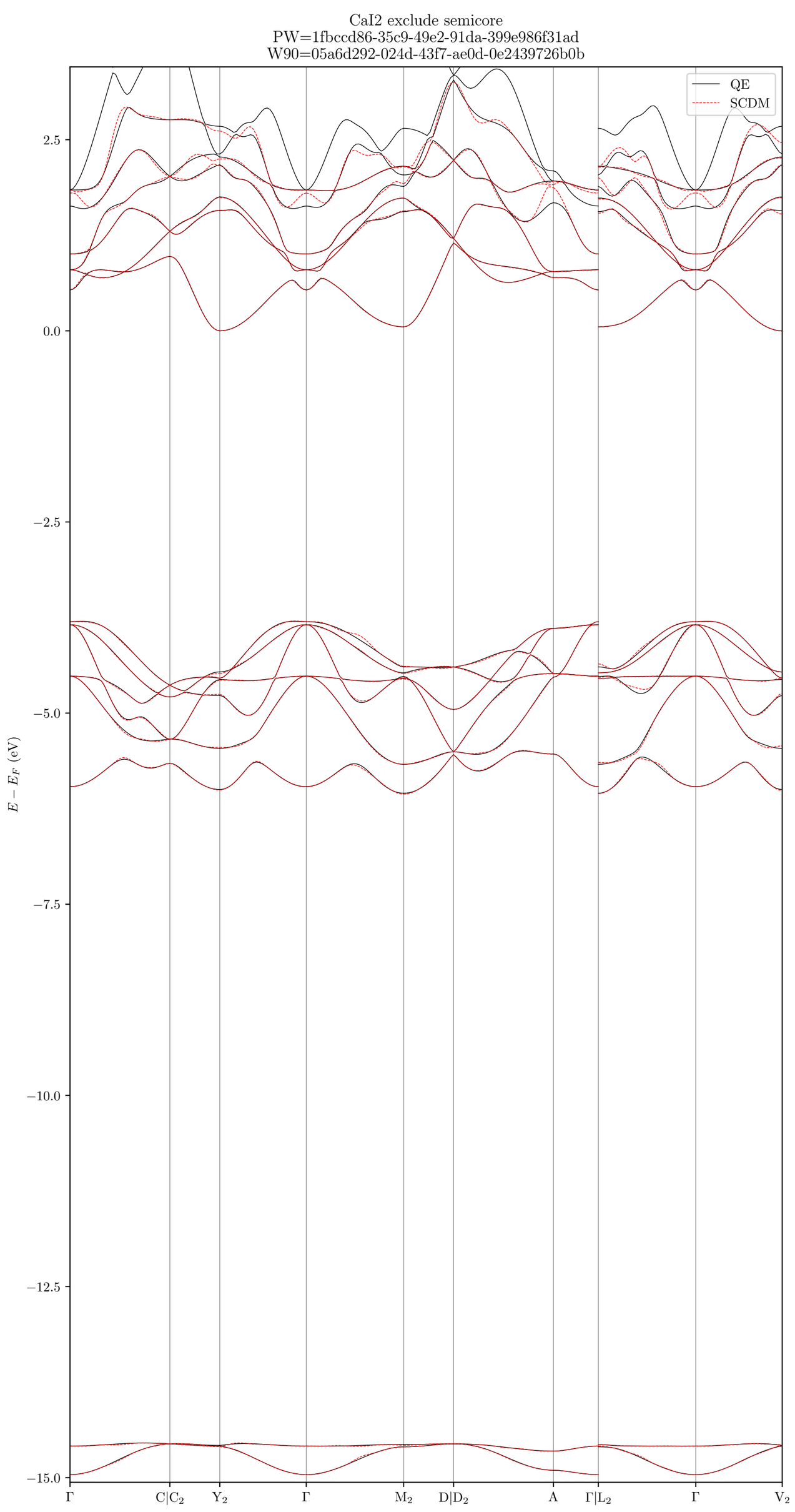
Hamiltonian decay





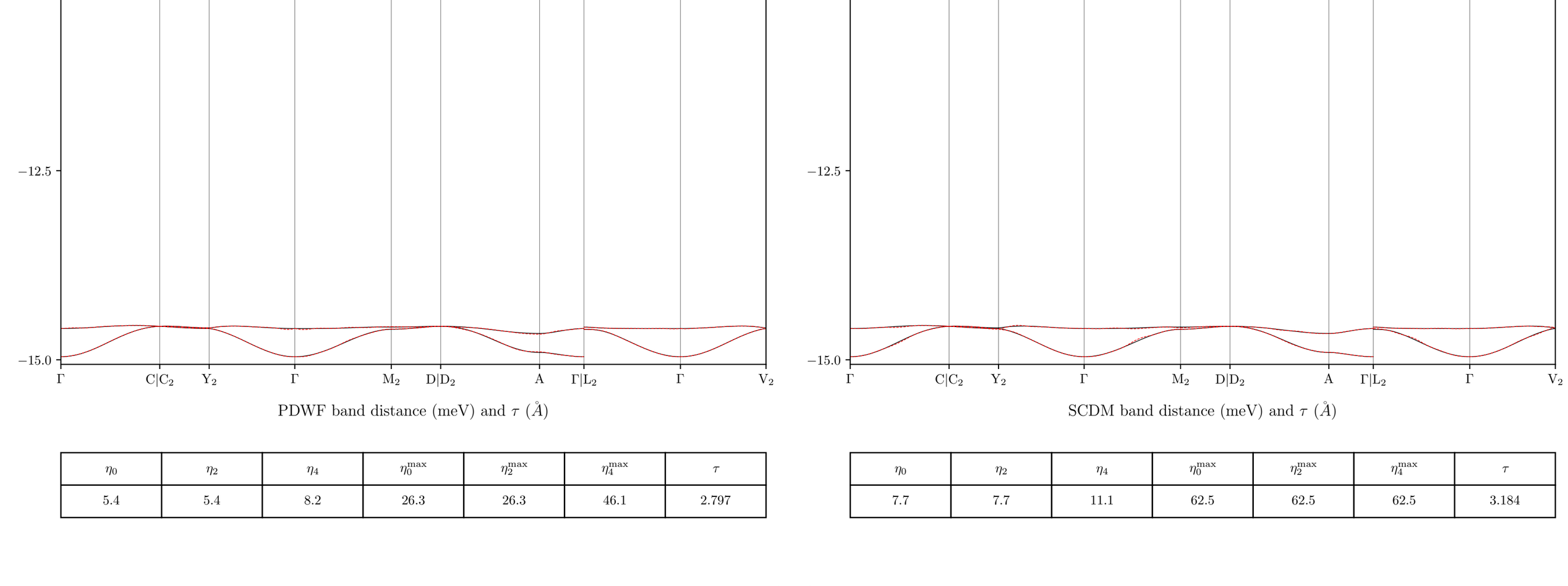

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

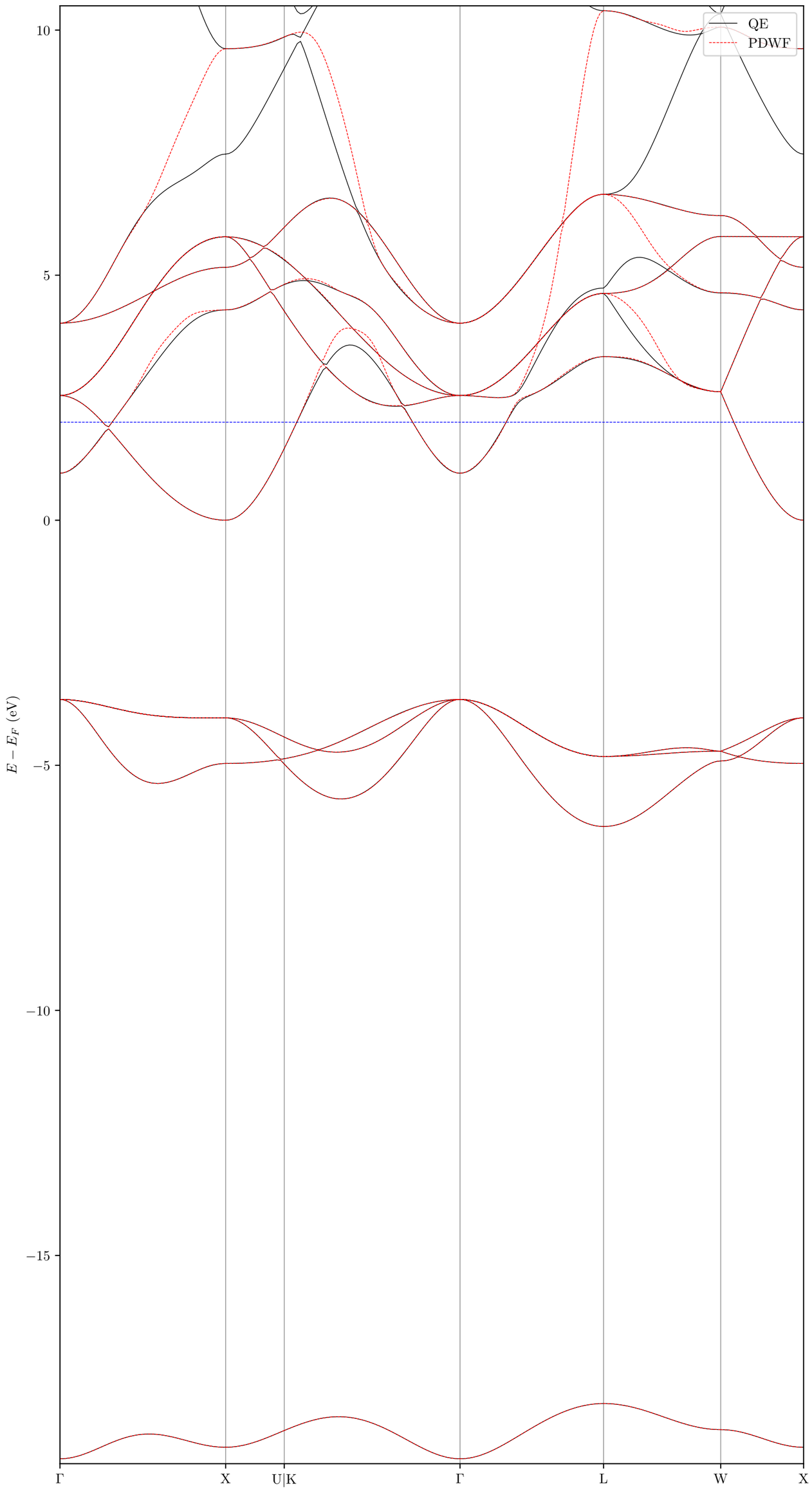
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.4 | 5.4 | 8.2 | 26.3 | 26.3 | 46.1 | 2.797 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

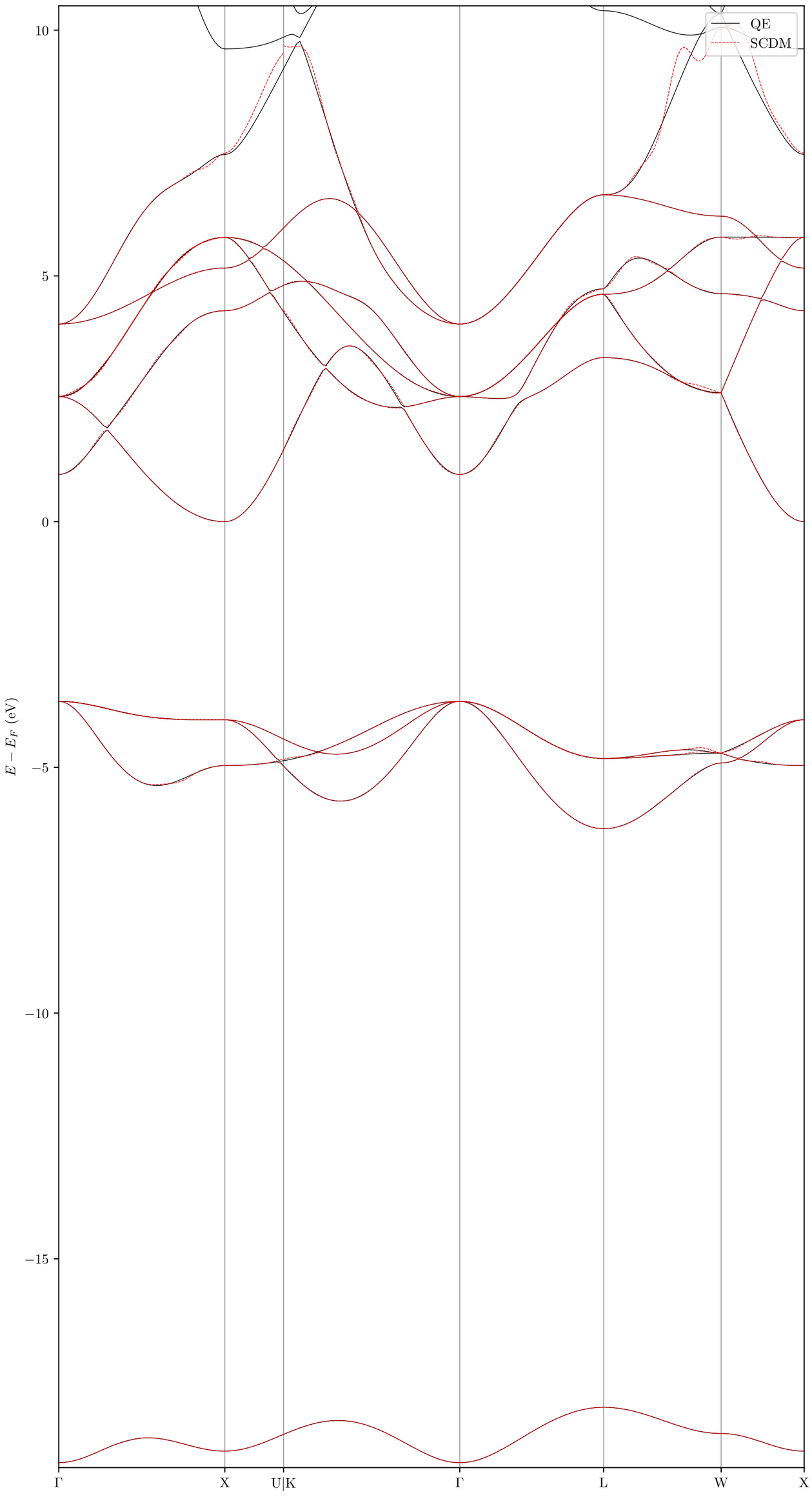
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.7 | 7.7 | 11.1 | 62.5 | 62.5 | 62.5 | 3.184 |





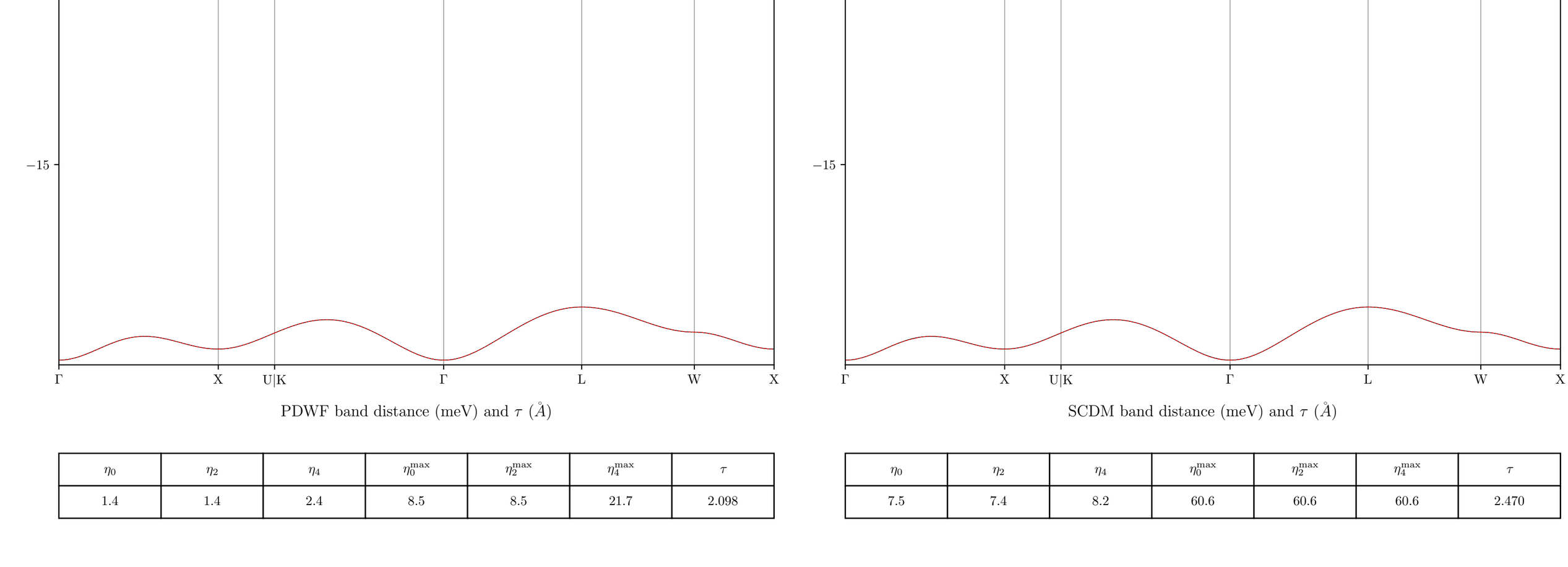

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.4 | 1.4 | 2.4 | 8.5 | 8.5 | 21.7 | 2.098 |

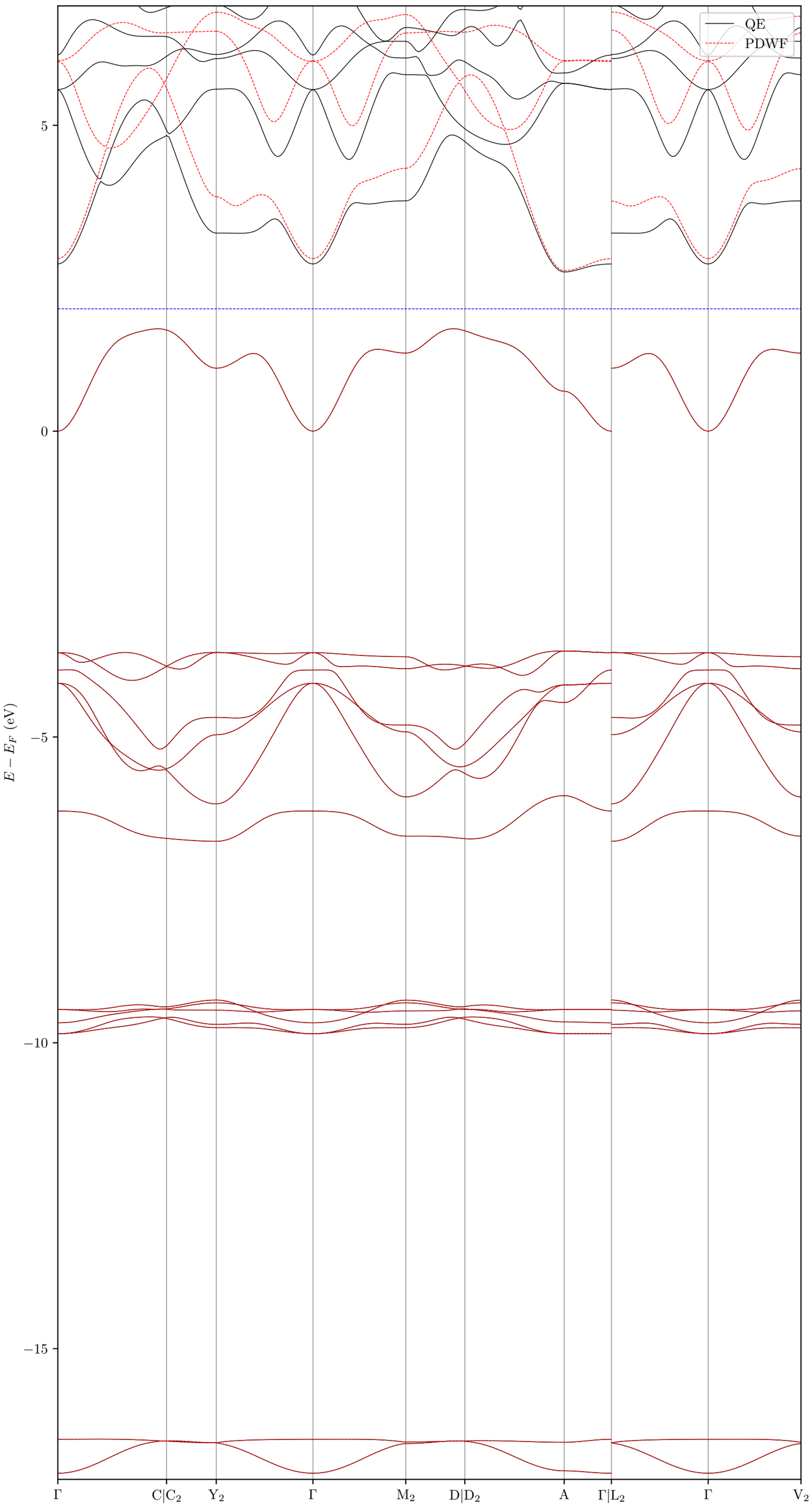



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.5 | 7.4 | 8.2 | 60.6 | 60.6 | 60.6 | 2.470 |



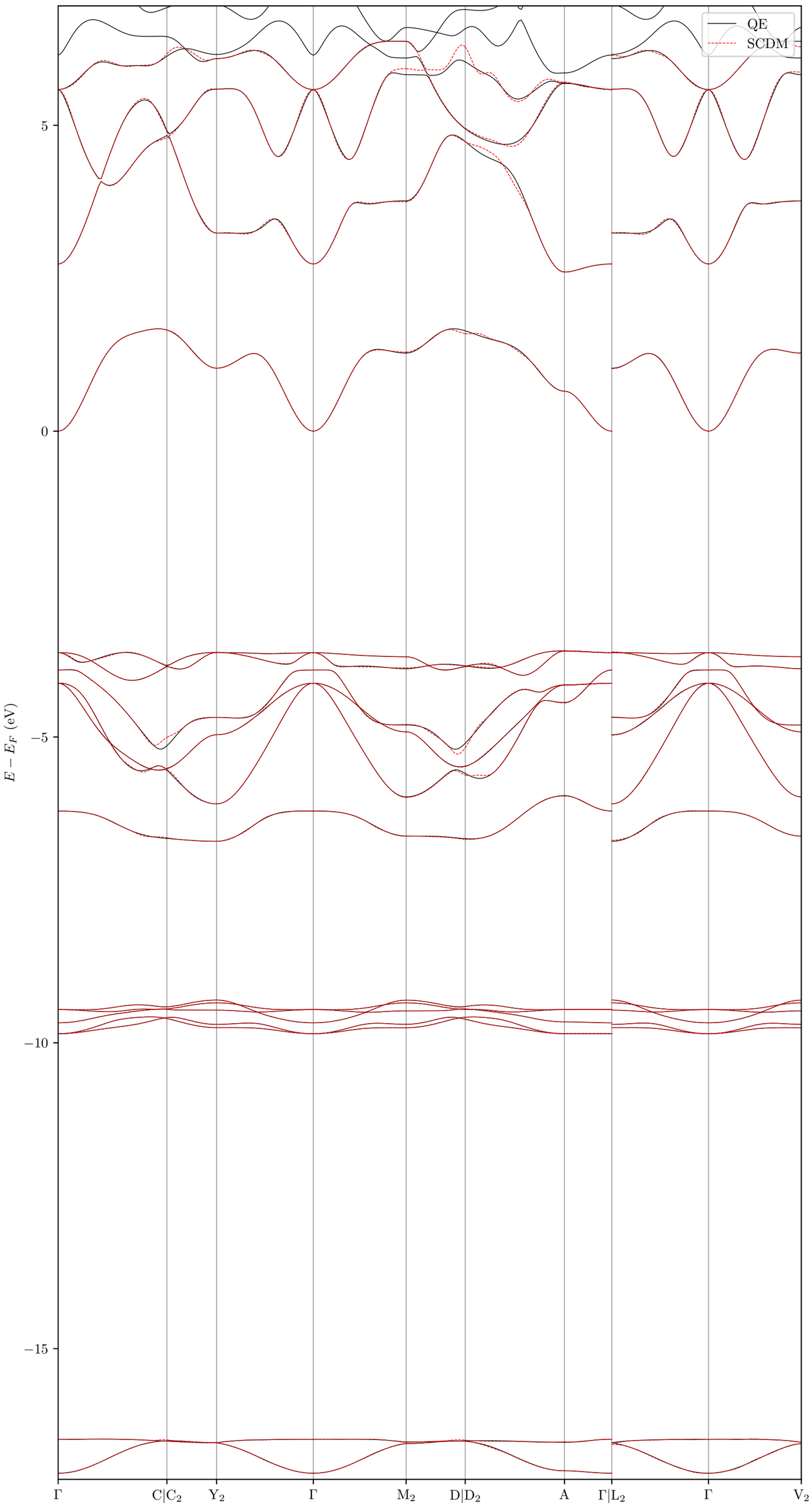
CdCl2 exclude semicore
PW=ae7d3965-255d-4fad-b4e9-8bc33ffe3d39
W90=ac415914-2a70-41b6-8f41-4e5286911bbb




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.4 | 0.4 | 0.5 | 3.0 | 3.0 | 3.0 | 2.226 |

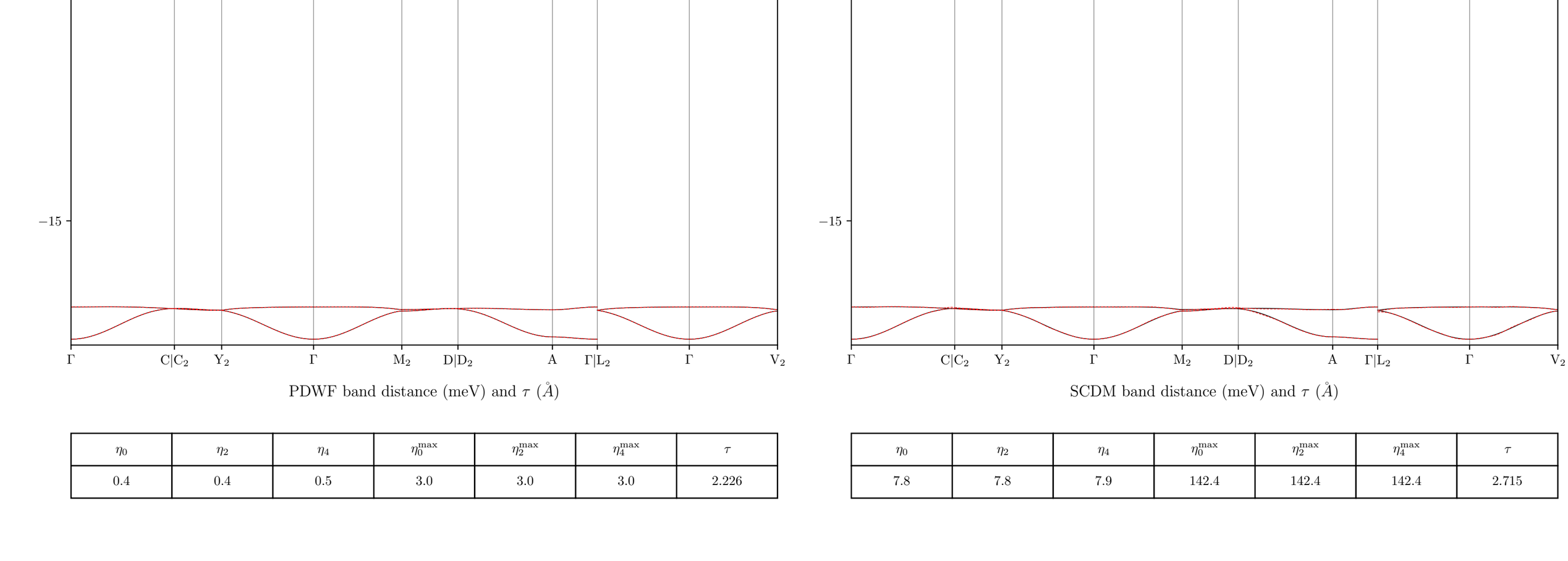
CdCl2 exclude semicore
PW=ae7d3965-255d-4fad-b4e9-8bc33ffe3d39
W90=d2687c98-ab55-42d3-8317-6b596a1a3e6c

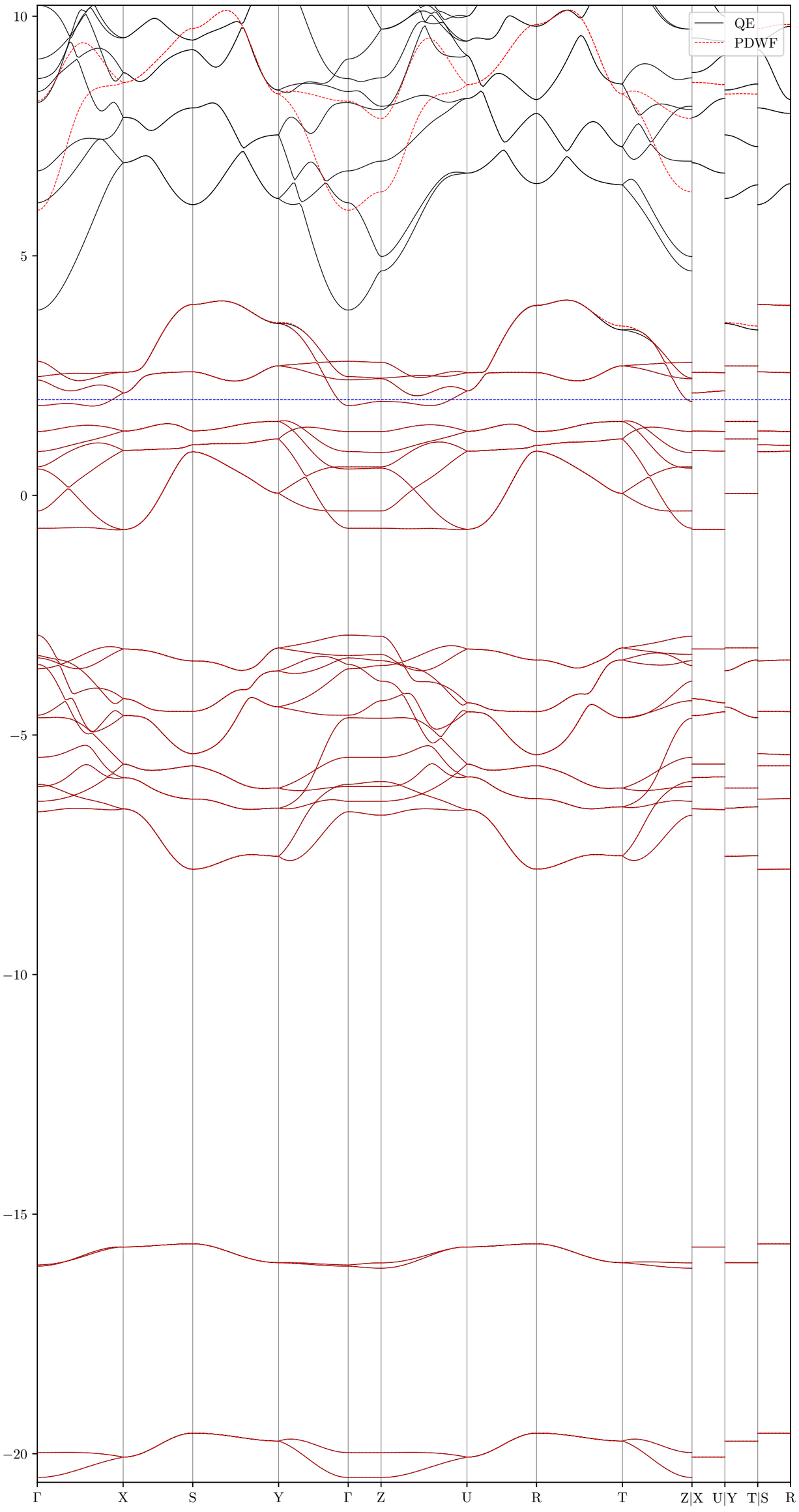



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.8 | 7.8 | 7.9 | 142.4 | 142.4 | 142.4 | 2.715 |

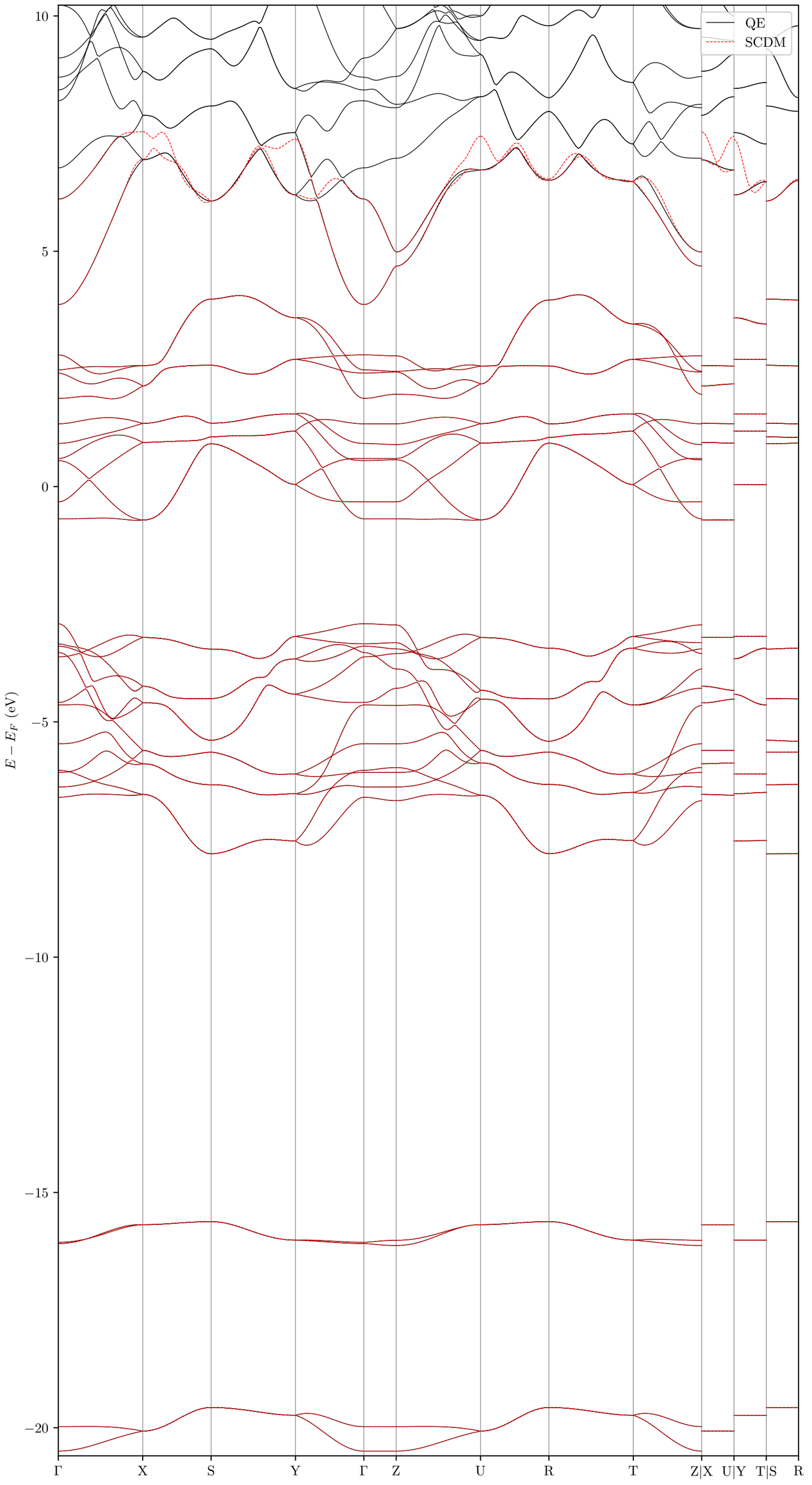
Hamiltonian decay





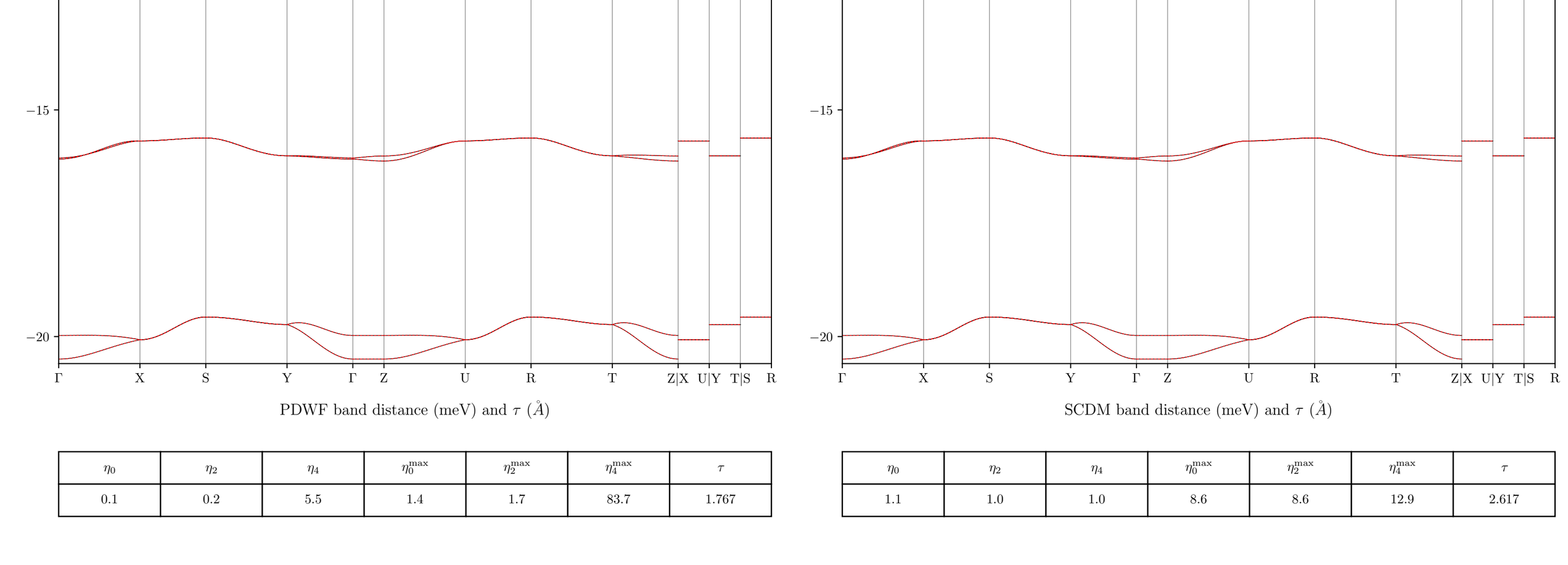

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.2 | 5.5 | 1.4 | 1.7 | 83.7 | 1.767 |

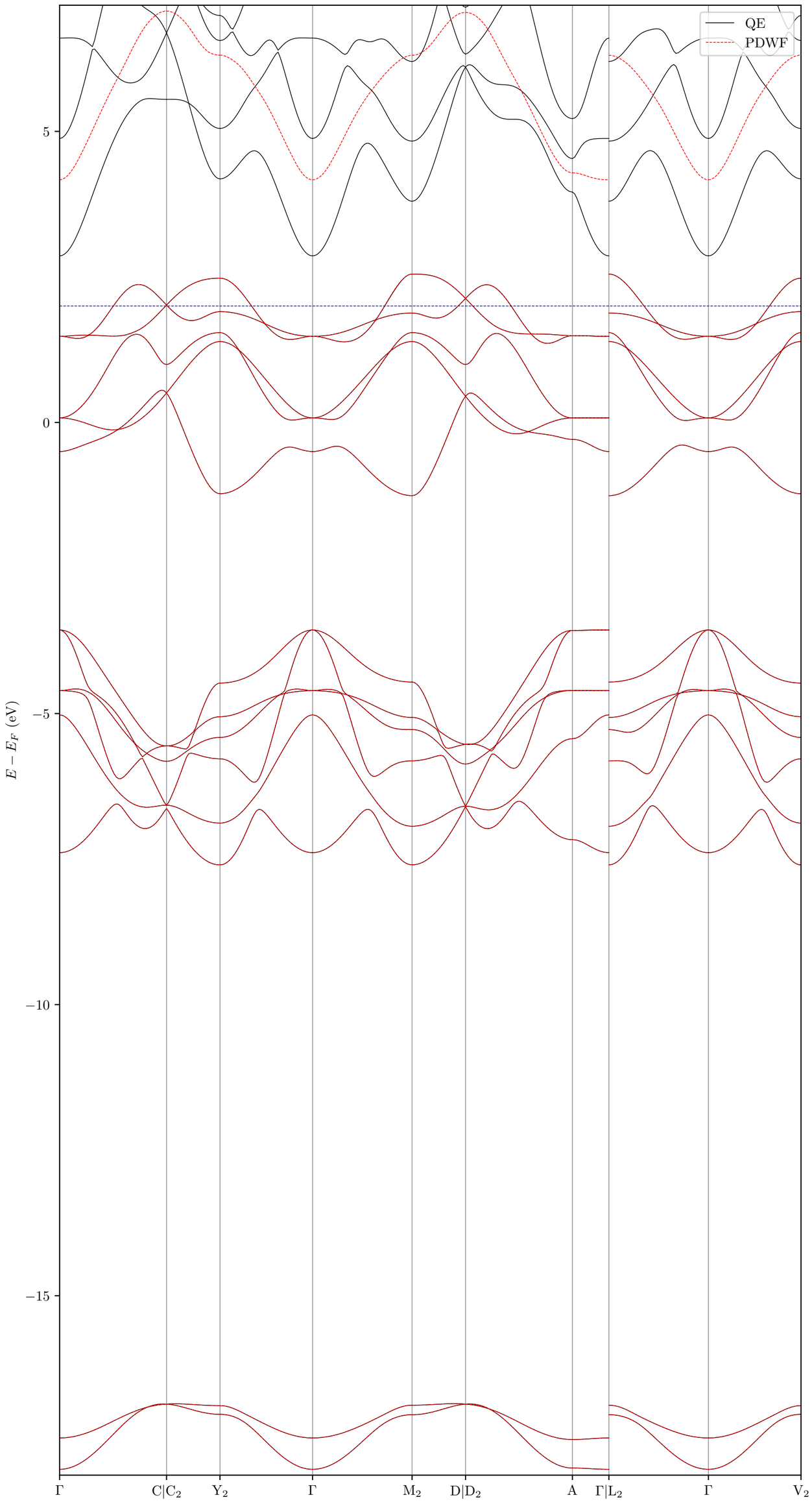



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.0 | 1.0 | 8.6 | 8.6 | 12.9 | 2.617 |



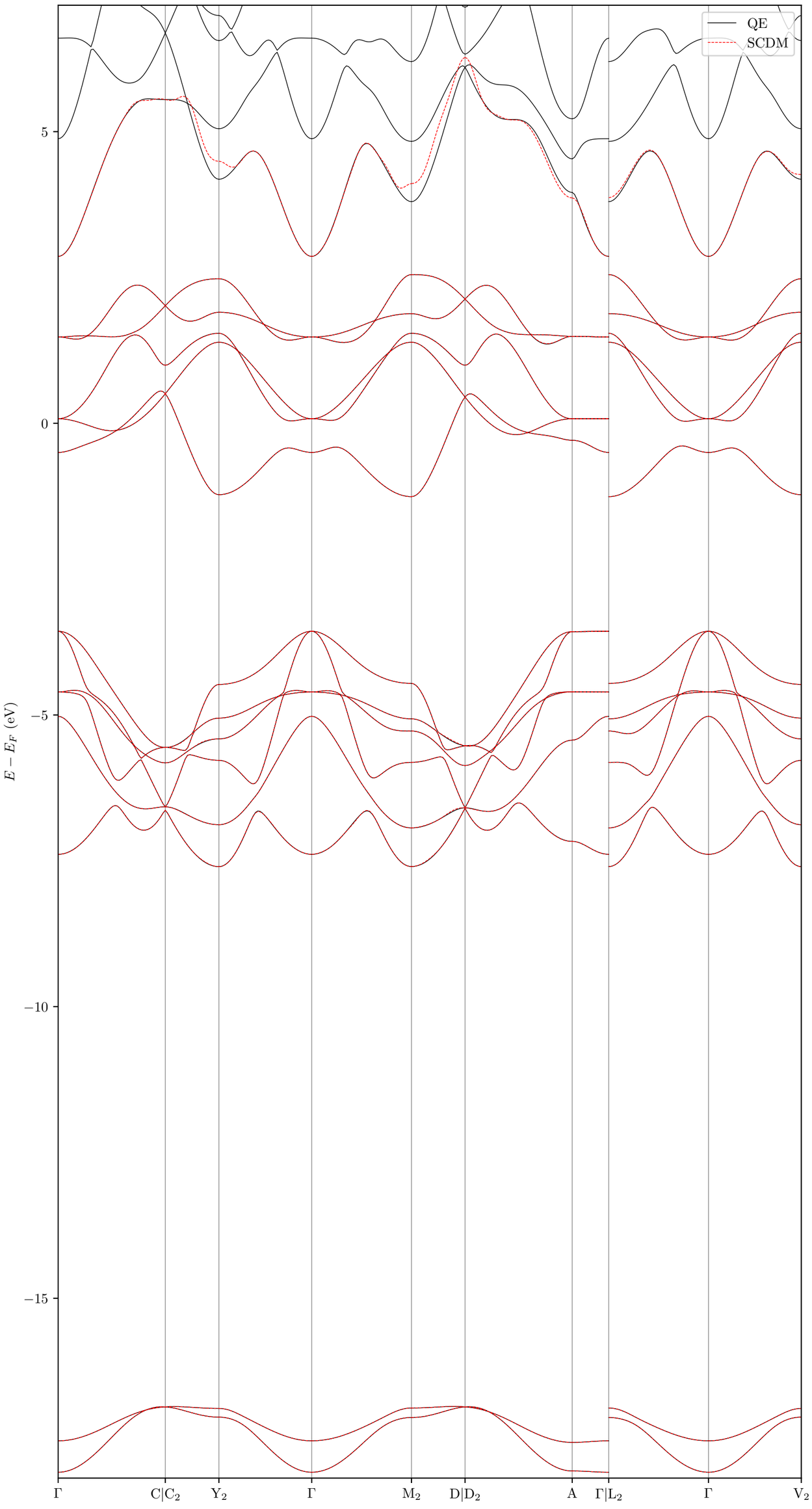
Cl2Ti exclude semicore
PW=d485a68f-5c0e-4f48-b08c-bbfc31b07253
W90=93ece50b-528a-4a93-b1bc-4c8974b0f5fc




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.3 | 74.6 | 0.7 | 3.2 | 495.8 | 2.031 |

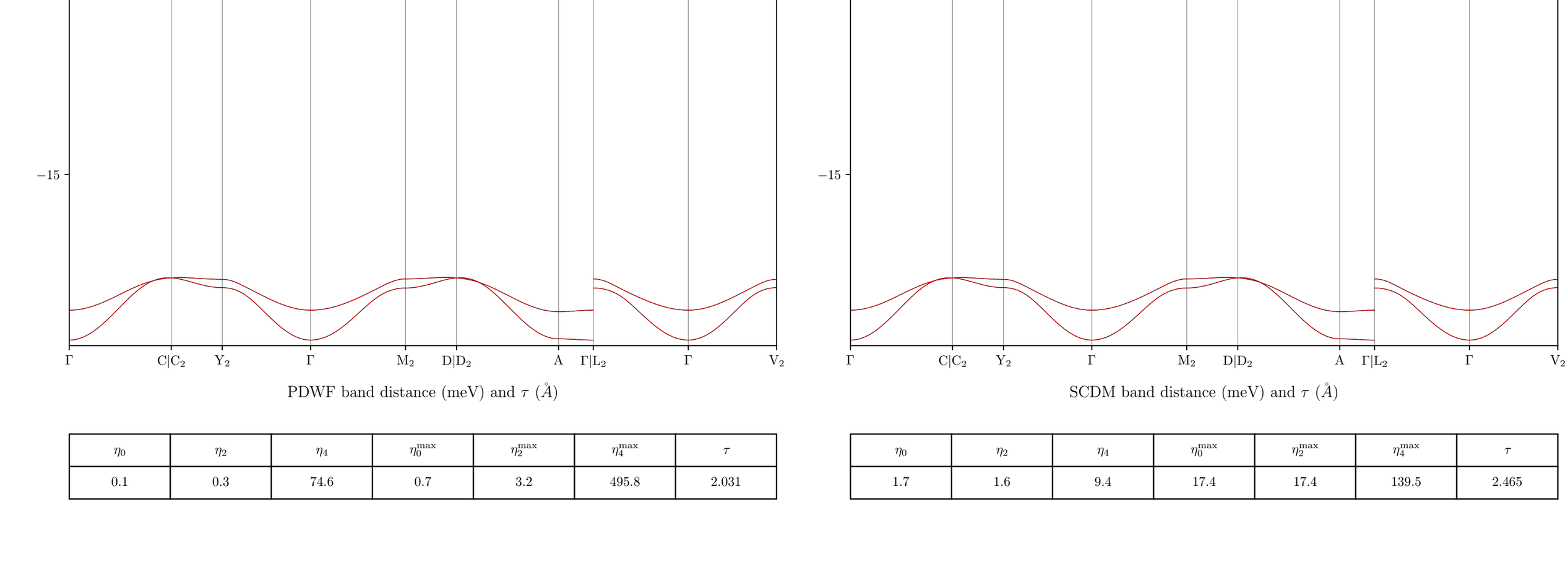
Cl2Ti exclude semicore
PW=d485a68f-5c0e-4f48-b08c-bbfc31b07253
W90=3e9a8c55-3d11-43b4-a298-5de88fc53d6e




SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.7 | 1.6 | 9.4 | 17.4 | 17.4 | 139.5 | 2.465 |

Hamiltonian decay



Cl2V exclude semicore
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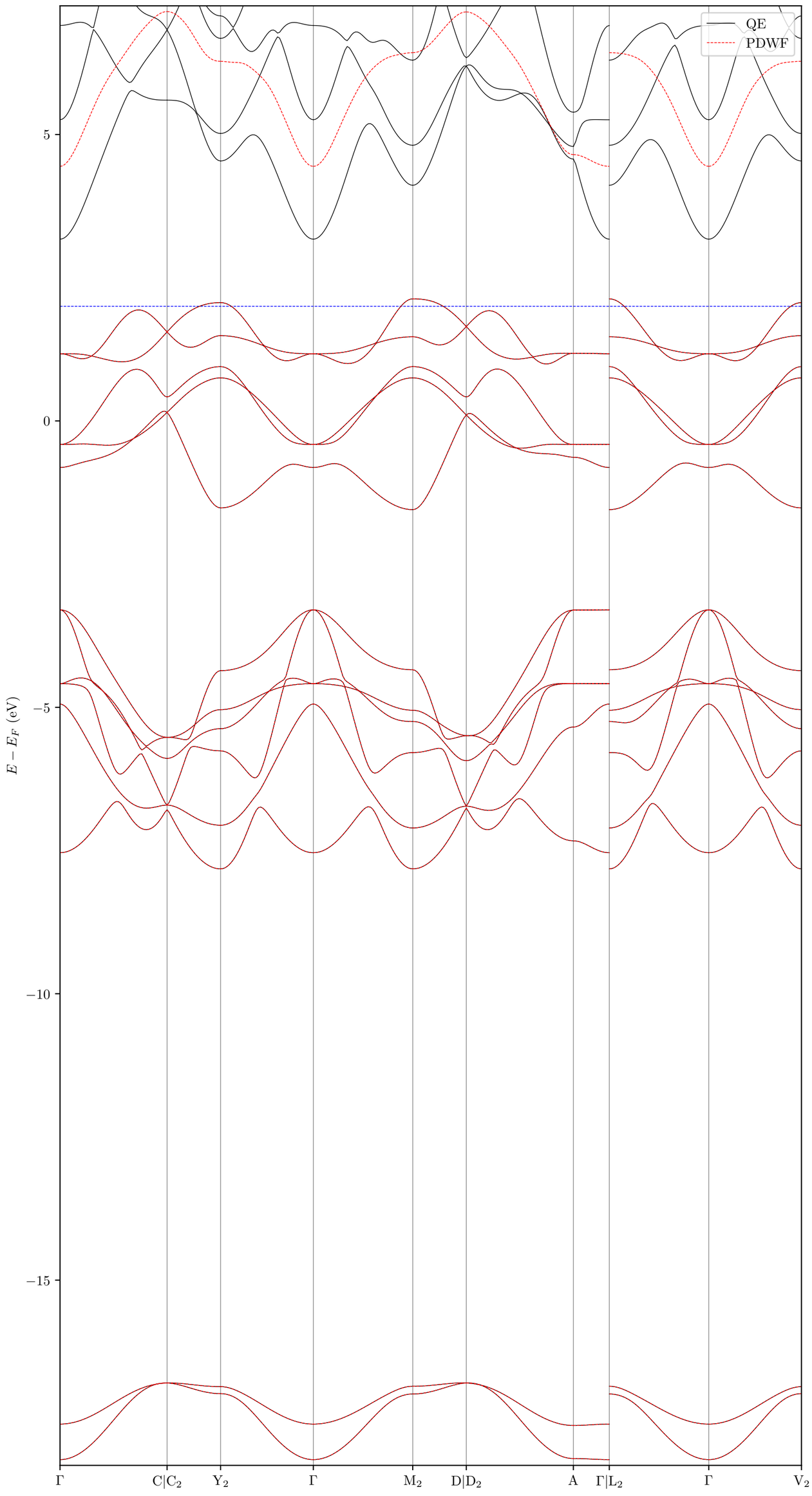
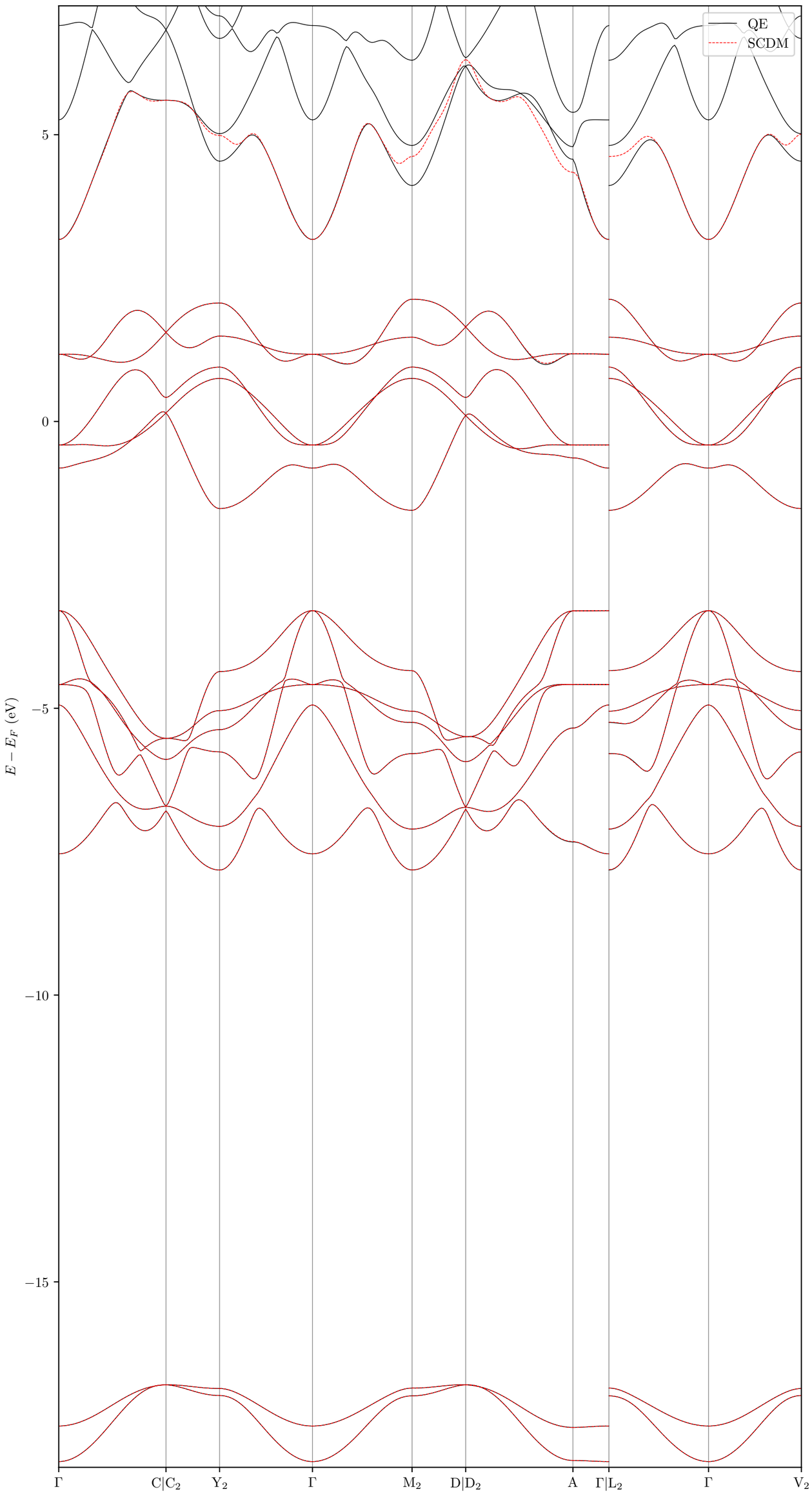
W90=f25bd102-1959-4a98-84e1-a58d6e61306b




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.1 | 36.2 | 1.0 | 1.0 | 137.0 | 1.925 |

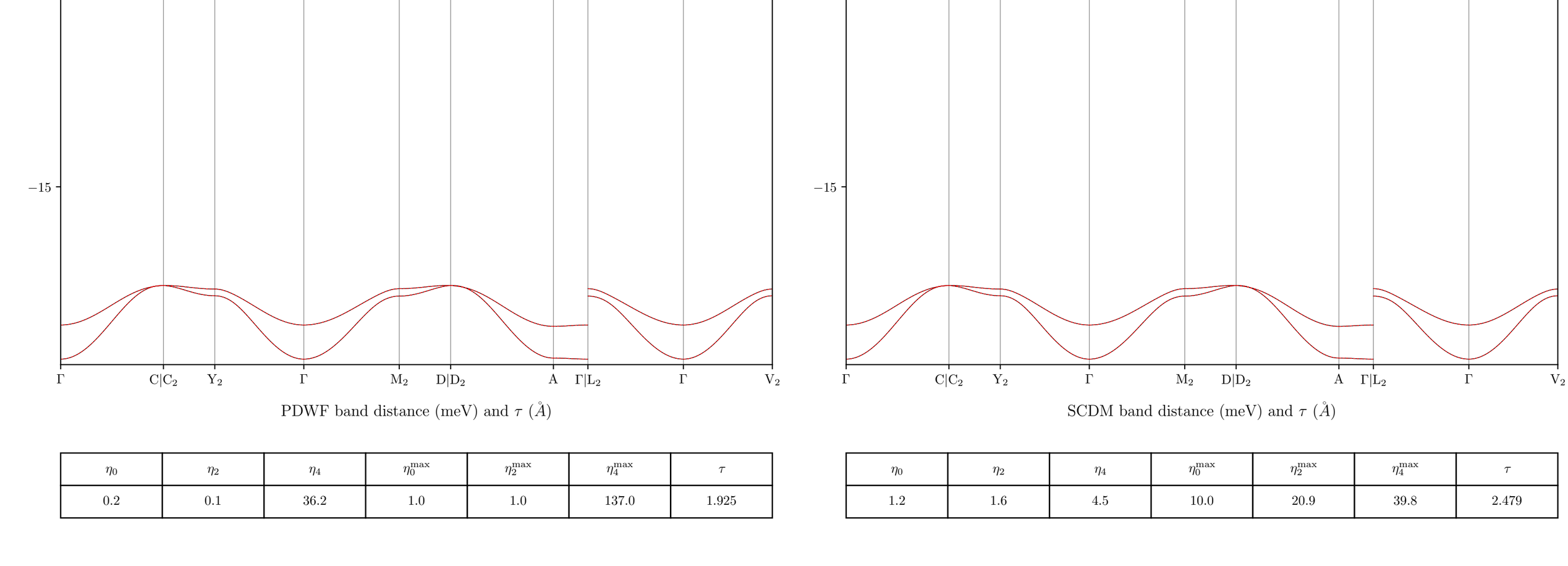
Cl2V exclude semicore
PW=3bd02544-19a7-490c-92bc-0205a3e1534d
W90=cedf3956-1aec-4811-8c80-bd26a593ea8d



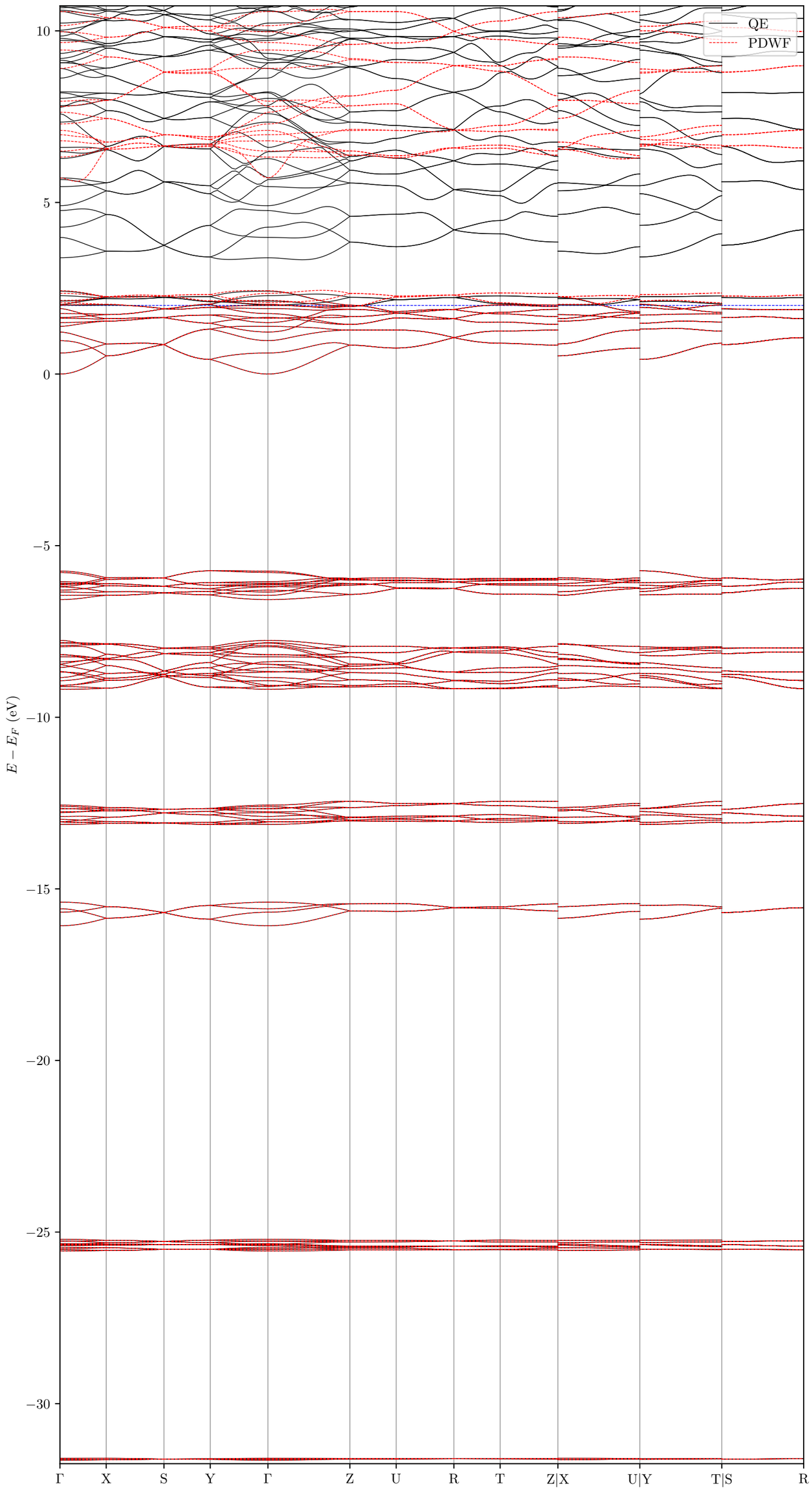

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.6 | 4.5 | 10.0 | 20.9 | 39.8 | 2.479 |

Hamiltonian decay



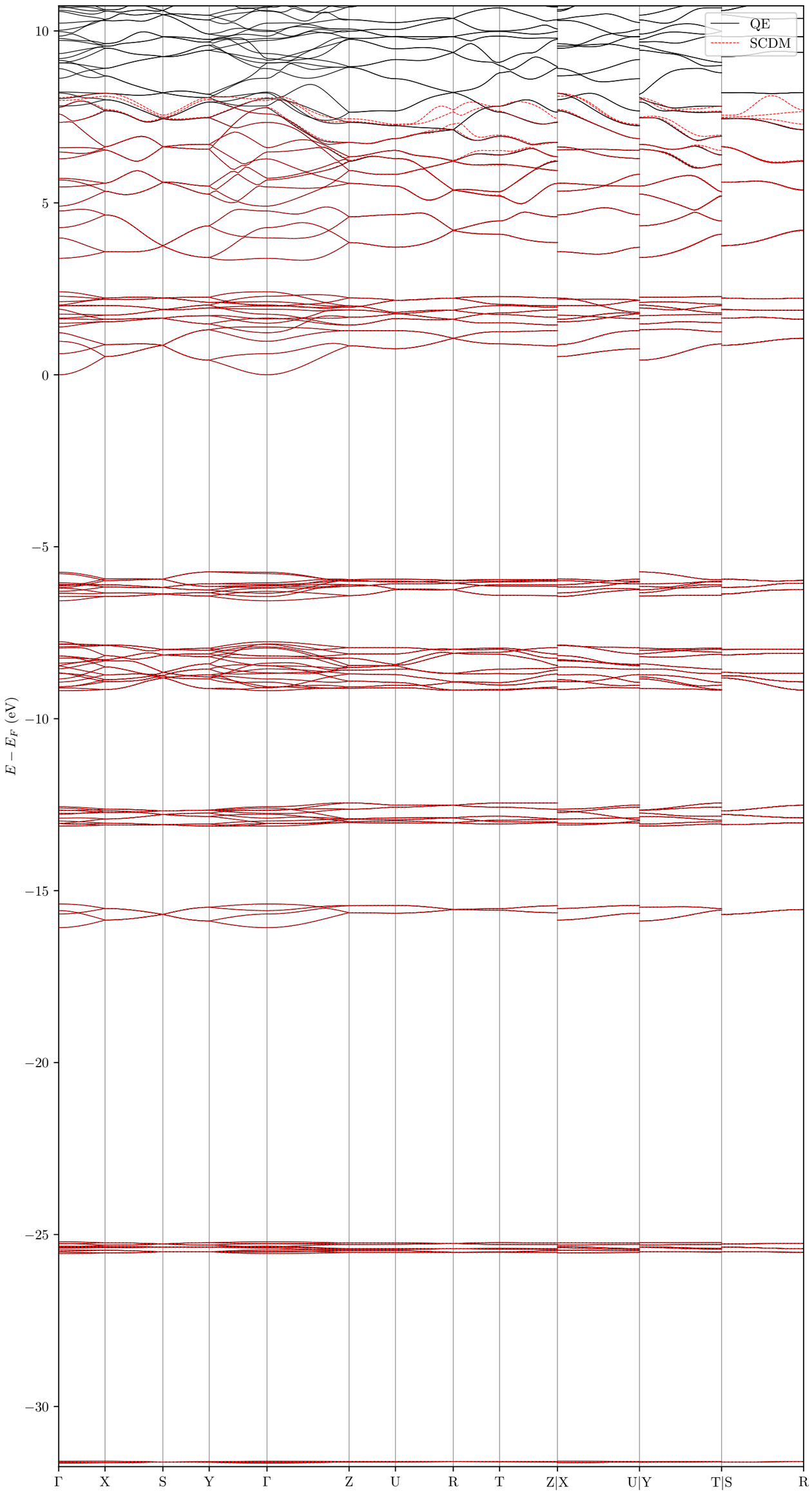
Cl4Li4O16 exclude semicore
PW=675fe60a-ad61-45f7-bbaf-74c12443c4e4
W90=8c4ccda0-1d16-4365-8696-30b48c55ee7f




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.2 | 0.2 | 1.6 | 1.6 | 1.6 | 2.397 |

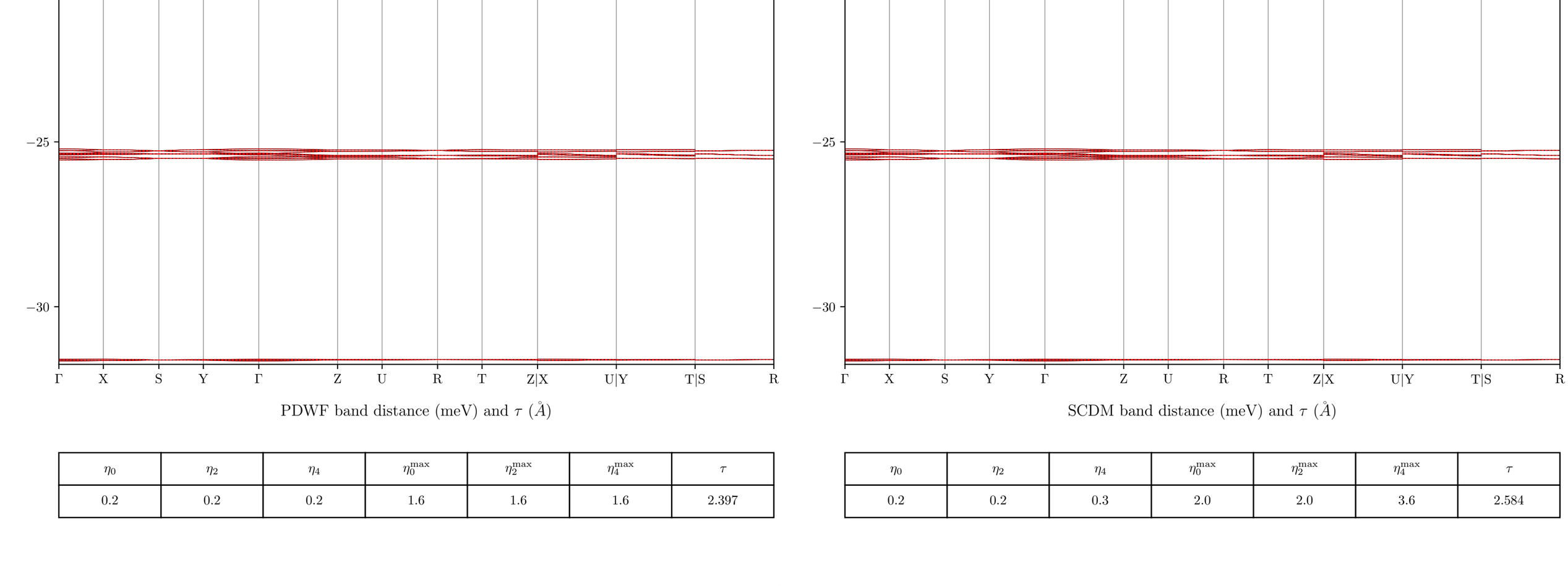
Cl4Li4O16 exclude semicore
PW=675fe60a-ad61-45f7-bbaf-74c12443c4e4
W90=9b6730dd-b592-4bd5-8bd5-87f54ac0eaf9



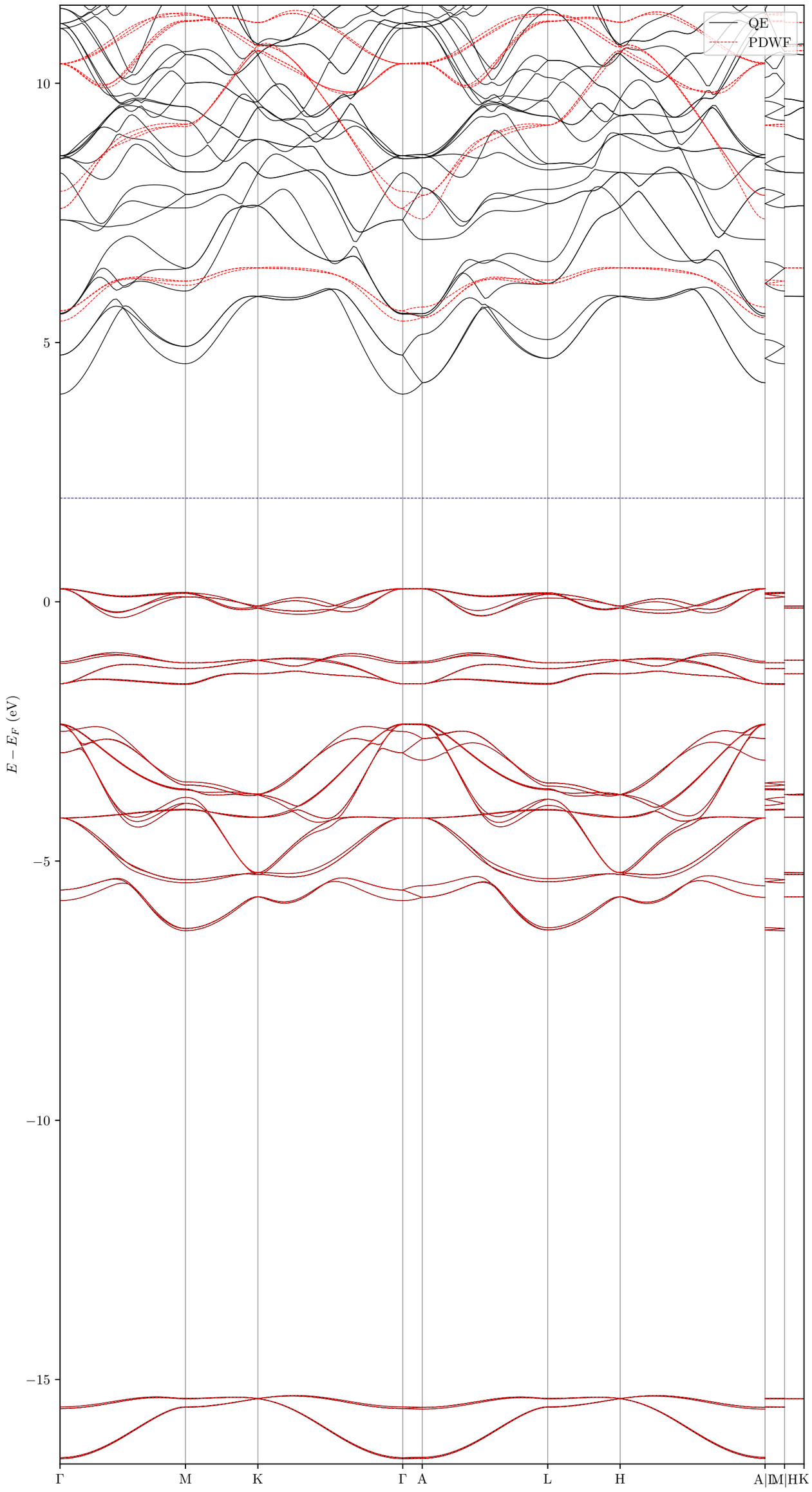

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.2 | 0.3 | 2.0 | 2.0 | 3.6 | 2.584 |

Hamiltonian decay



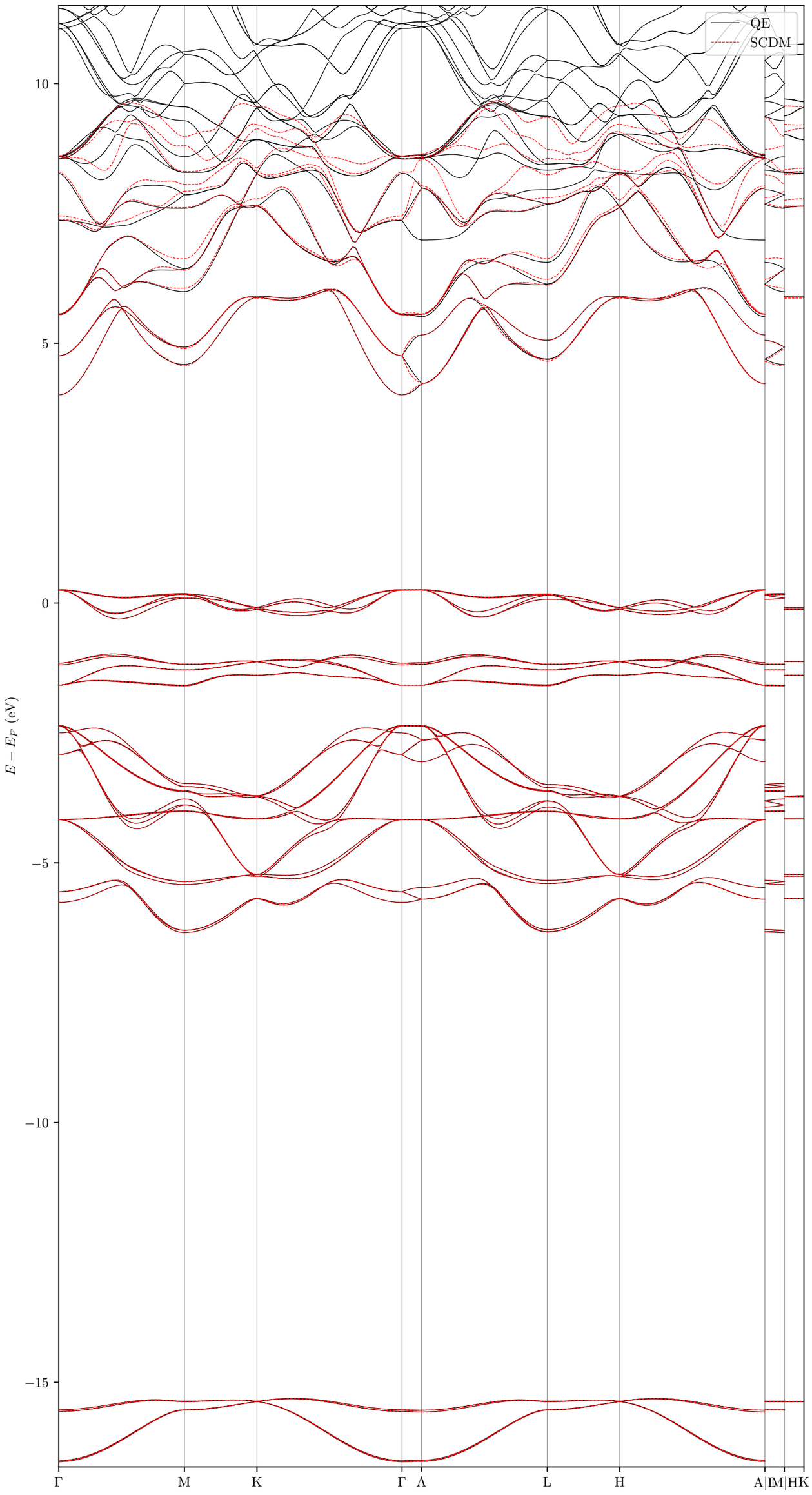
Cl6Ni3 exclude semicore
PW=3ede2fb5-0a18-4927-a899-8cc2c4633cc0
W90=3e7ffe95-fc30-4215-8352-61b18204baed




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.2 | 1.5 | 2.0 | 2.0 | 2.0 | 2.432 |

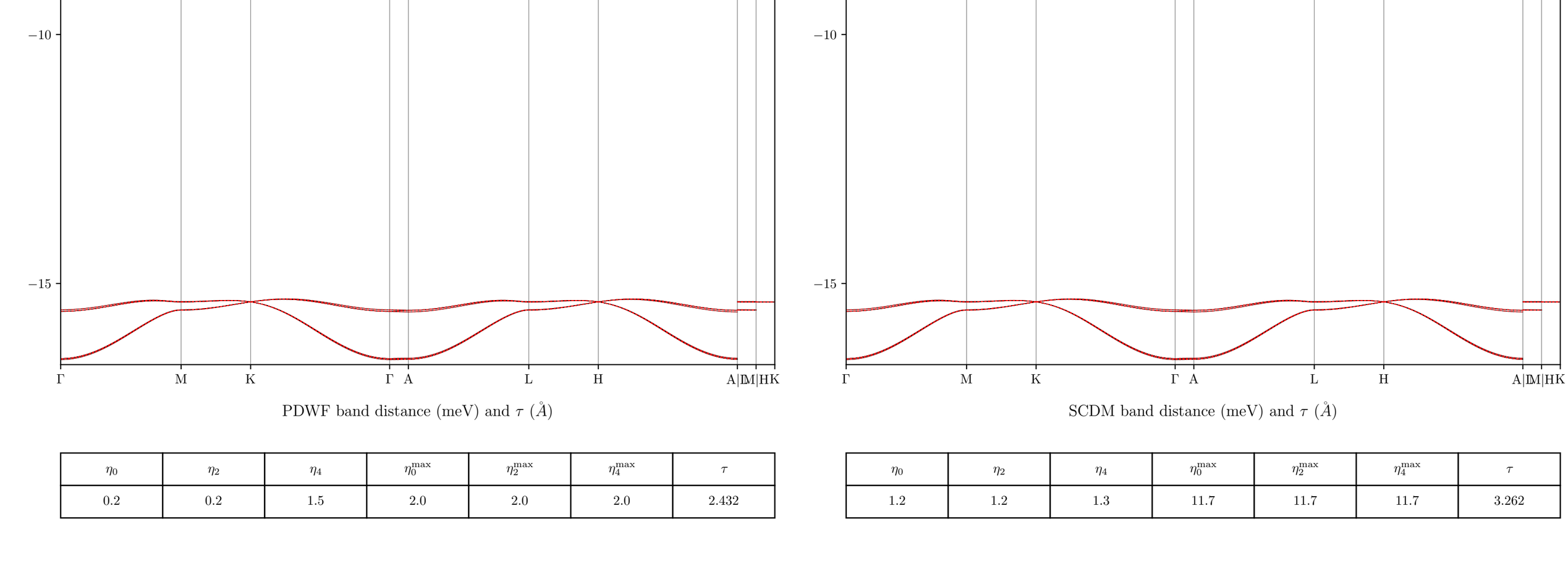
Cl6Ni3 exclude semicore
PW=3ede2fb5-0a18-4927-a899-8cc2c4633cc0
W90=0ea1228f-cc89-49a7-8a42-f8046ec3b73f

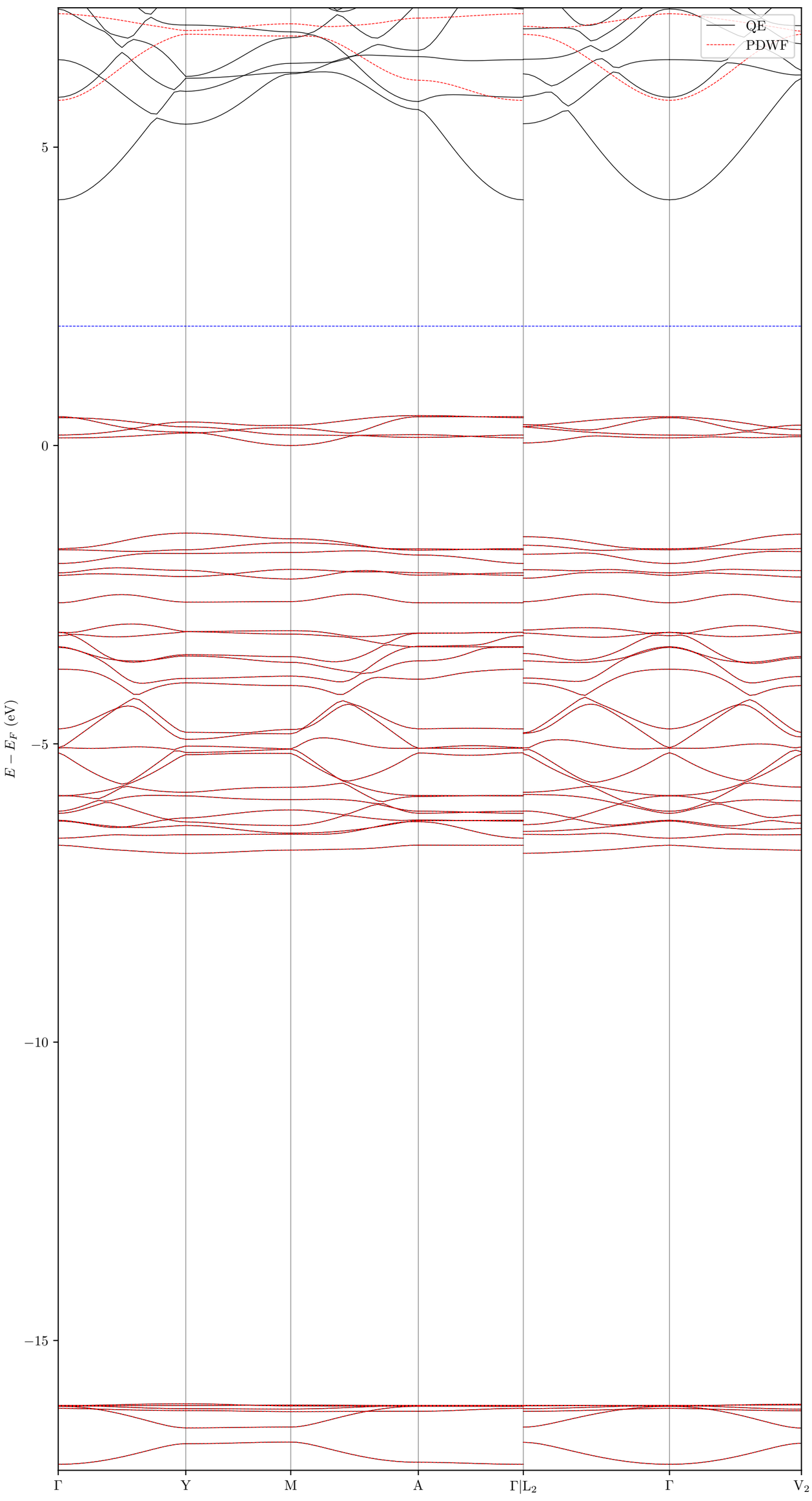



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.2 | 1.3 | 11.7 | 11.7 | 11.7 | 3.262 |

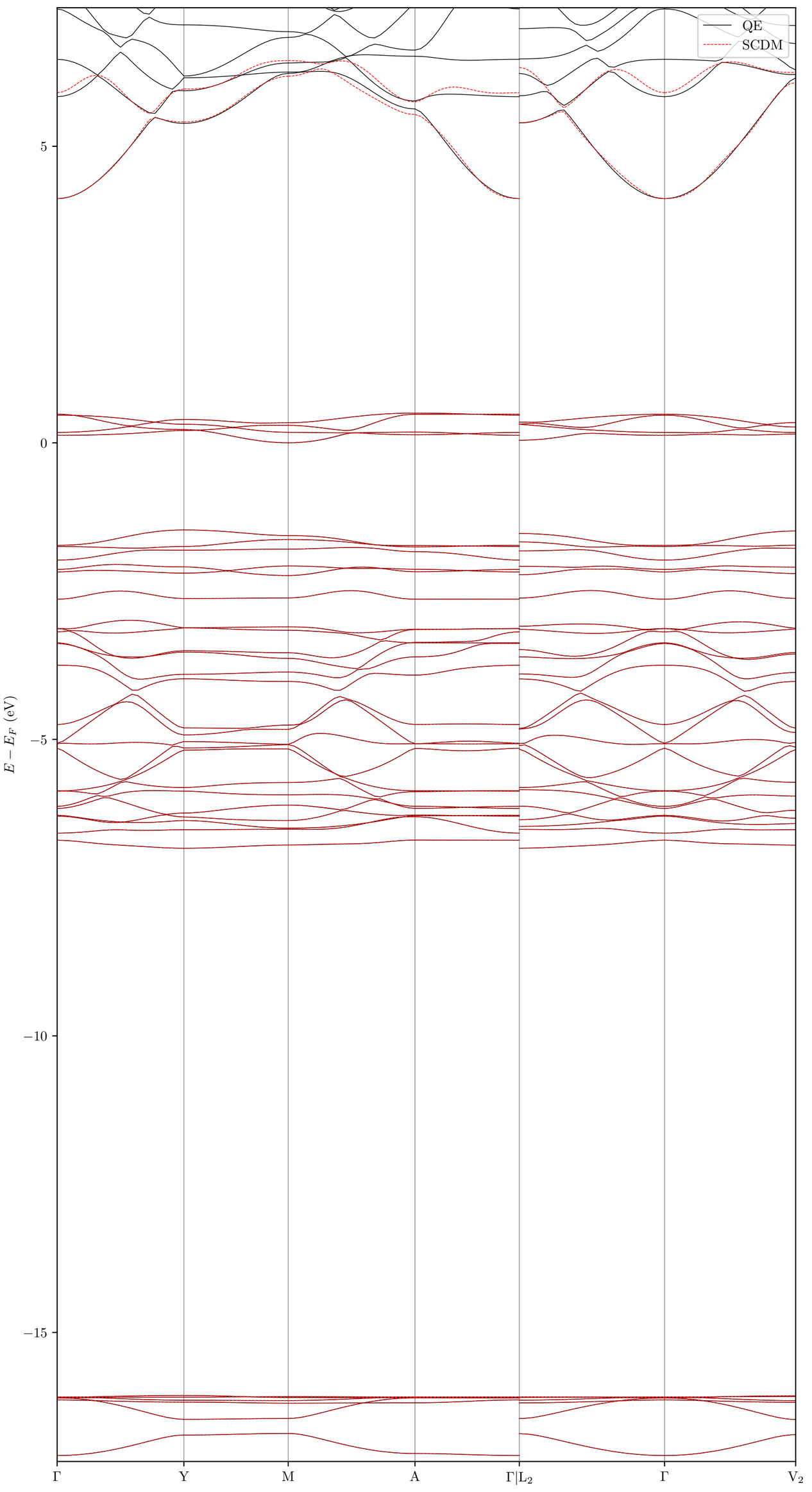
Hamiltonian decay





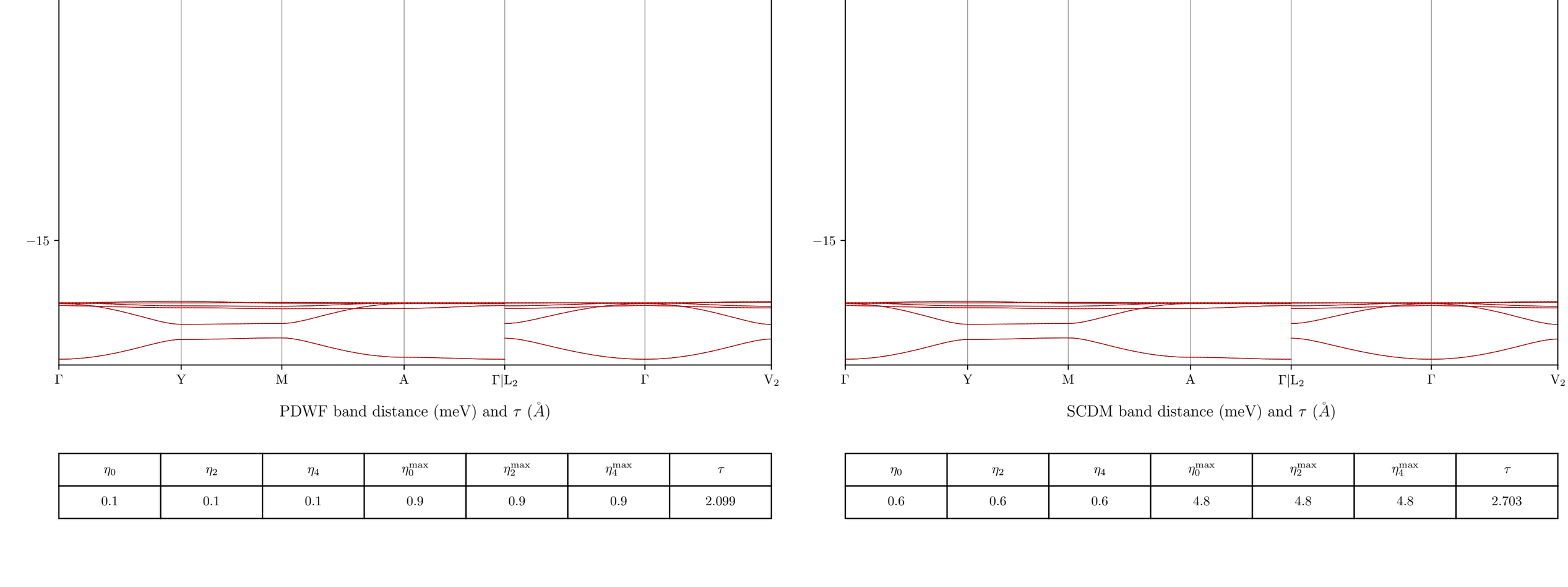

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.1 | 0.1 | 0.9 | 0.9 | 0.9 | 2.099 |

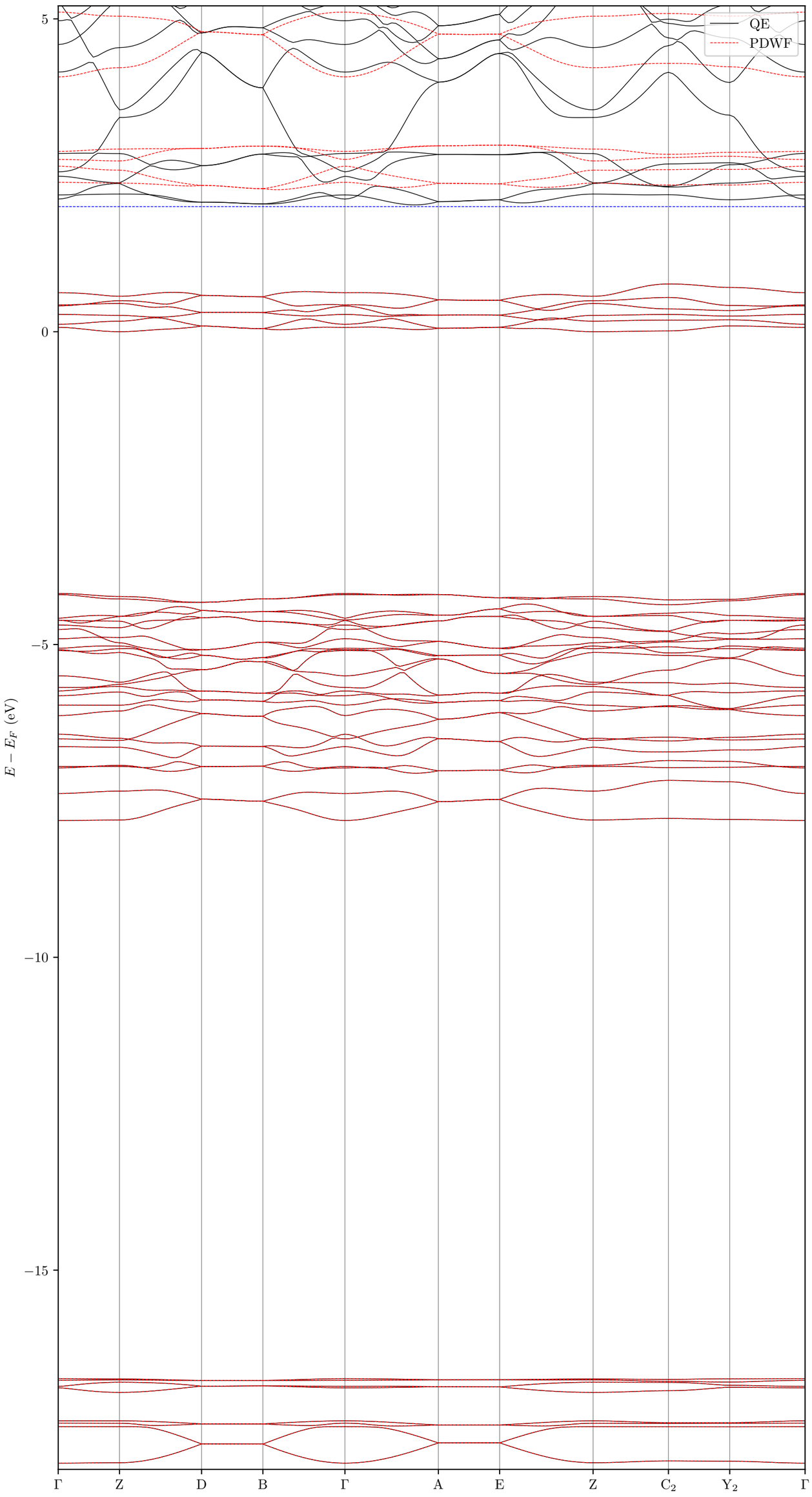



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 0.6 | 4.8 | 4.8 | 4.8 | 2.703 |



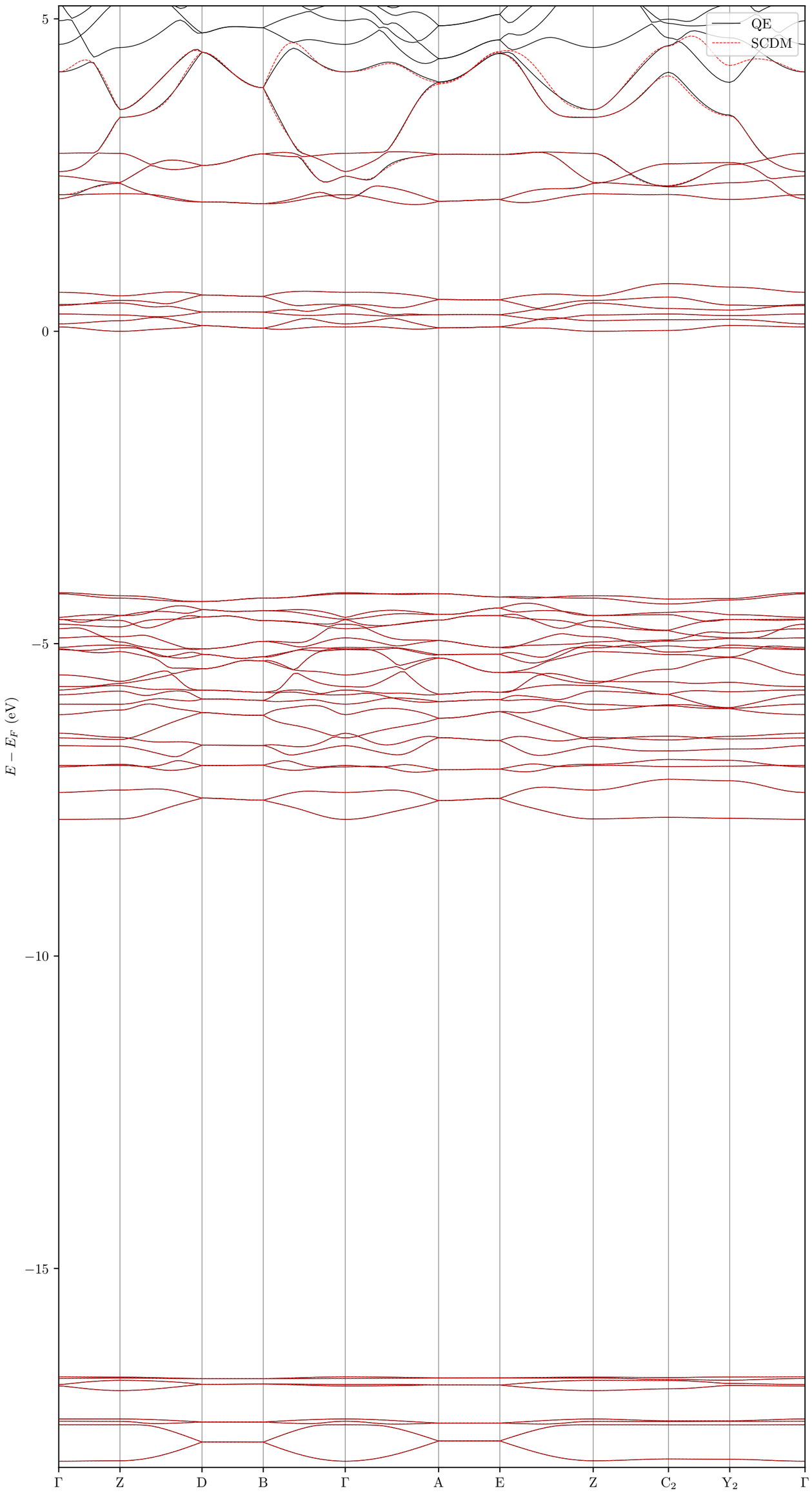
Cl8Hf2 exclude semicore
PW=bfda724e-ec3e-4fa7-8424-47f9949ff93e
W90=1e108ca0-81dd-45cc-96c3-b797e40392b6




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.7 | 76.6 | 0.6 | 0.6 | 460.3 | 2.080 |

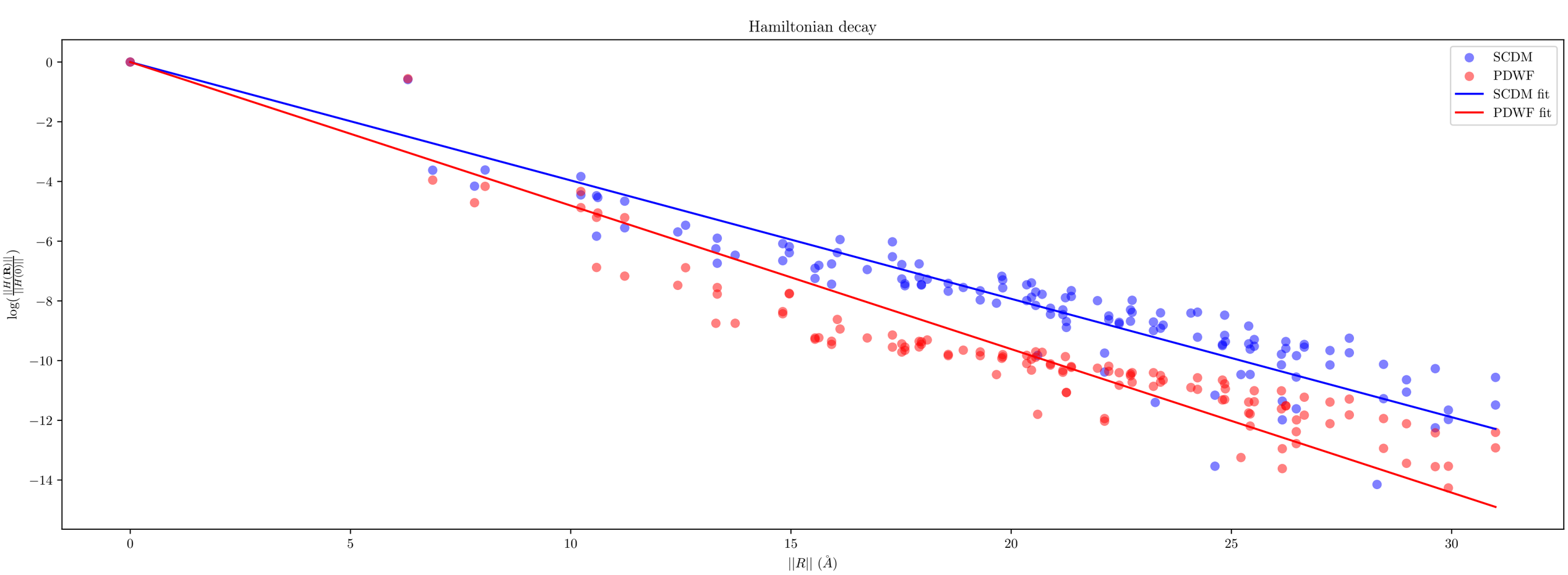
Cl8Hf2 exclude semicore
PW=bfda724e-ec3e-4fa7-8424-47f9949ff93e
W90=c096ffba-61a8-4c5b-b65a-f5d0cf79cc94



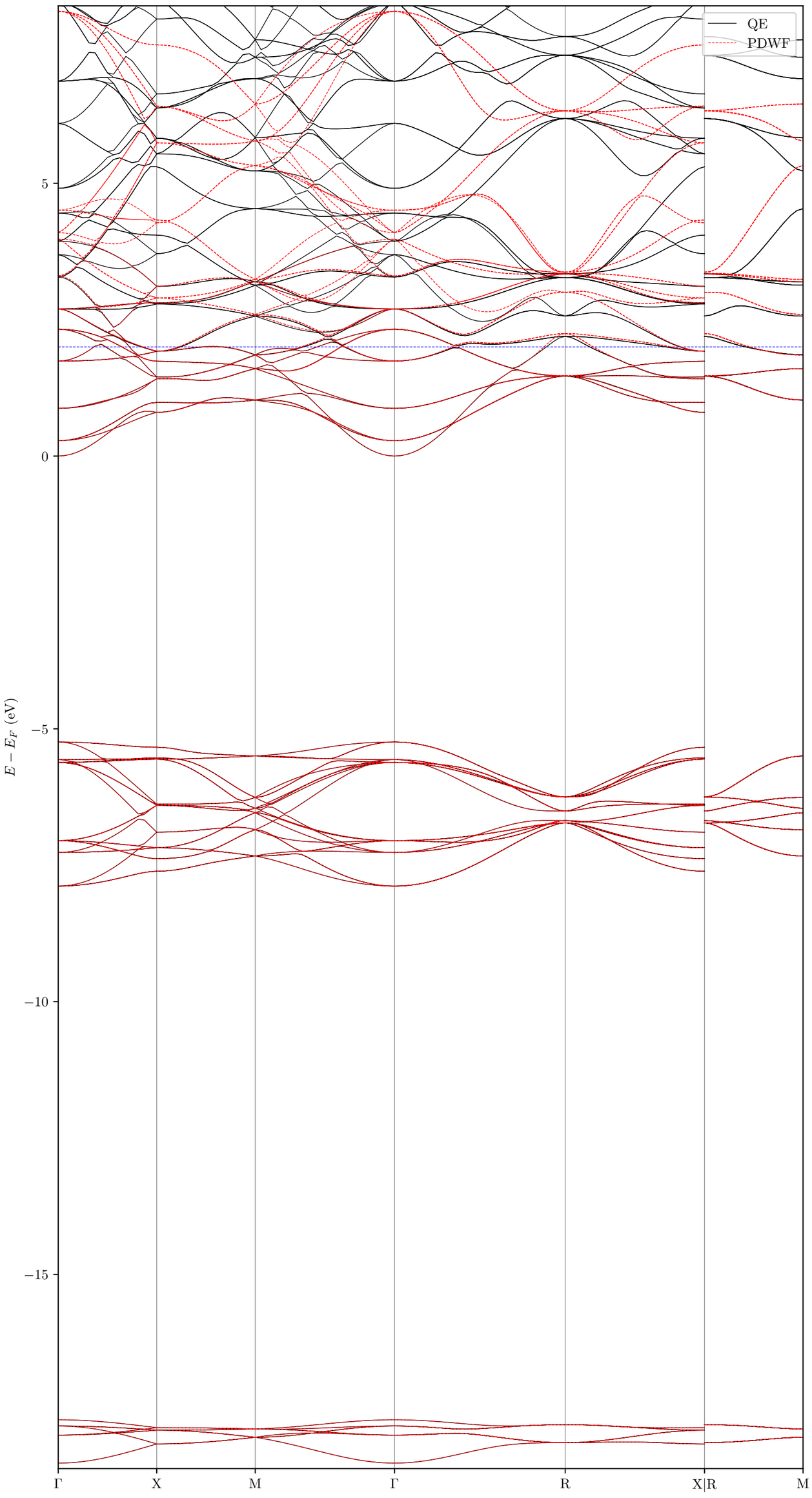

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.5 | 1.6 | 5.1 | 5.1 | 27.1 | 2.522 |

Hamiltonian decay



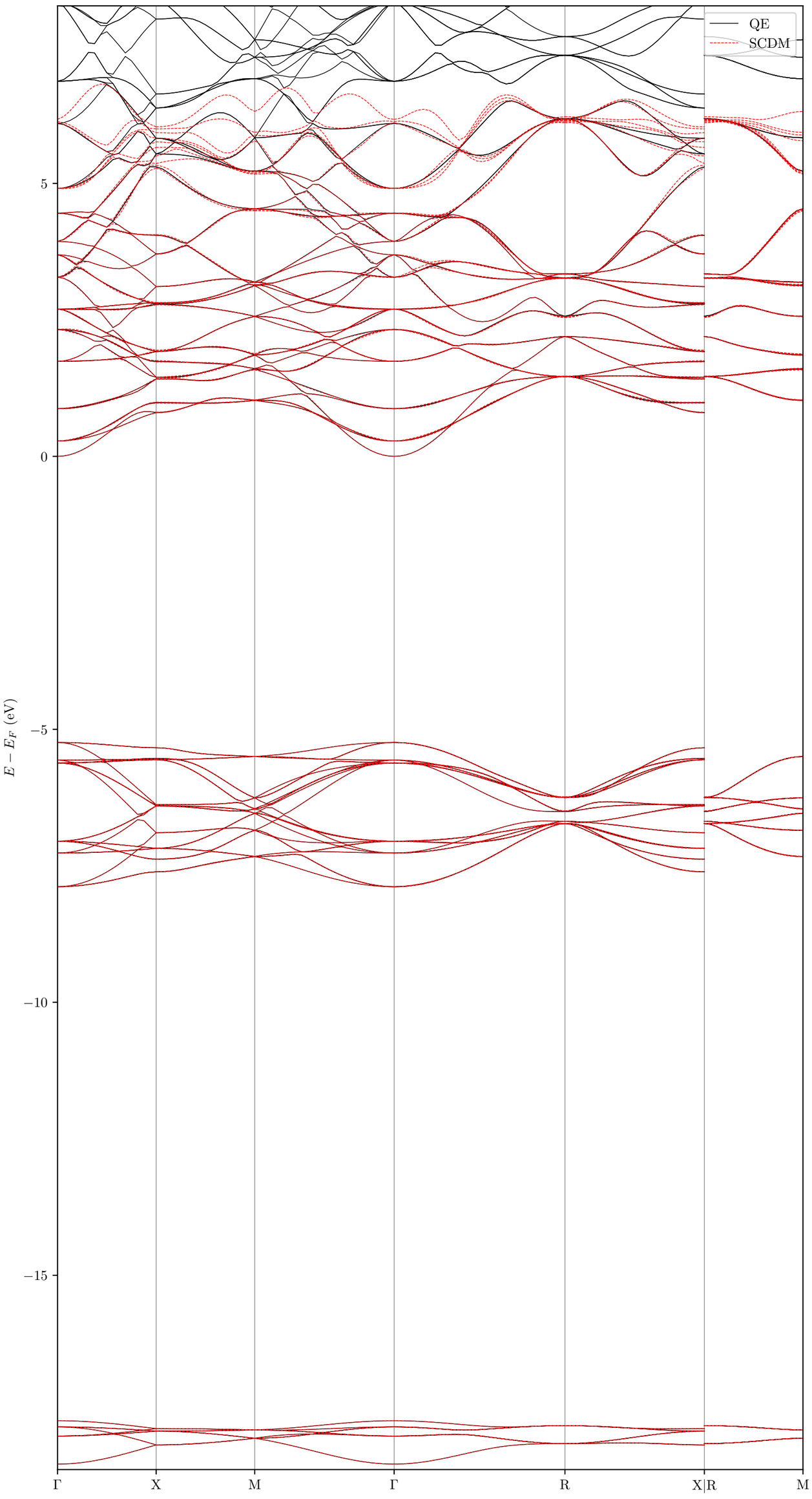
Cl8Sr4 exclude semicore
PW=5b3b9fff-736c-47a7-b3c7-1b5fe6dc92cf
W90=12397093-56f9-4a3a-a10c-80333e64d9be




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 7.1 | 4.0 | 4.0 | 44.6 | 2.641 |

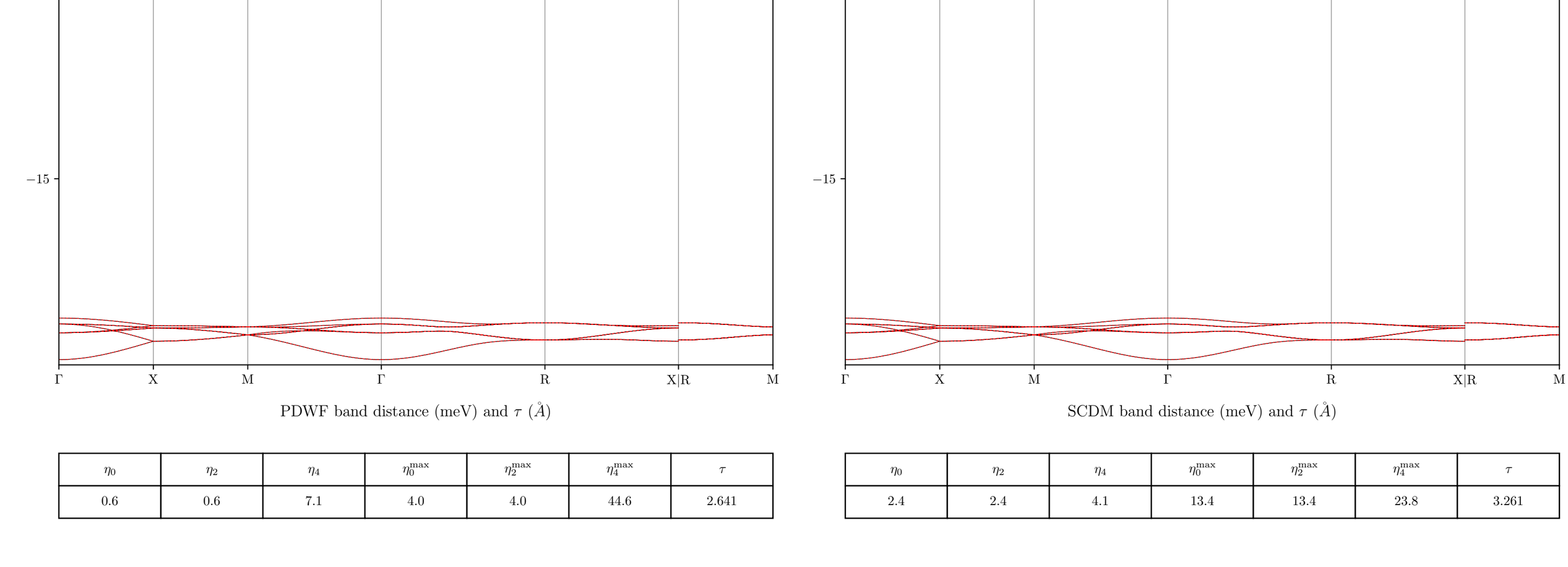
Cl8Sr4 exclude semicore
PW=5b3b9fff-736c-47a7-b3c7-1b5fe6dc92cf
W90=8d096c0d-332e-4df3-8800-ba6850f0c805



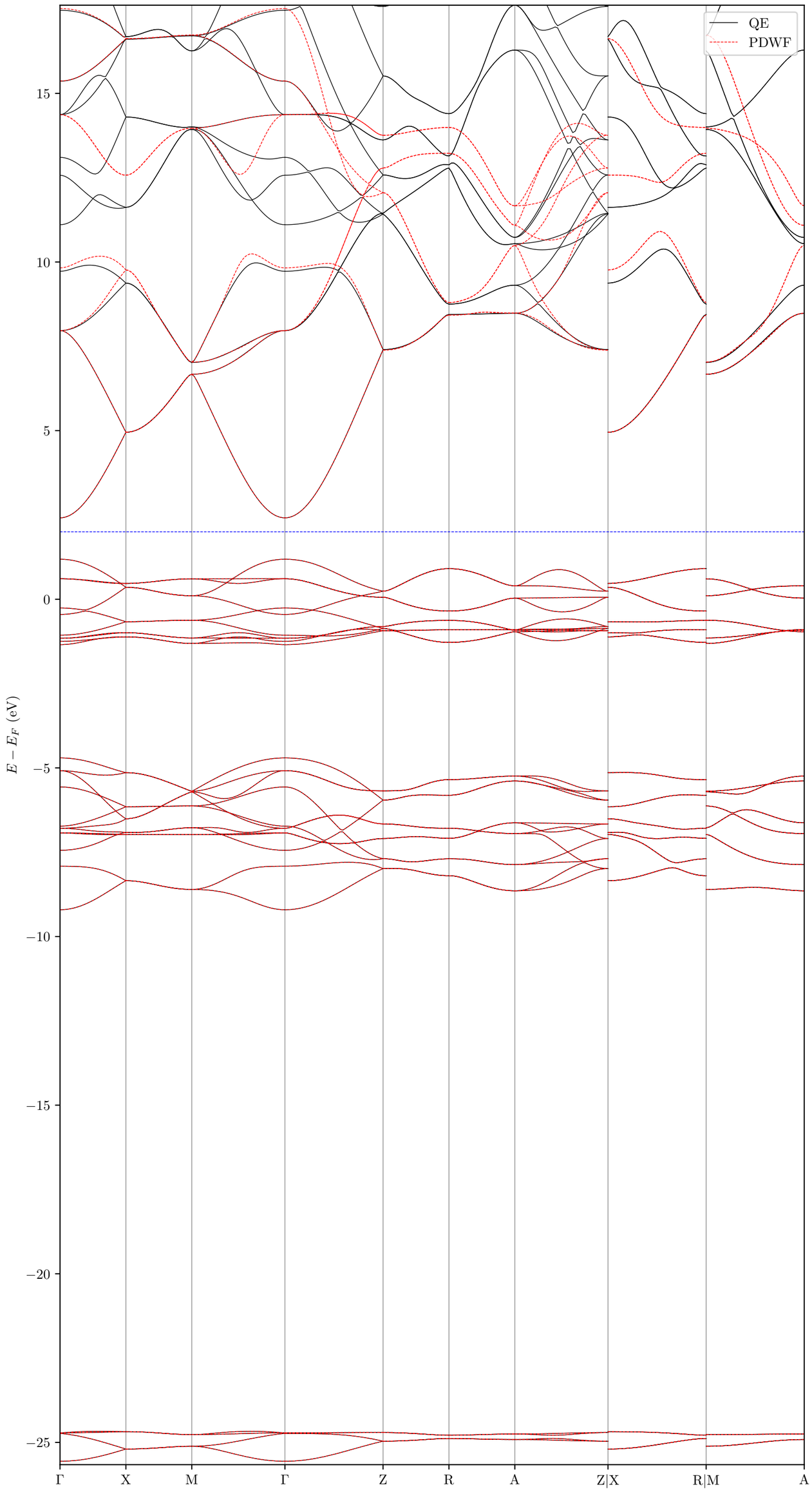

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.4 | 2.4 | 4.1 | 13.4 | 13.4 | 23.8 | 3.261 |

Hamiltonian decay



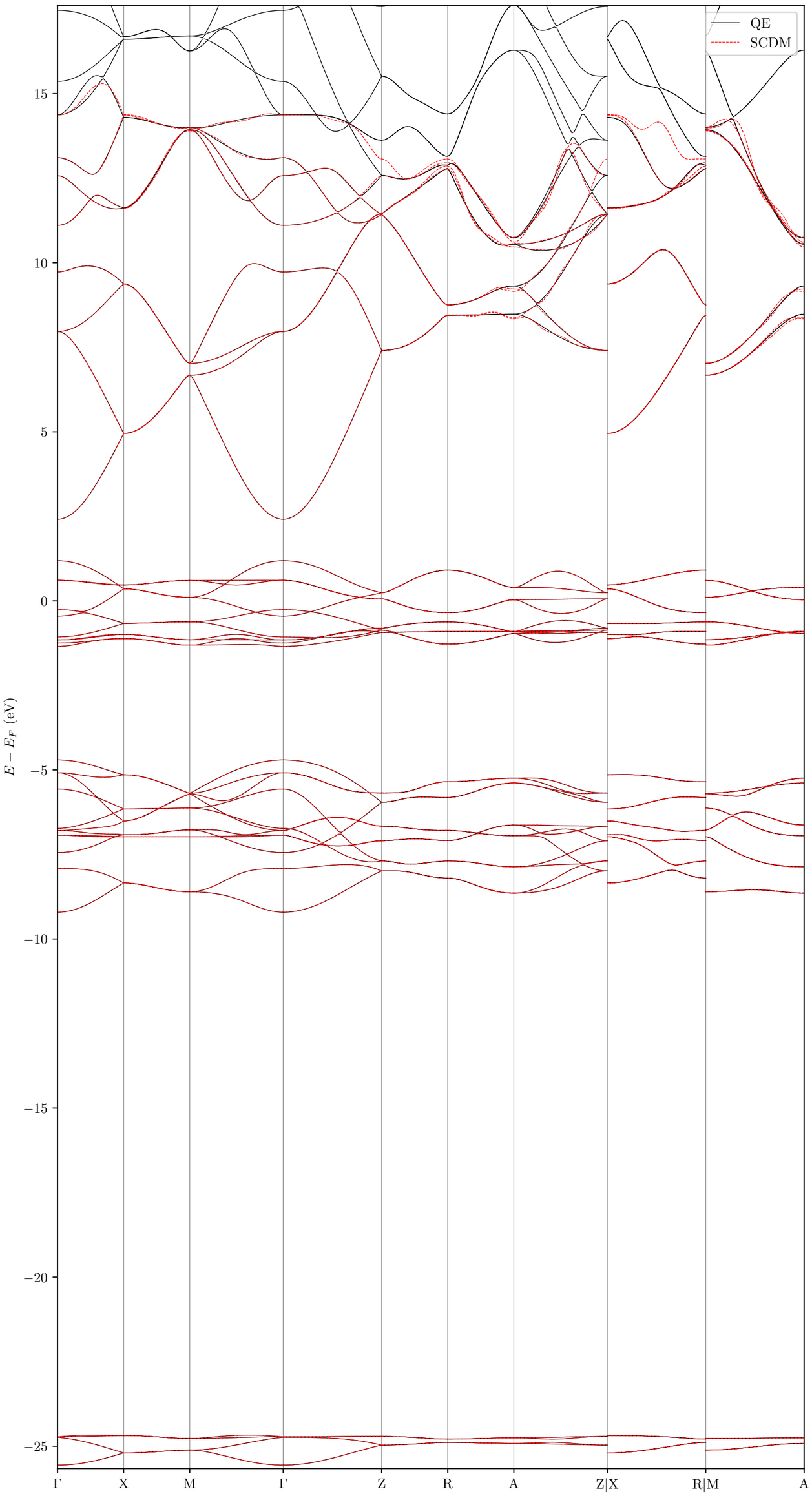
Co2F4 exclude semicore
PW=0367f773-03a2-4363-9627-e793f376317e
W90=f222d064-71a8-4070-95e7-9b3b0d346071




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.5 | 0.5 | 3.5 | 3.5 | 3.5 | 2.056 |

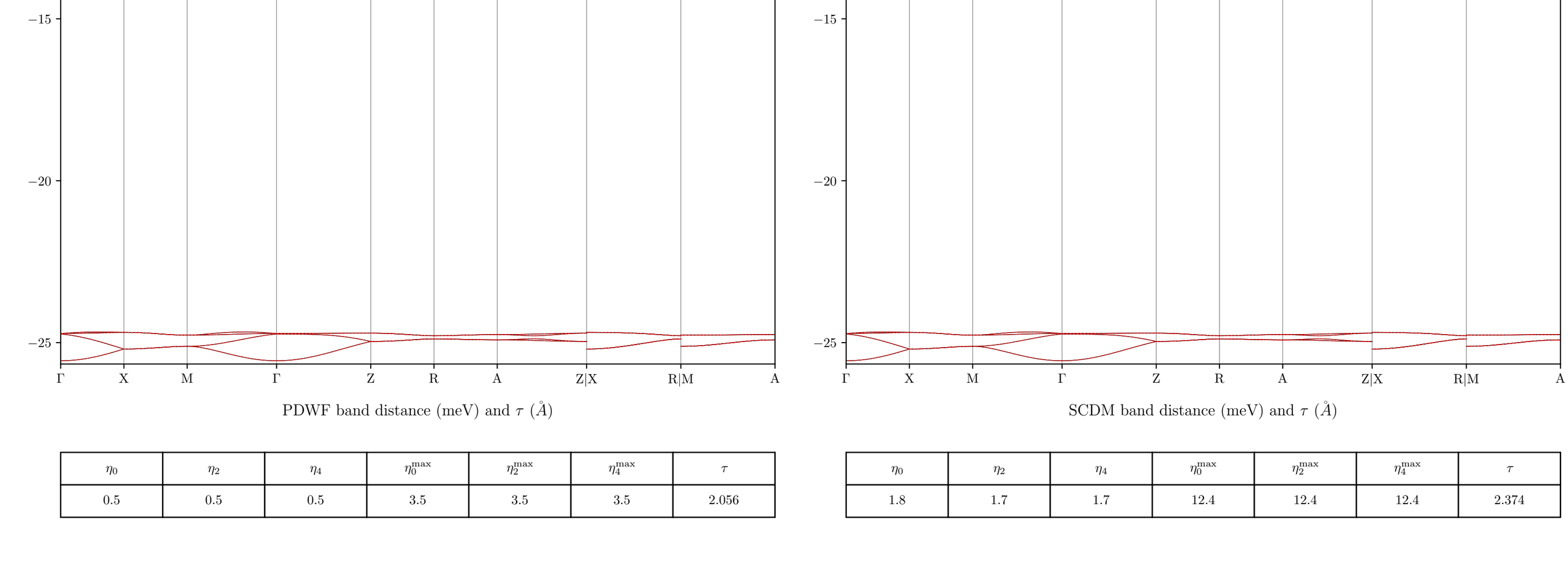
Co2F4 exclude semicore
PW=0367f773-03a2-4363-9627-e793f376317e
W90=38a6f23c-59f8-49ba-8a5e-707a4721e927



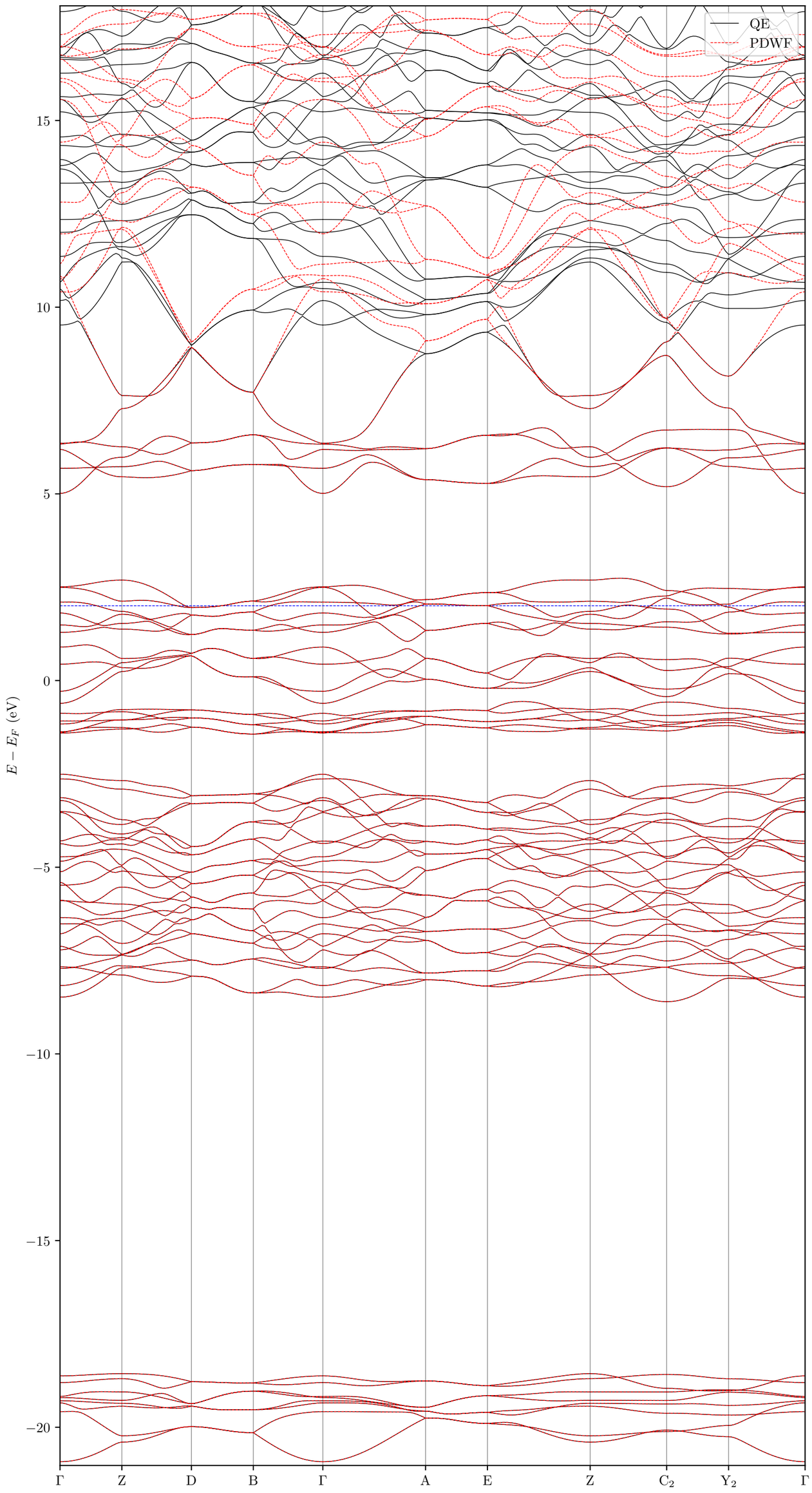

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.8 | 1.7 | 1.7 | 12.4 | 12.4 | 12.4 | 2.374 |

Hamiltonian decay



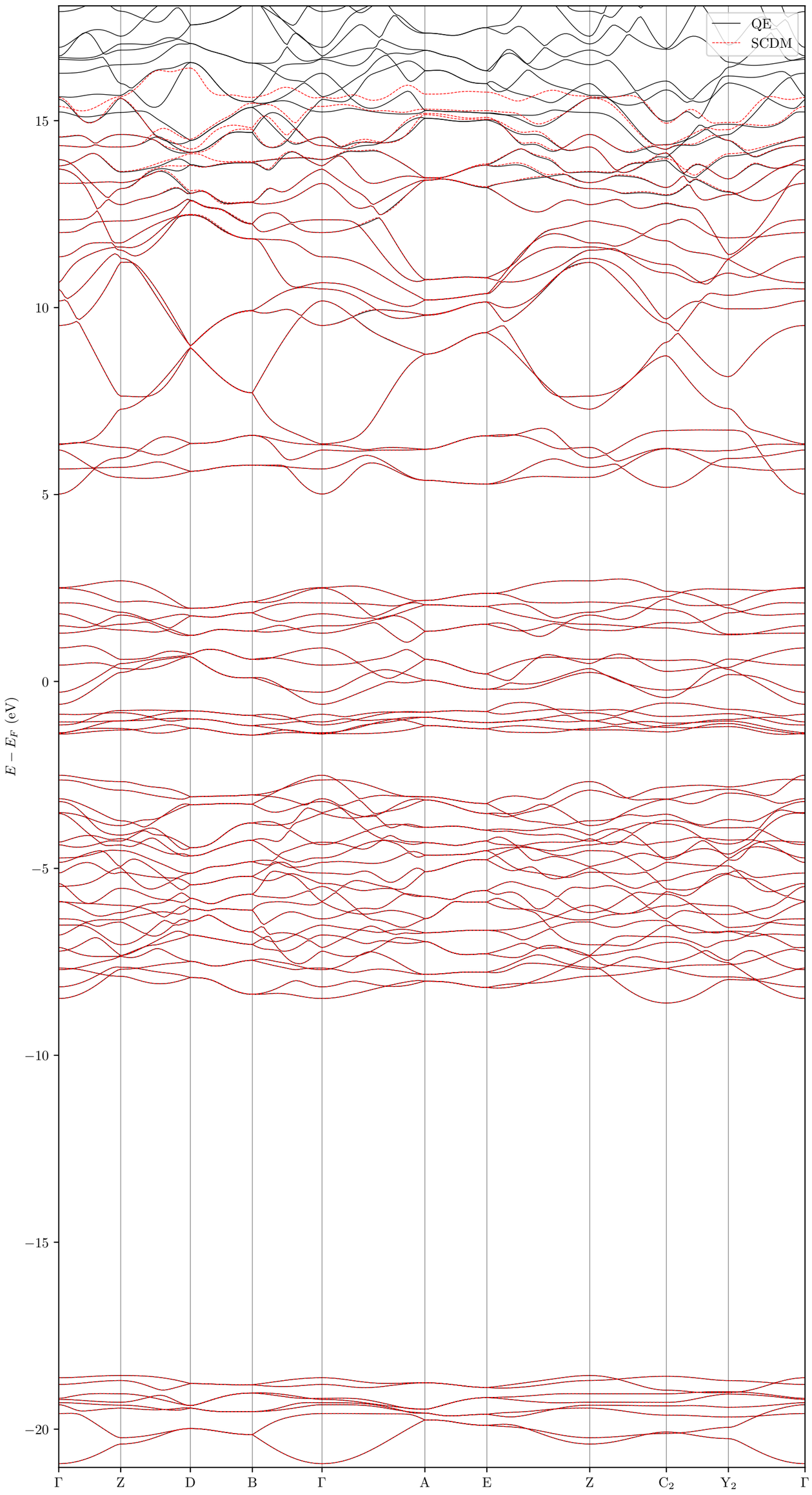
Co2O8W2 exclude semicore
PW=30faa125-ed9e-4abc-8367-ea5809c0be84
W90=476578bd-dda9-4c0e-a950-b82a8db9c9a7




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 0.3 | 1.9 | 1.9 | 1.9 | 2.164 |

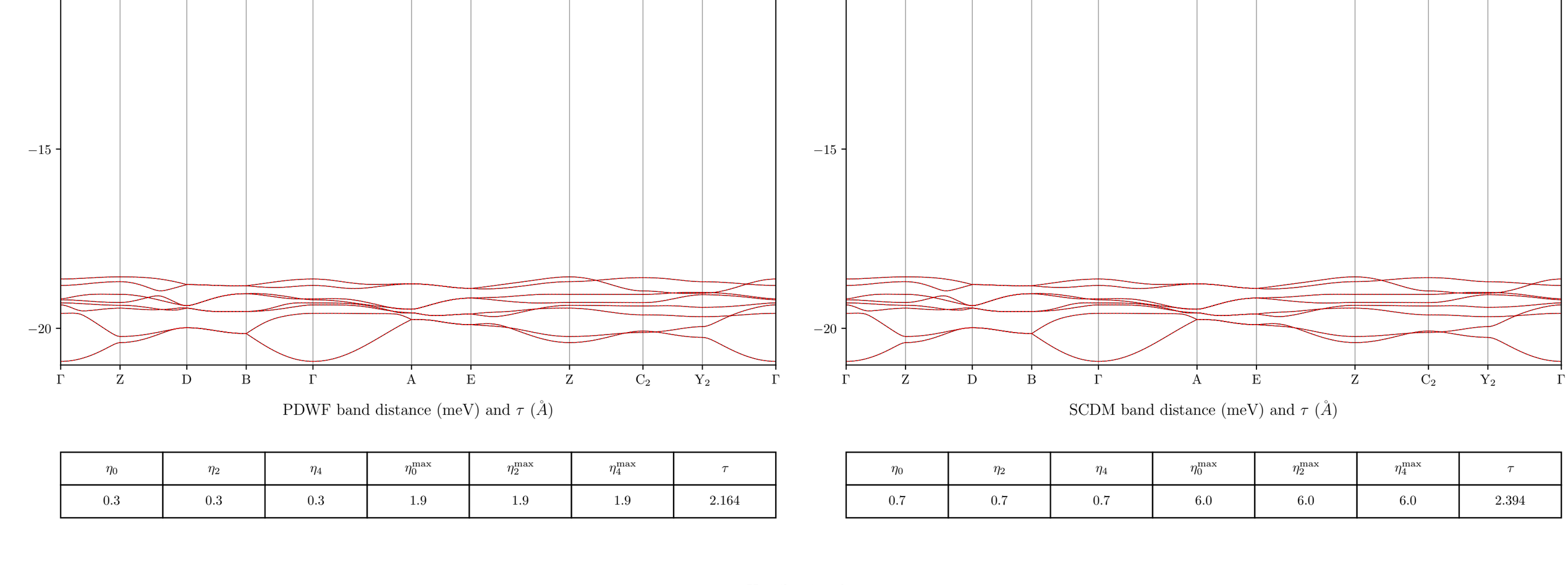
Co2O8W2 exclude semicore
PW=30faa125-ed9e-4abc-8367-ea5809c0be84
W90=c8e35a2e-a10d-45e9-b344-96ca7a11b7c2



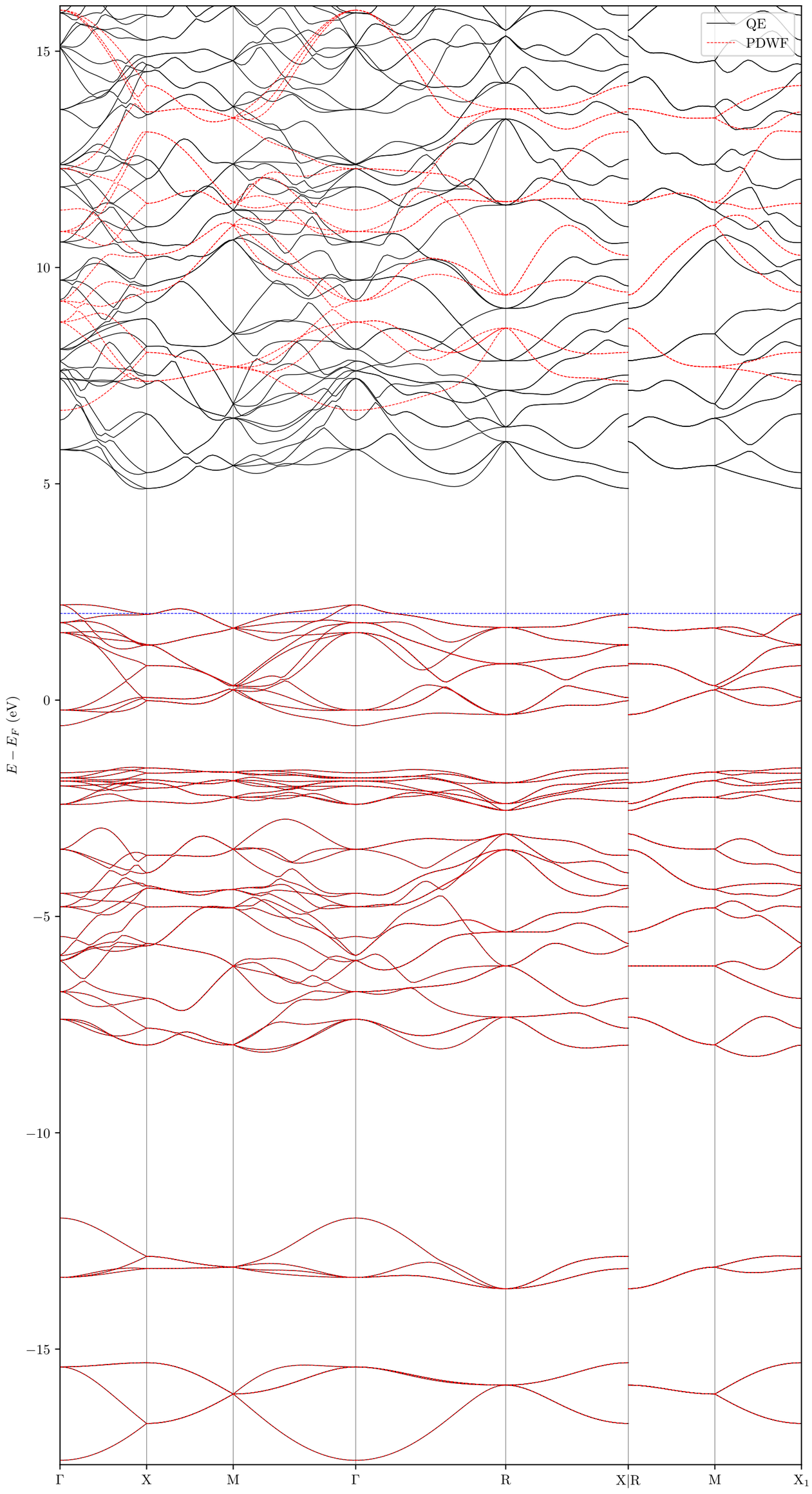

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 0.7 | 0.7 | 6.0 | 6.0 | 6.0 | 2.394 |

Hamiltonian decay



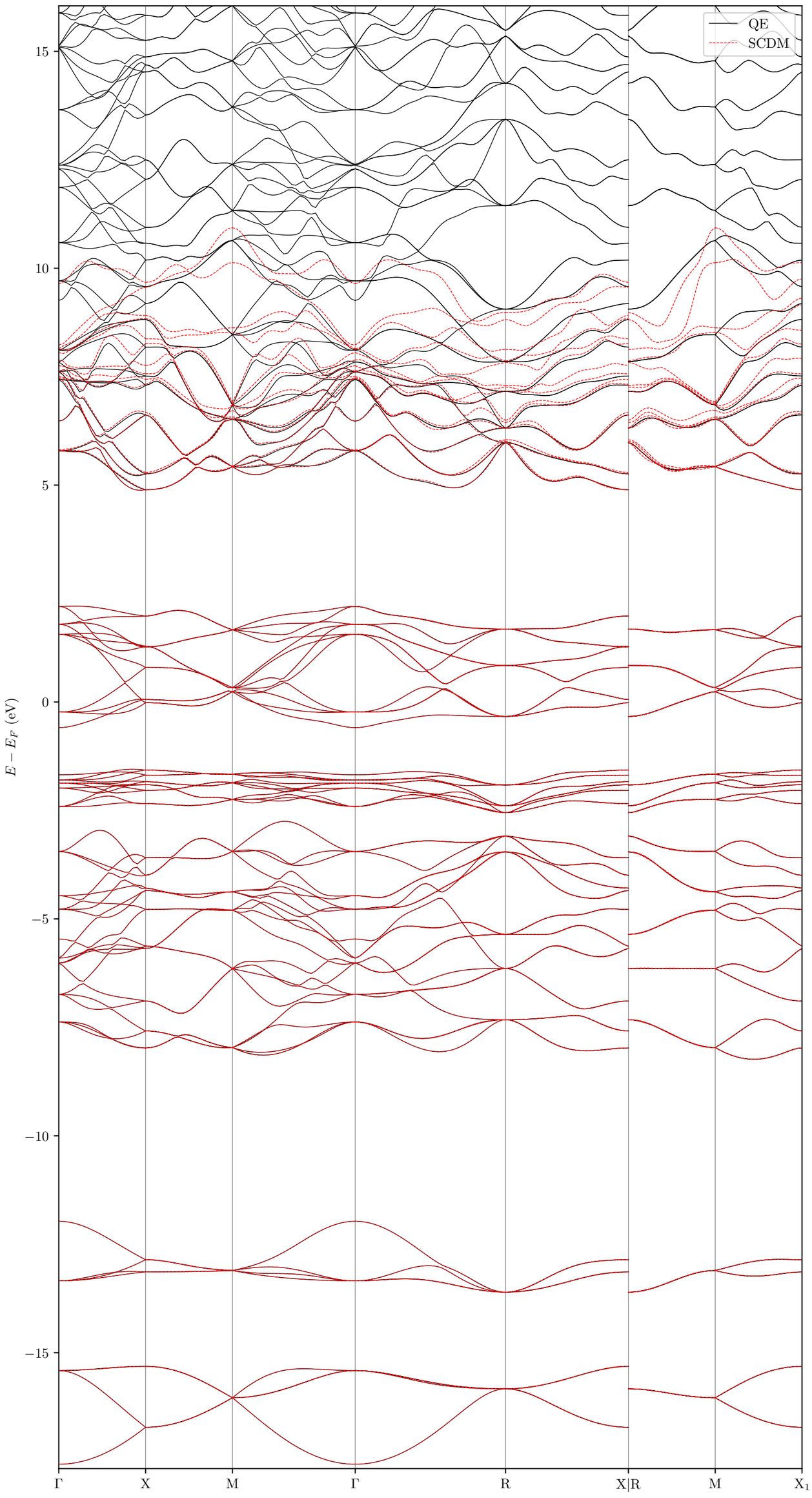
Co4S8 exclude semicore
PW=8b559b37-7c83-4e4f-b37d-0ce603be575c
W90=45789162-e646-4848-80d6-4a805269c37d




PDWF band distance (meV) and $\tau$ ($\AA$)

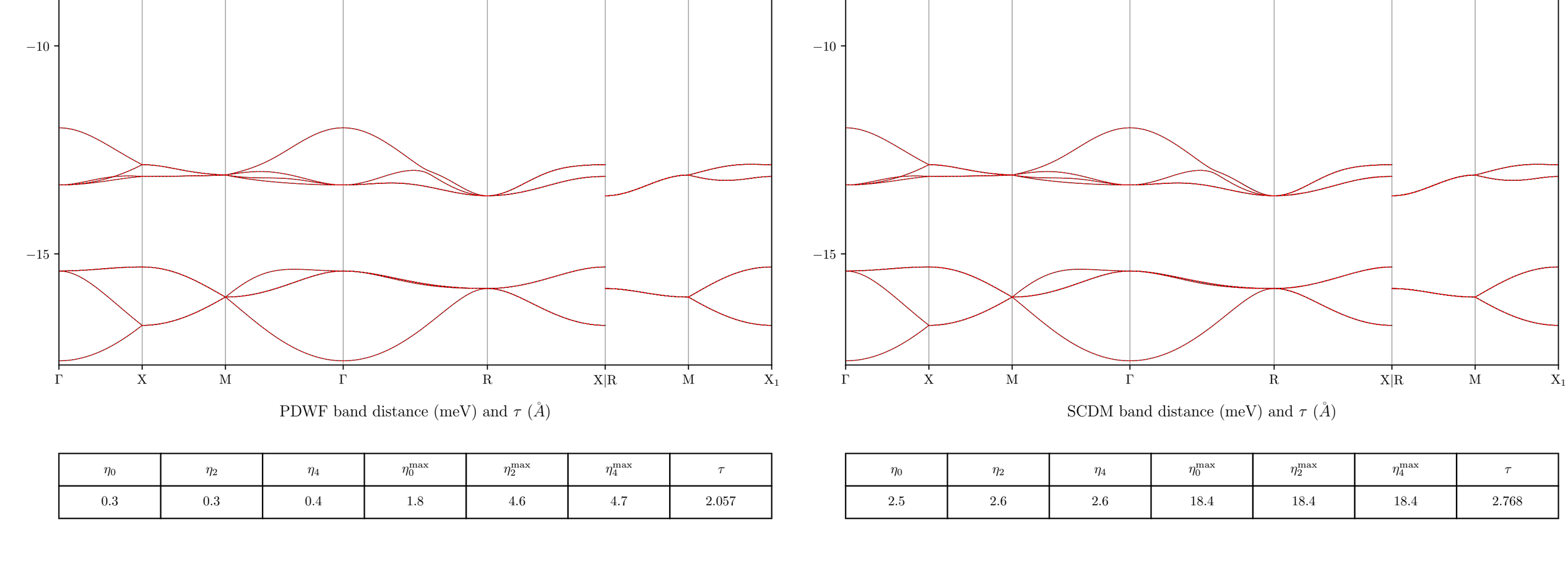
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 0.4 | 1.8 | 4.6 | 4.7 | 2.057 |

Co4S8 exclude semicore
PW=8b559b37-7c83-4e4f-b37d-0ce603be575c
W90=42c1220a-94bf-4715-a943-cd1b8b27c211

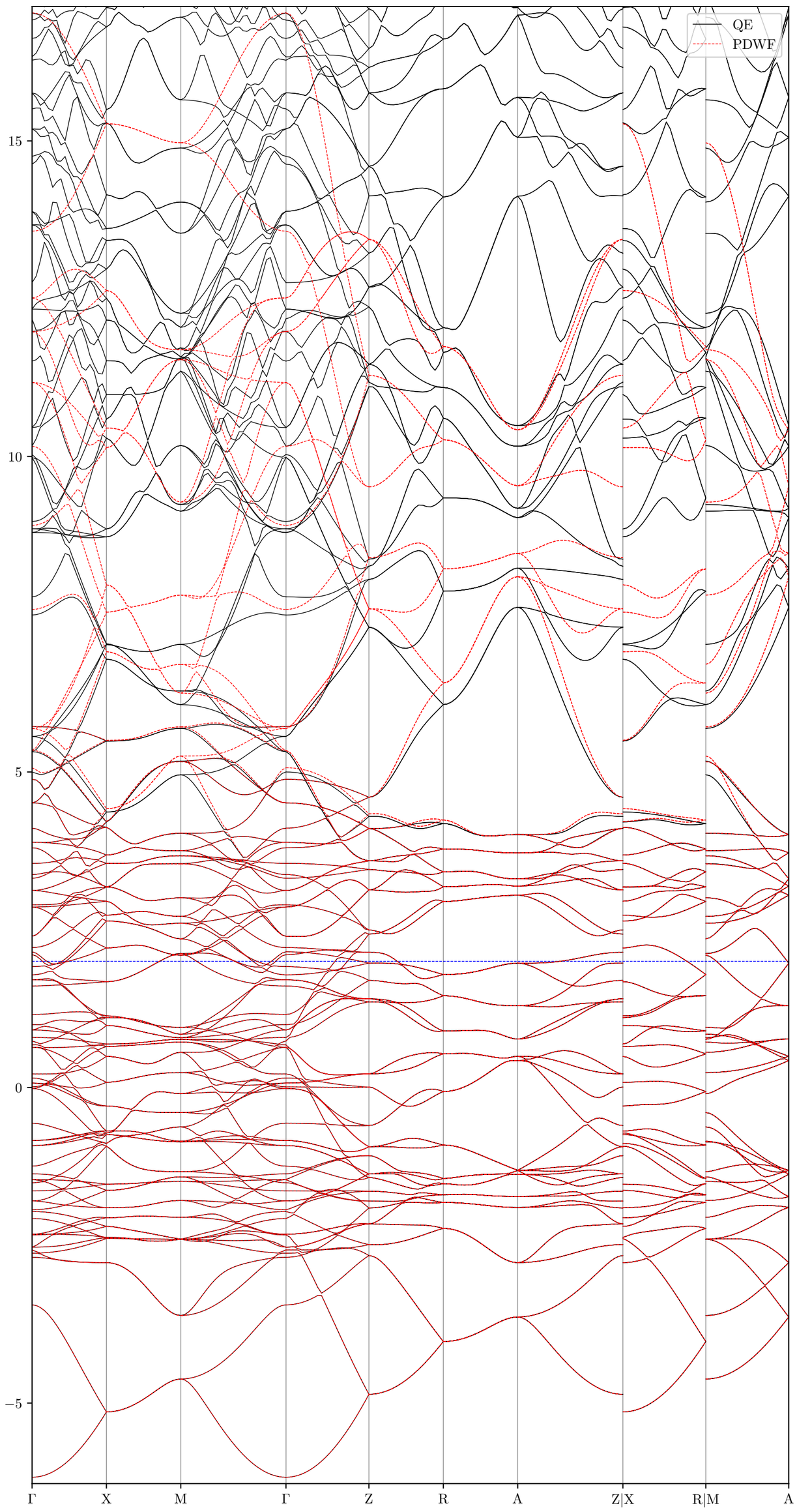



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.5 | 2.6 | 2.6 | 18.4 | 18.4 | 18.4 | 2.768 |



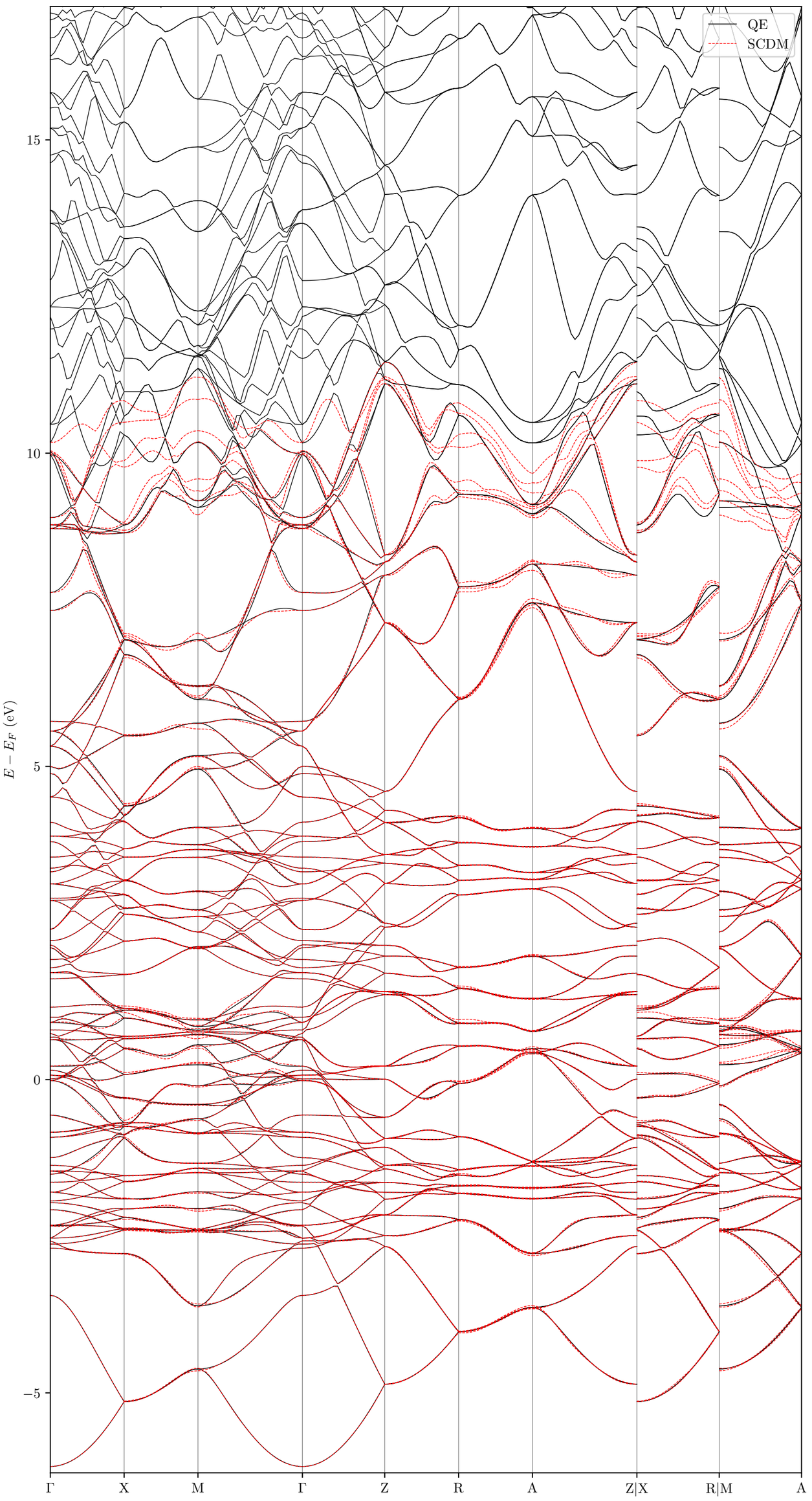
Co4Sc8 exclude semicore
PW=92f5d7f9-bd0d-4376-8e0e-89c20e6dee47
W90=2871875f-19a8-4b2d-bc60-b2e0f7496621




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.6 | 2.1 | 5.1 | 5.1 | 19.6 | 2.231 |

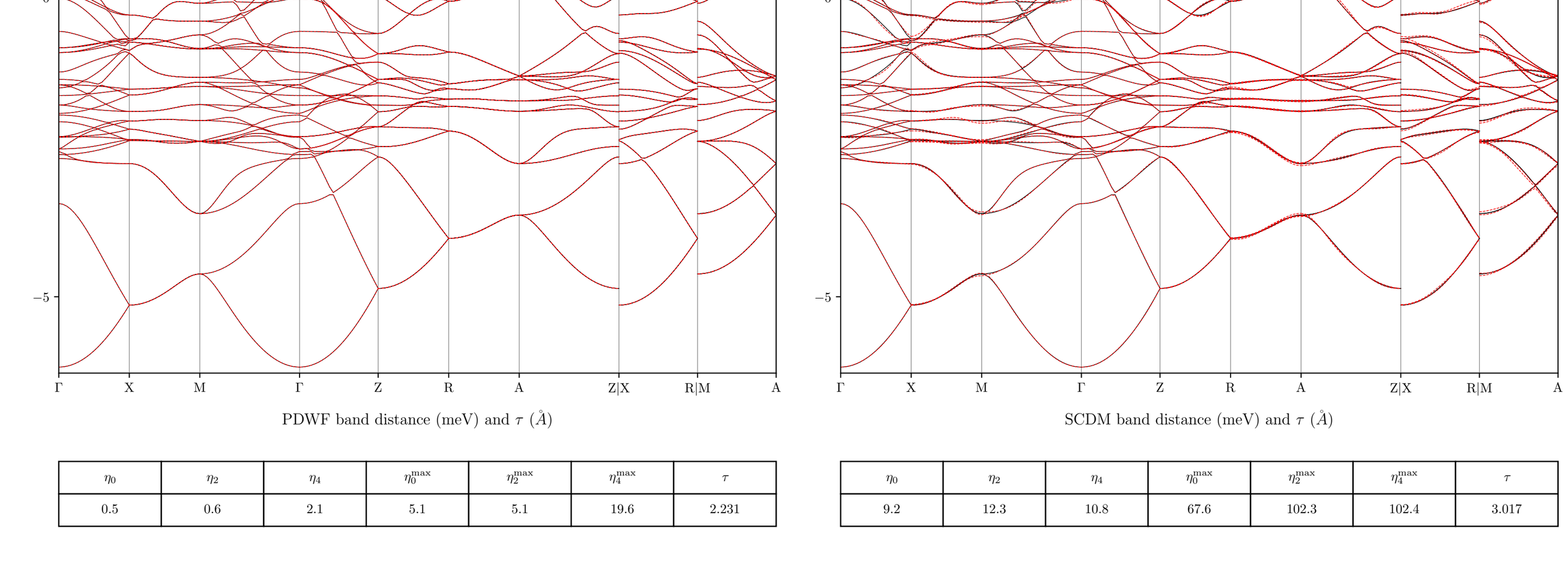
Co4Sc8 exclude semicore
PW=92f5d7f9-bd0d-4376-8e0e-89c20e6dee47
W90=4761d7fe-7579-426b-b997-c14dff12672e



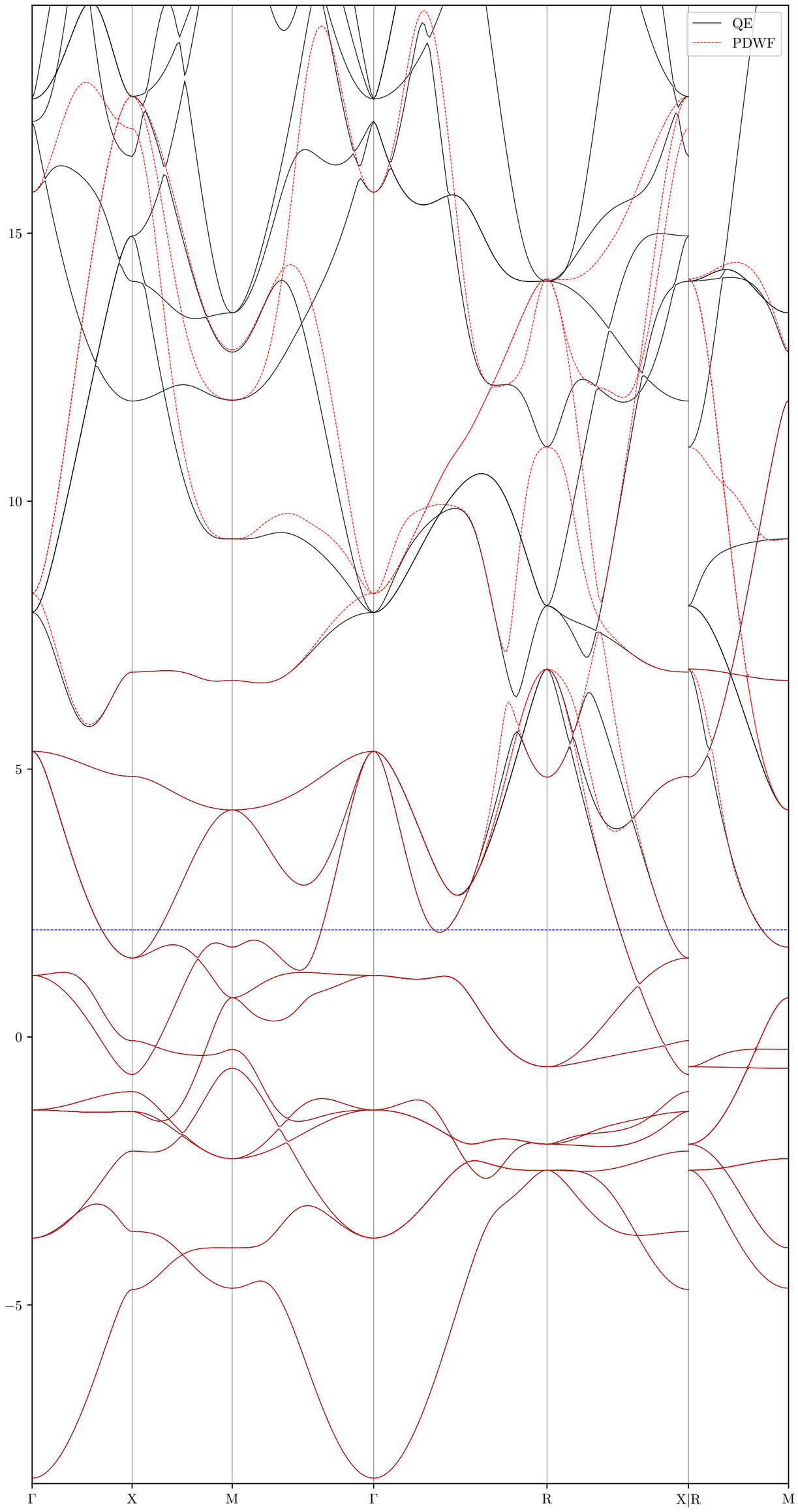

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 9.2 | 12.3 | 10.8 | 67.6 | 102.3 | 102.4 | 3.017 |

Hamiltonian decay



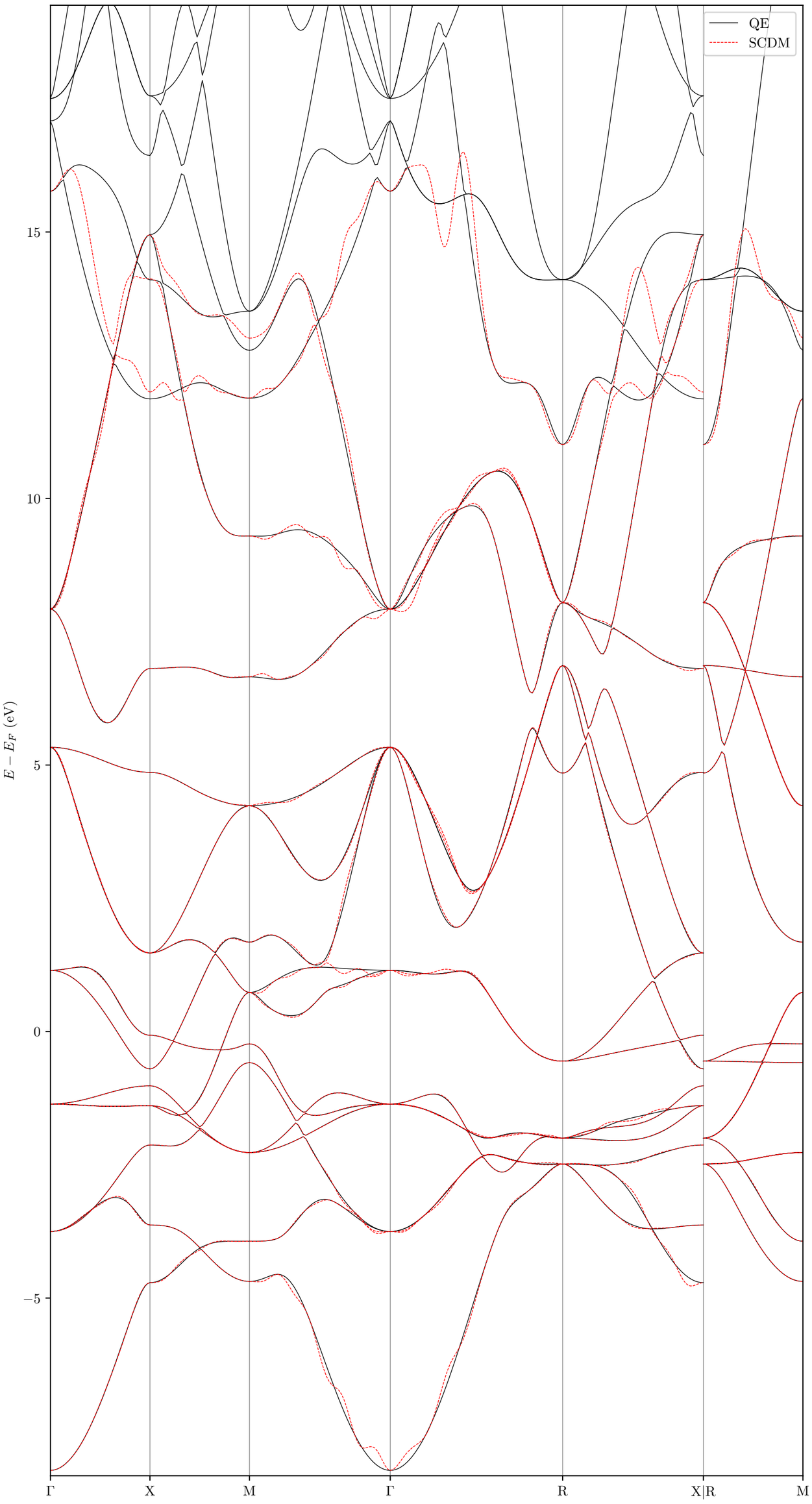
CoHf exclude semicore
PW=025b9bd8-20ed-48d5-86e2-042ea9ae5497
W90=26536c9f-959a-44d7-9914-2e08e21719d6




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.4 | 1.6 | 9.6 | 9.8 | 10.2 | 110.1 | 1.835 |

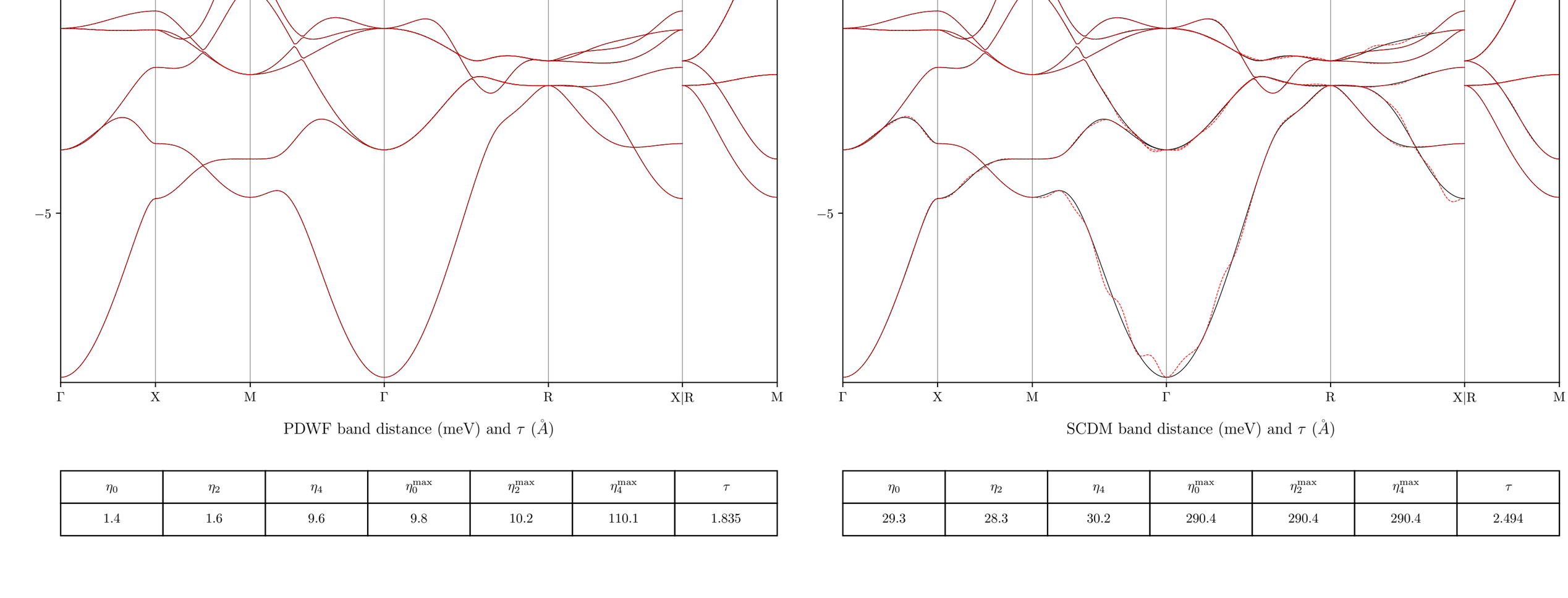
CoHf exclude semicore
PW=025b9bd8-20ed-48d5-86e2-042ea9ae5497
W90=d6483e96-6400-45f1-8642-9f10e84a651b



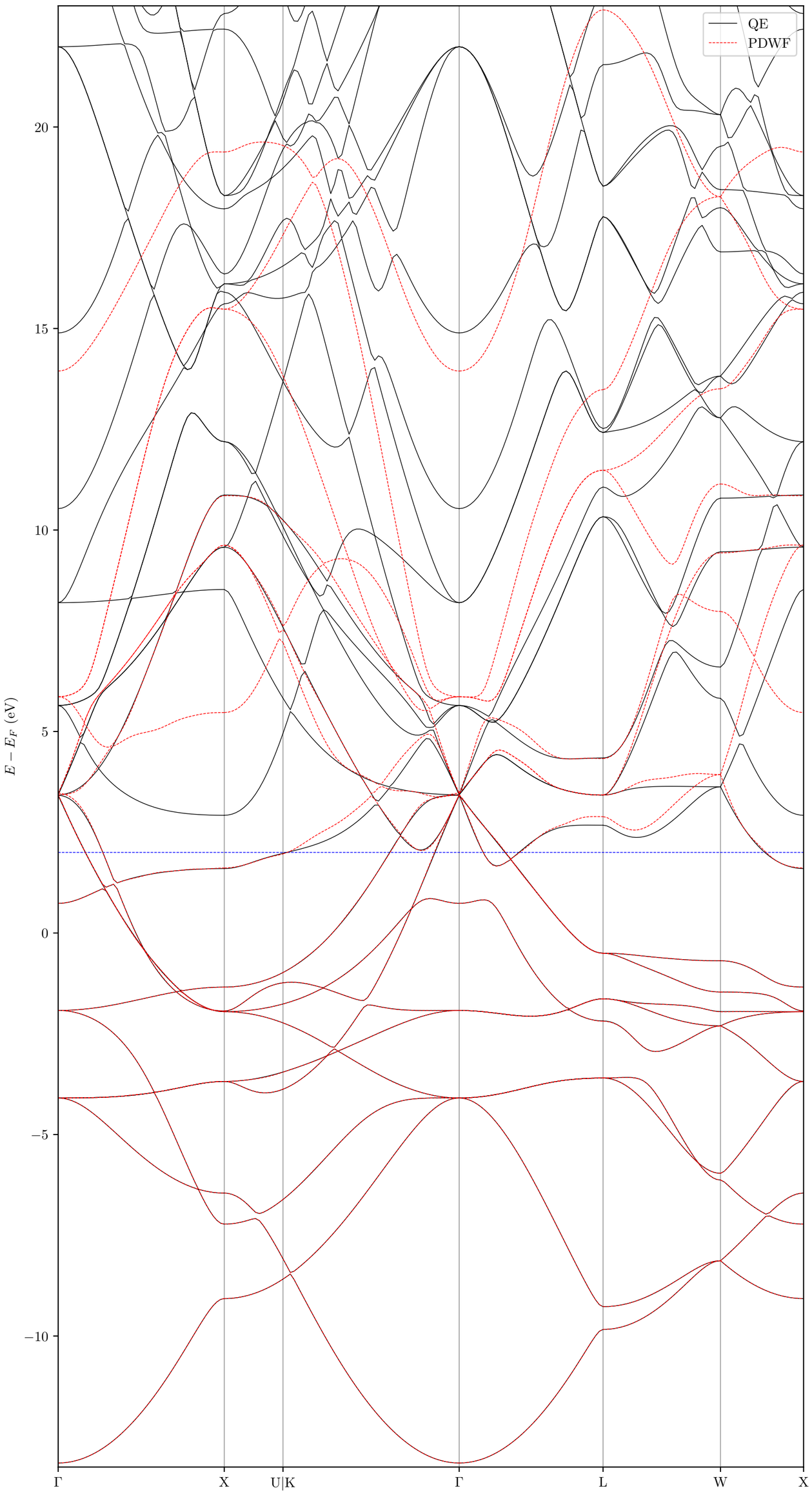

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 29.3 | 28.3 | 30.2 | 290.4 | 290.4 | 290.4 | 2.494 |

Hamiltonian decay



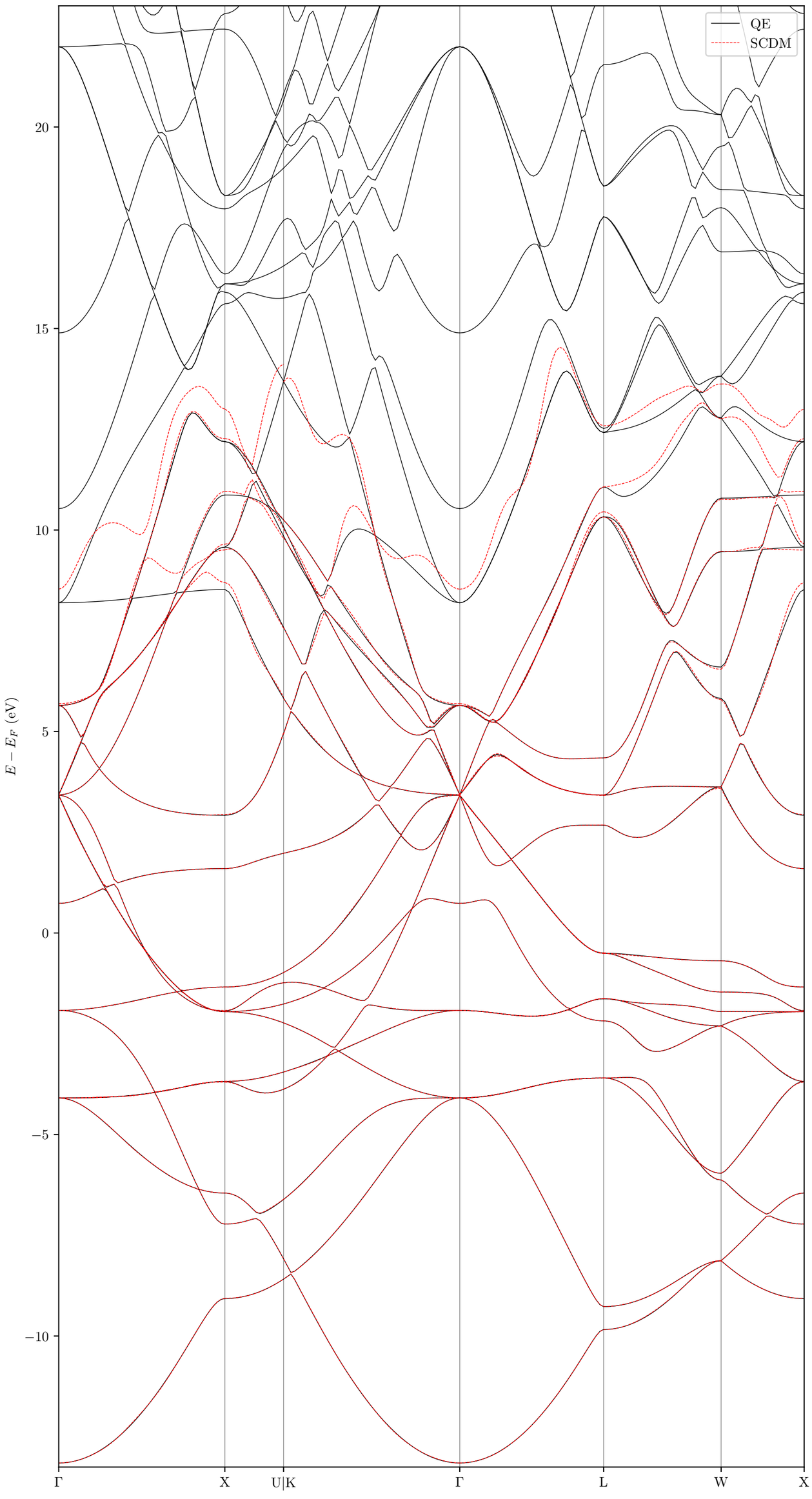
CoSi2 exclude semicore
PW=56cd322e-500e-45fe-bdc9-f774ed01d688
W90=70816441-cb97-4615-876b-b2fc0b110308




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.7 | 5.0 | 58.1 | 13.4 | 25.0 | 384.0 | 2.396 |

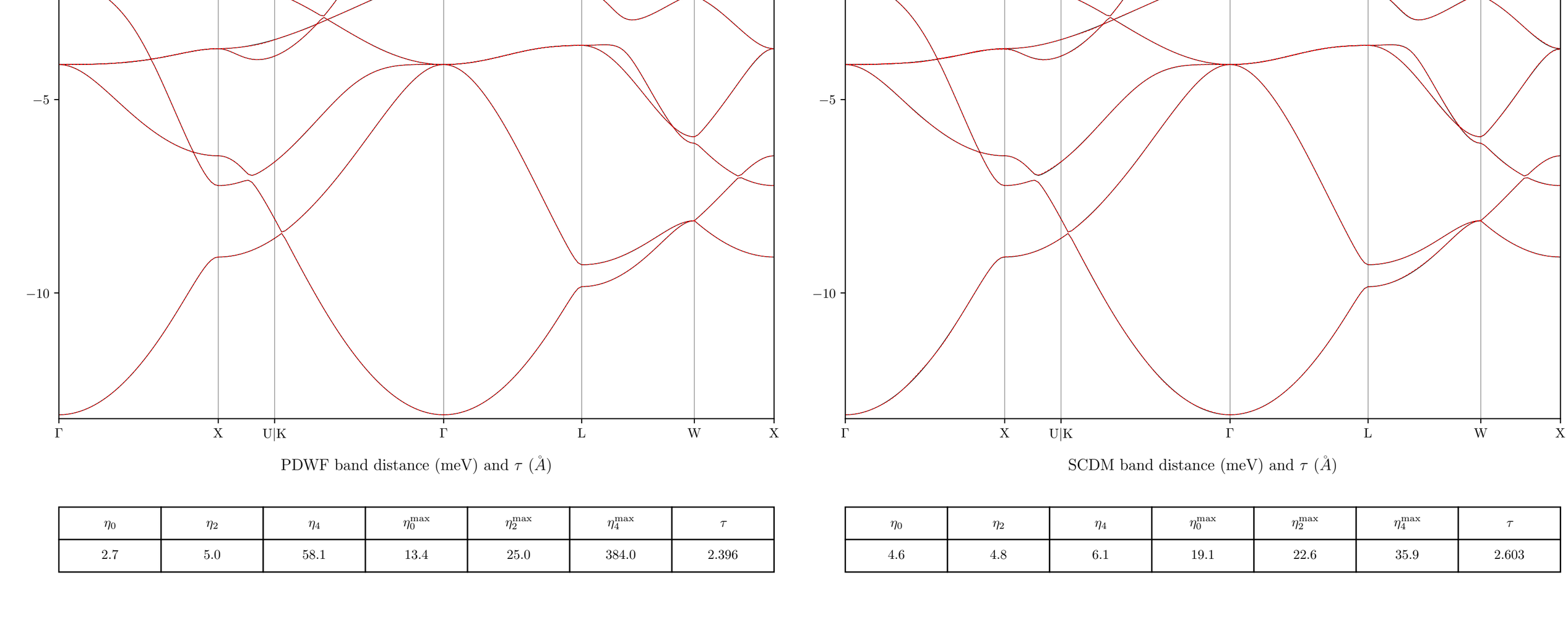
CoSi2 exclude semicore
PW=56cd322e-500e-45fe-bdc9-f774ed01d688
W90=89954637-e98c-4726-bcbc-6e09ff99af76



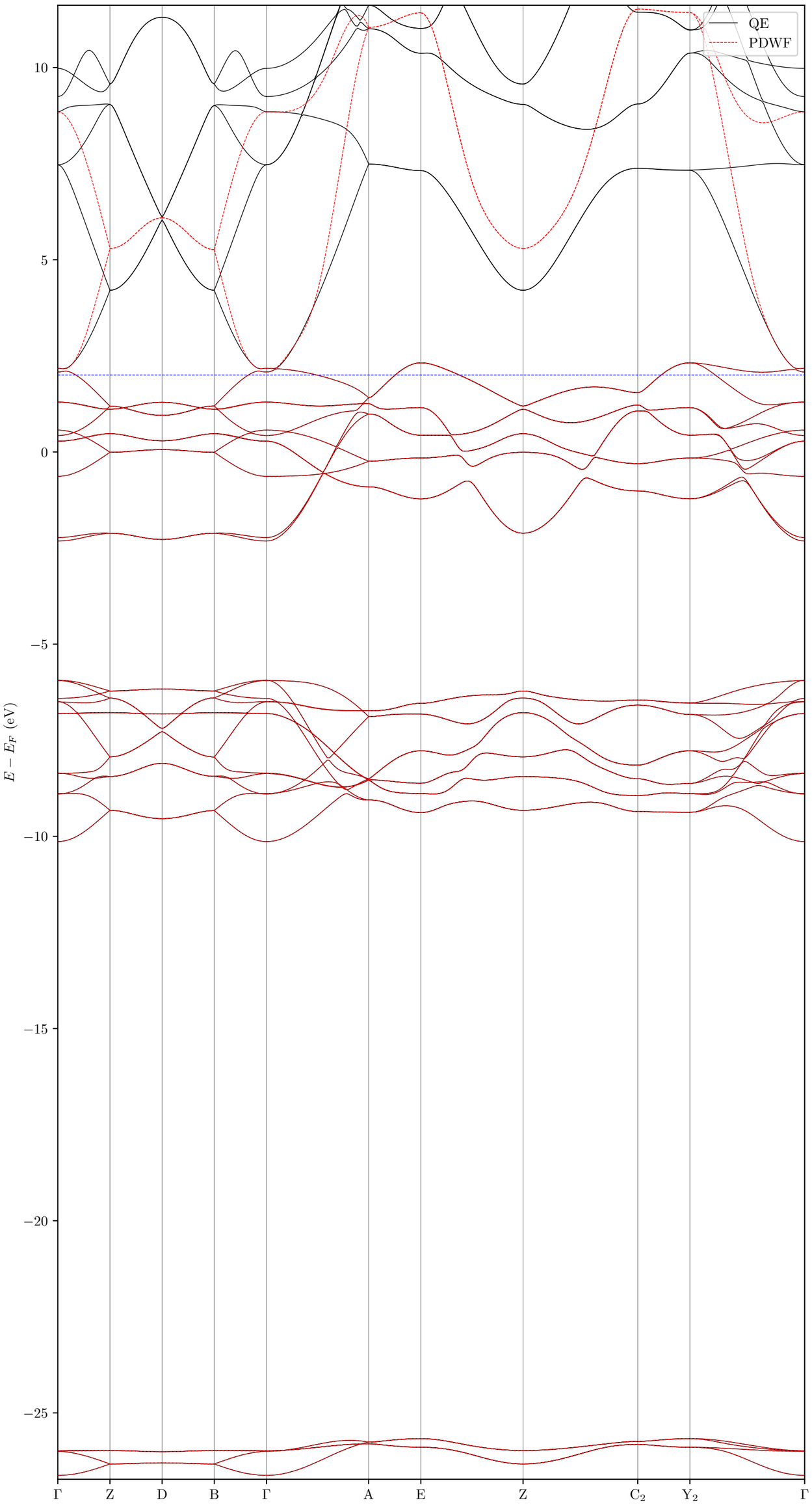

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.6 | 4.8 | 6.1 | 19.1 | 22.6 | 35.9 | 2.603 |

Hamiltonian decay



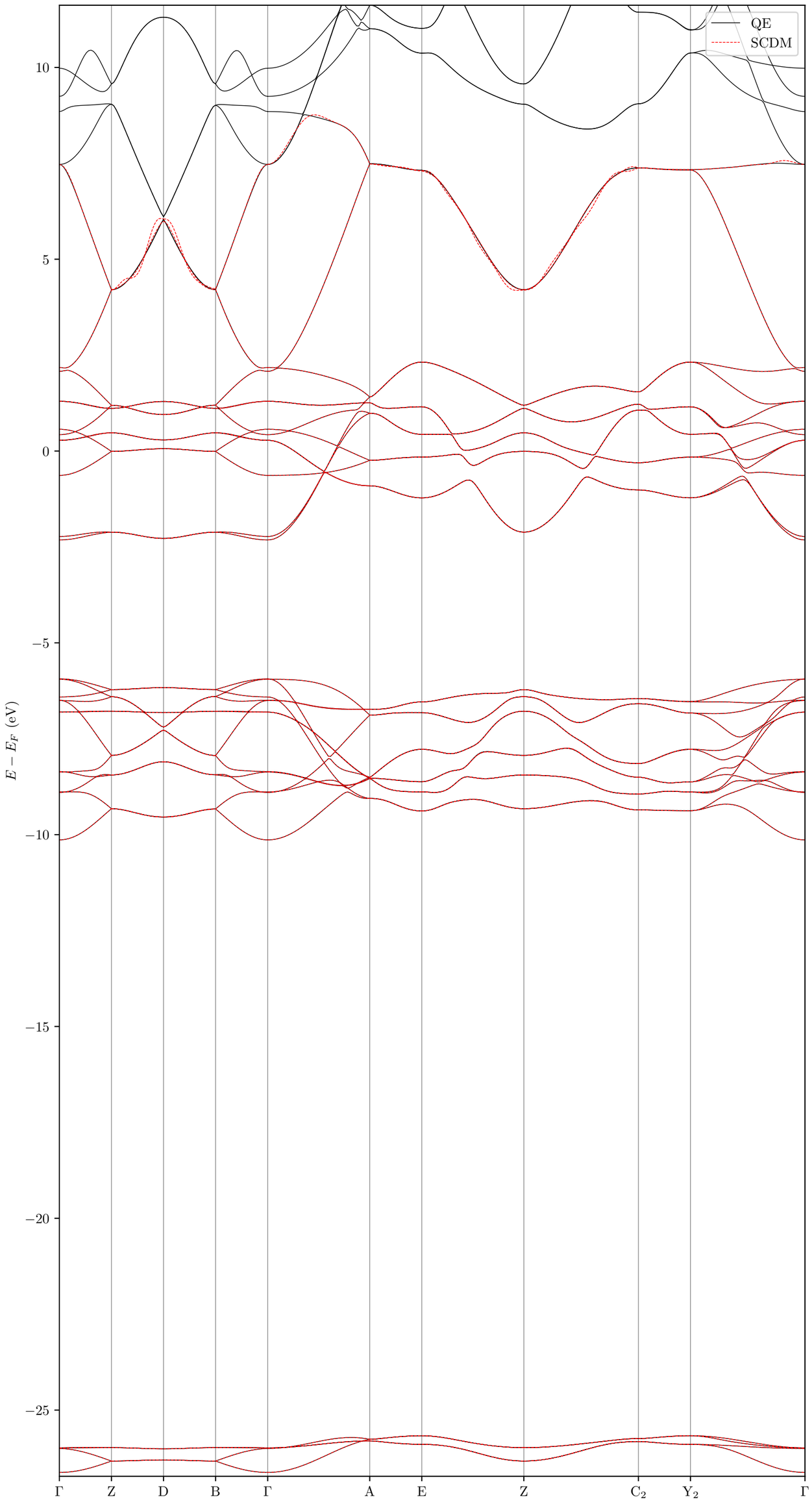
Cr2F4 exclude semicore
PW=953a29f1-9842-4d36-ab3f-1ca12fc6f62c
W90=4e78f7fa-0f9b-46ee-b31e-78fa4a144c1a




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.2 | 17.4 | 0.6 | 2.1 | 515.4 | 1.868 |

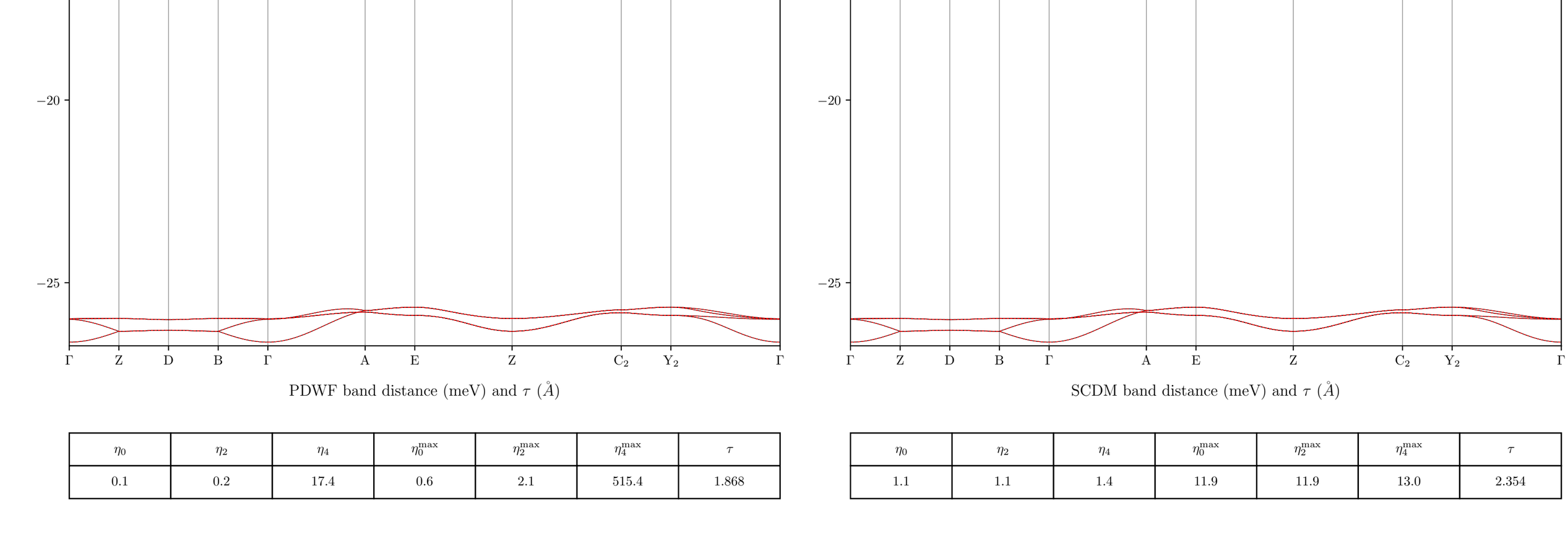
Cr2F4 exclude semicore
PW=953a29f1-9842-4d36-ab3f-1ca12fc6f62c
W90=fd83ab9e-897e-4063-be76-36a09cf204a0

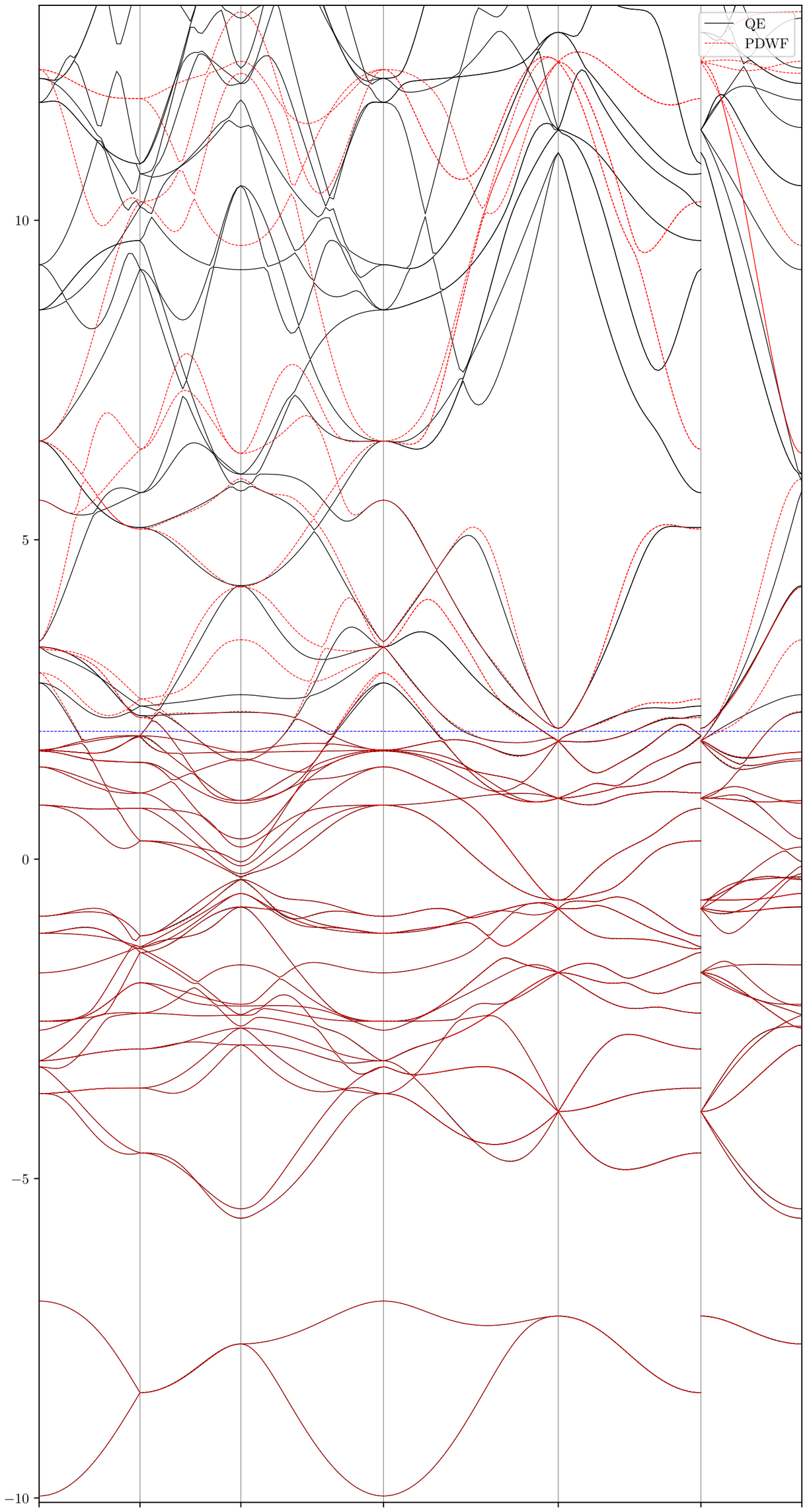



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.1 | 1.4 | 11.9 | 11.9 | 13.0 | 2.354 |

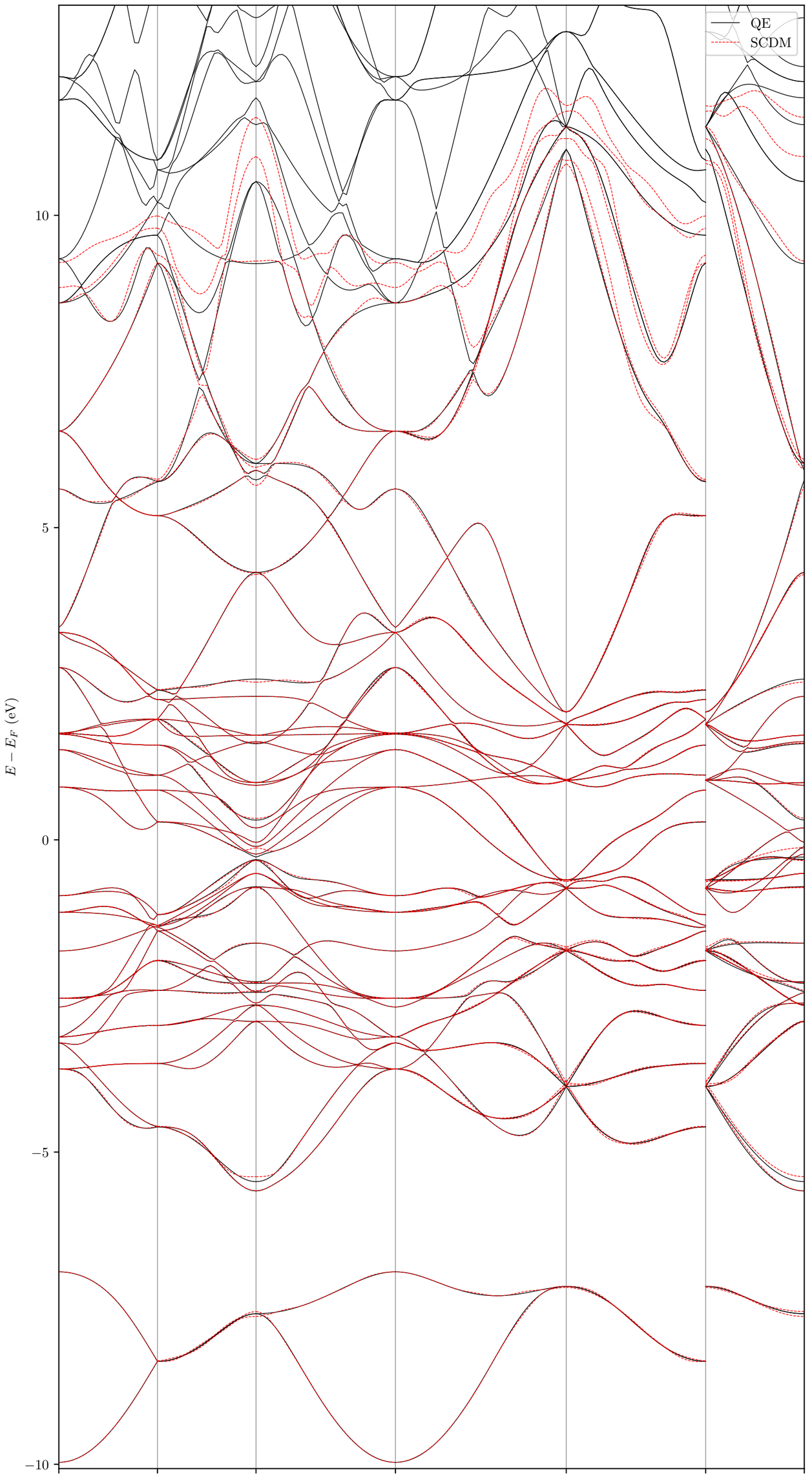
Hamiltonian decay





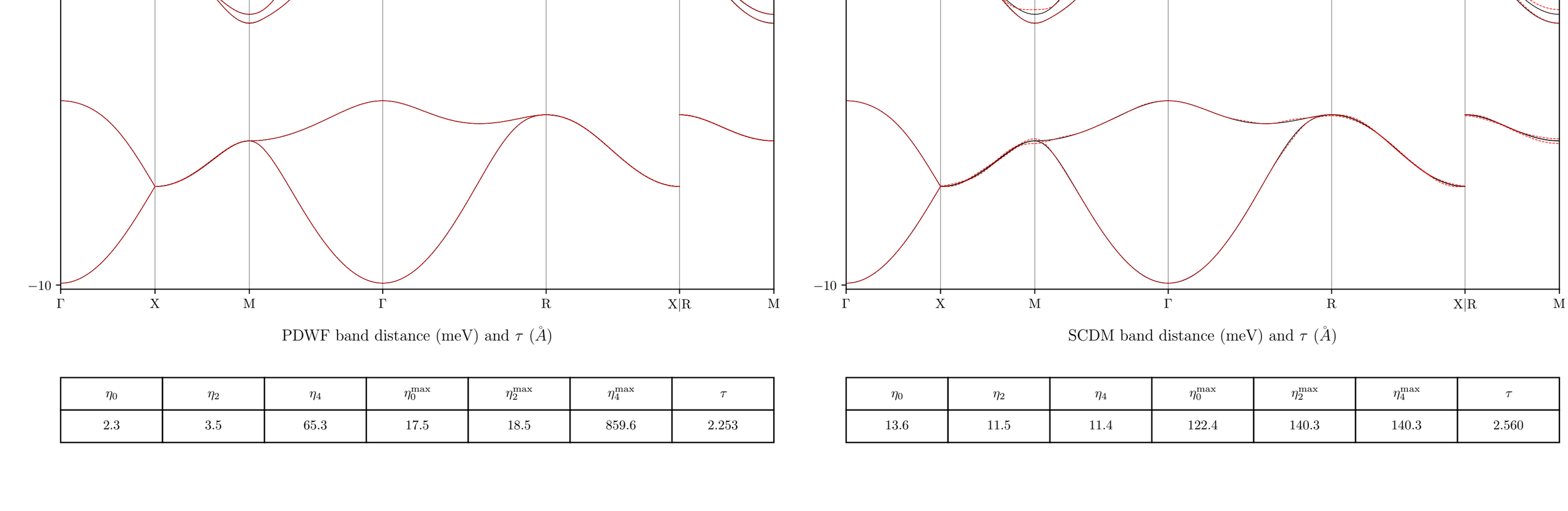

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.3 | 3.5 | 65.3 | 17.5 | 18.5 | 859.6 | 2.253 |

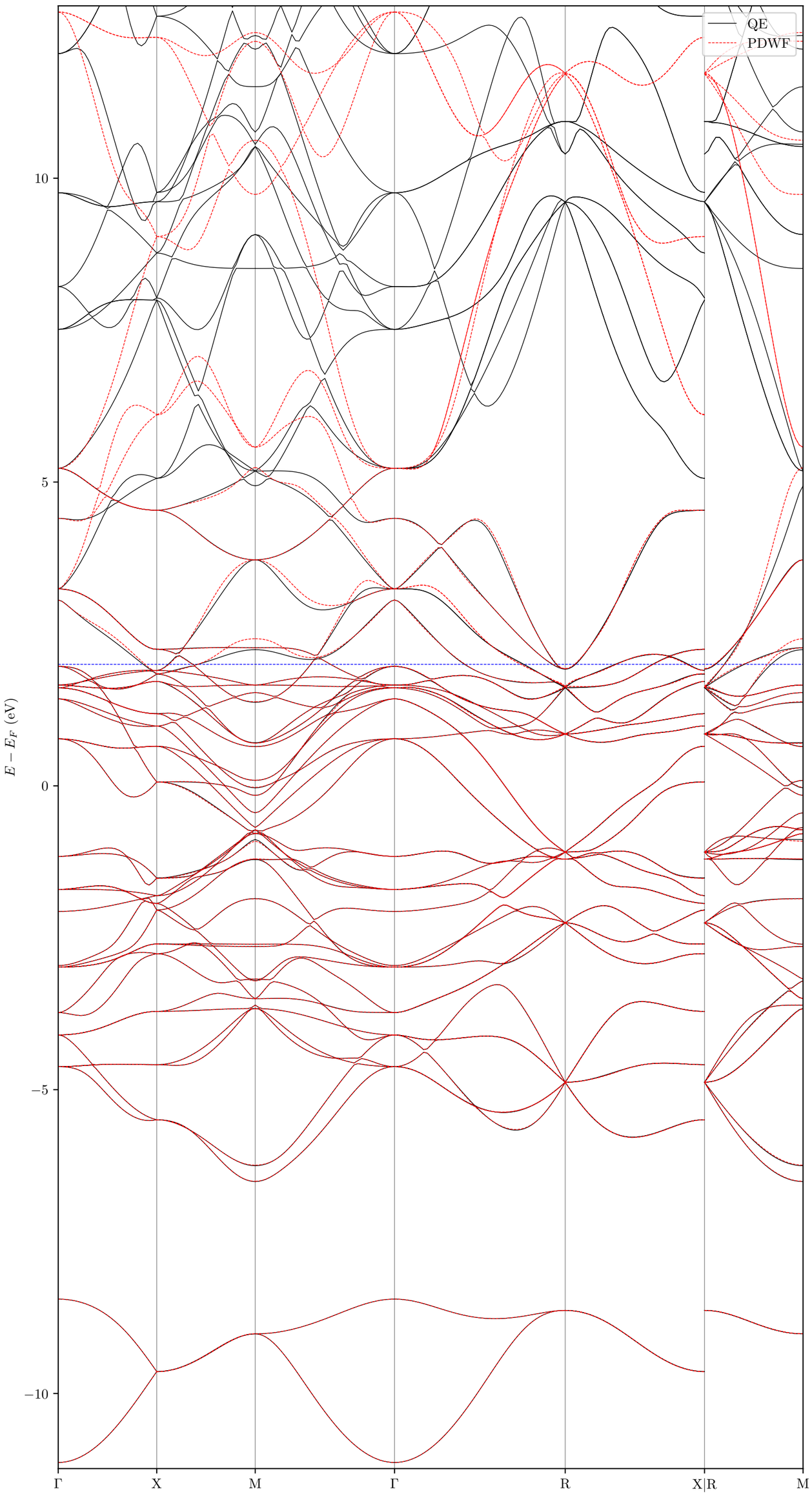



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 13.6 | 11.5 | 11.4 | 122.4 | 140.3 | 140.3 | 2.560 |



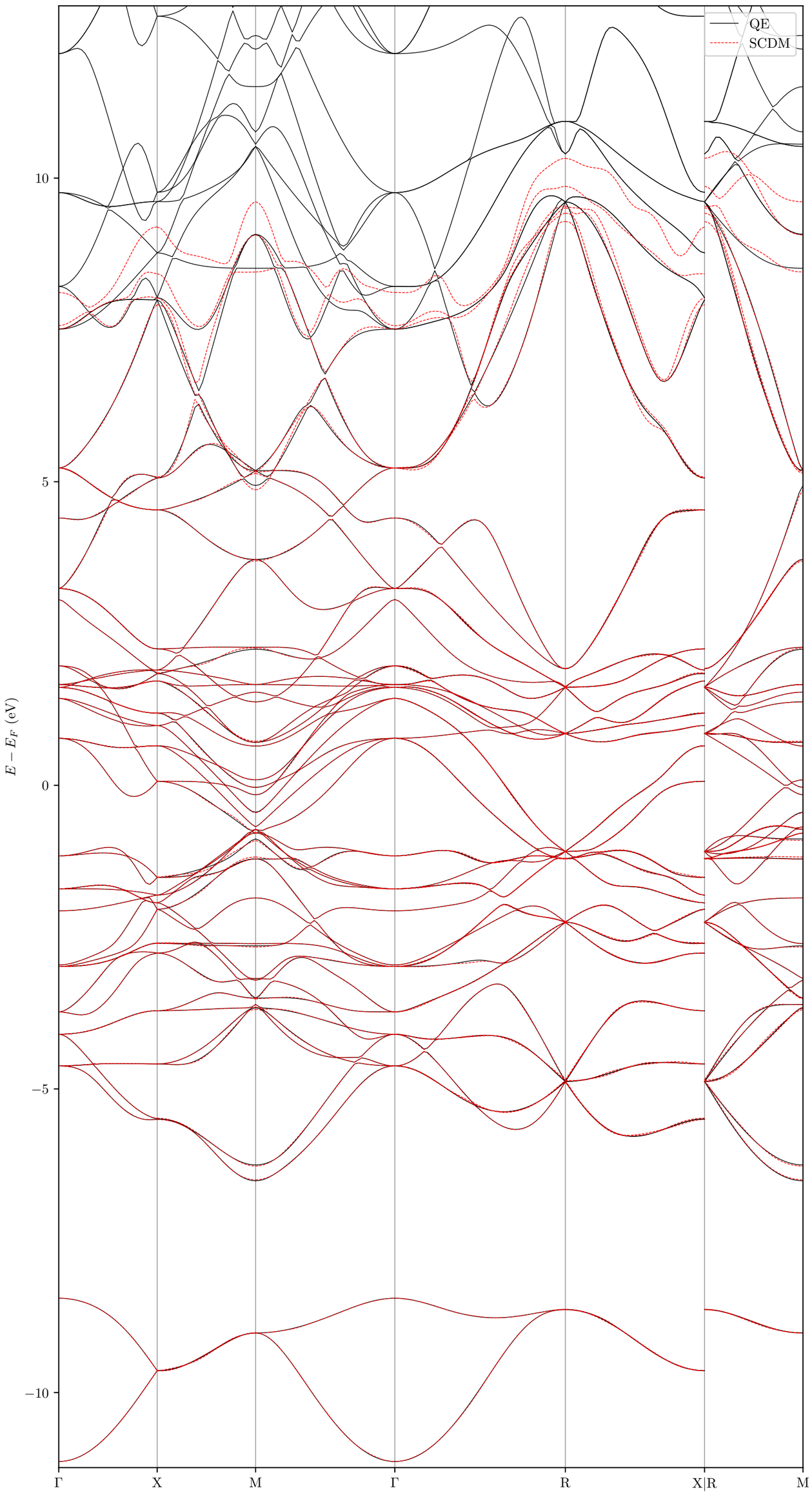
Cr6Si2 exclude semicore
PW=4beda044-05ad-4af0-bb32-44a2211a67dd
W90=0fcfcabe-38fc-4793-94cb-d2c59ae4b5cf




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.7 | 4.3 | 17.2 | 27.3 | 35.2 | 319.2 | 2.236 |

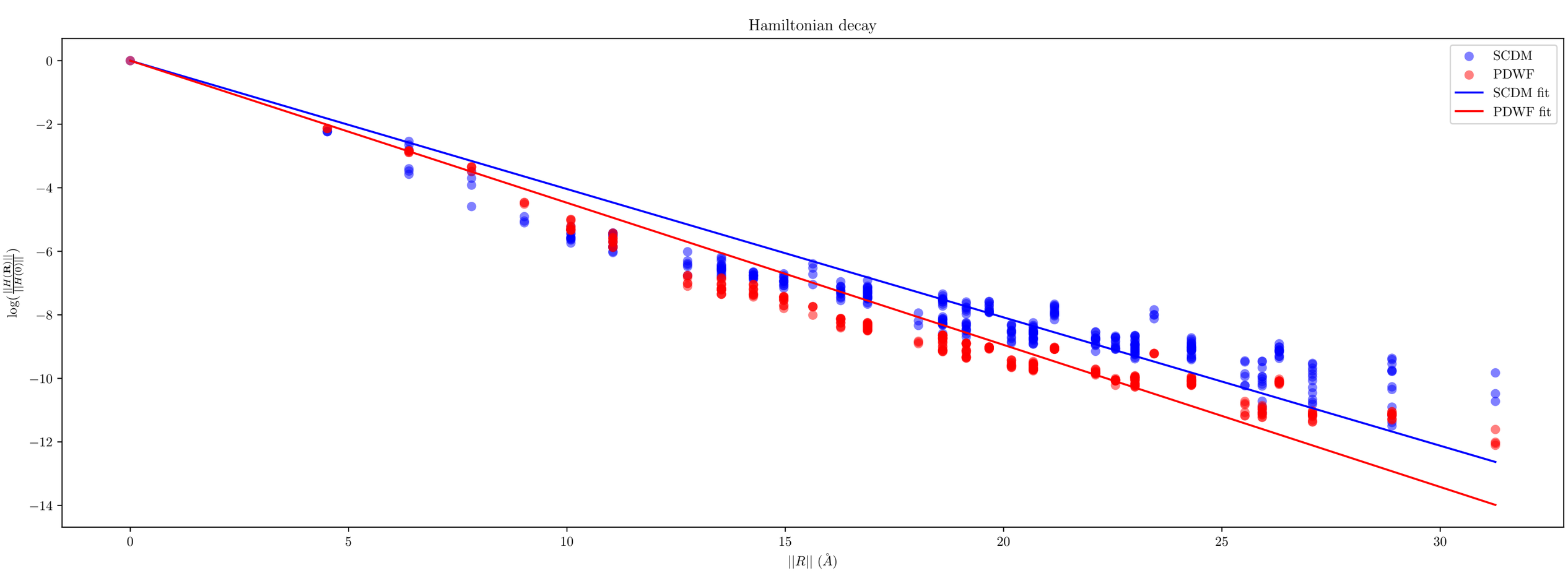
Cr6Si2 exclude semicore
PW=4beda044-05ad-4af0-bb32-44a2211a67dd
W90=3c15c3f3-fd1b-412b-b61f-499b16a2e653



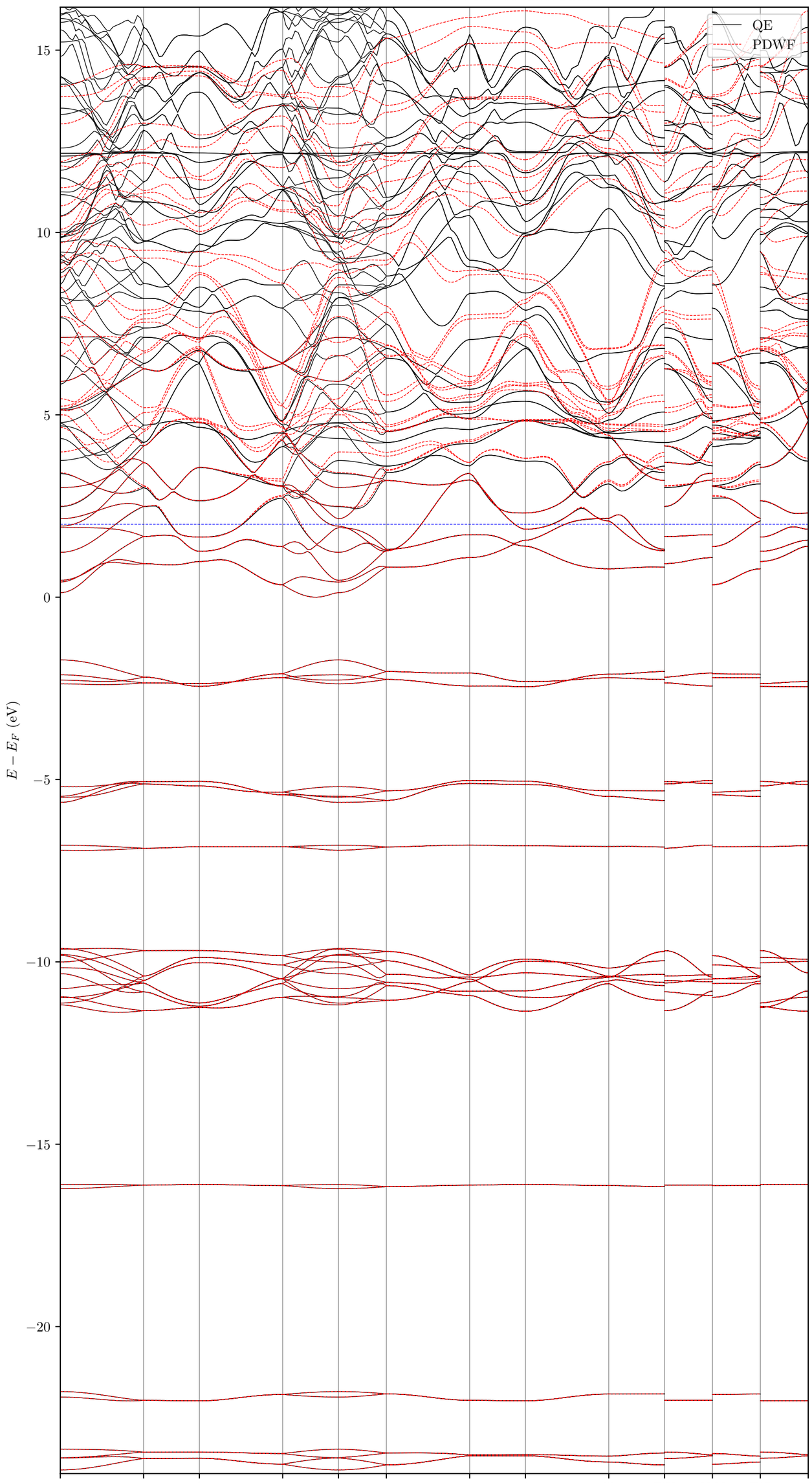

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.8 | 5.9 | 6.1 | 42.0 | 42.0 | 42.0 | 2.475 |

Hamiltonian decay



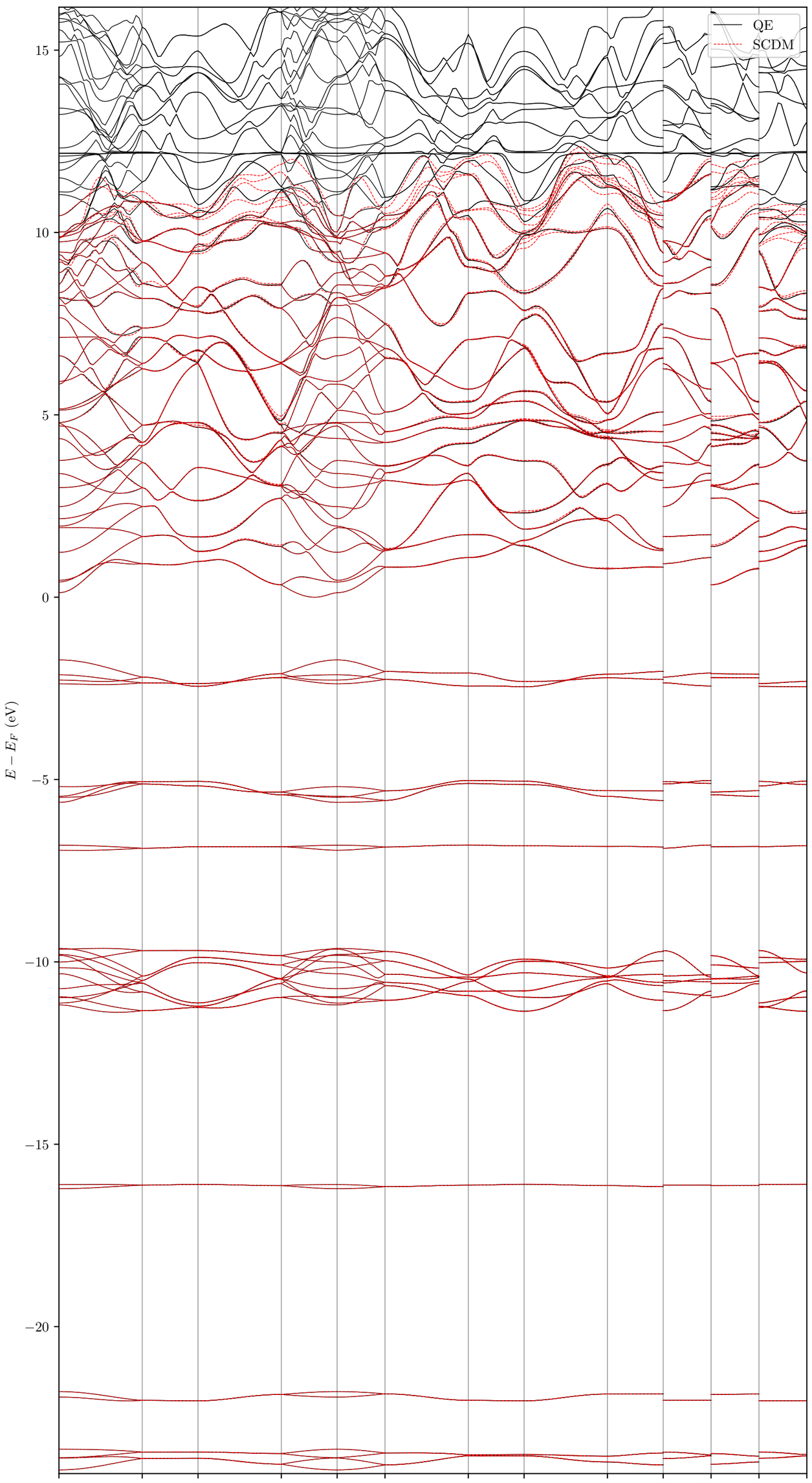
Cs4O4 **INCLUDE** semicore
PW=57eb31c9-3e55-4aca-acd2-e333a26caba3
W90=99da46b7-d768-4bb6-84d9-b552ac61dddb




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.3 | 7.8 | 8.0 | 11.1 | 113.7 | 2.683 |

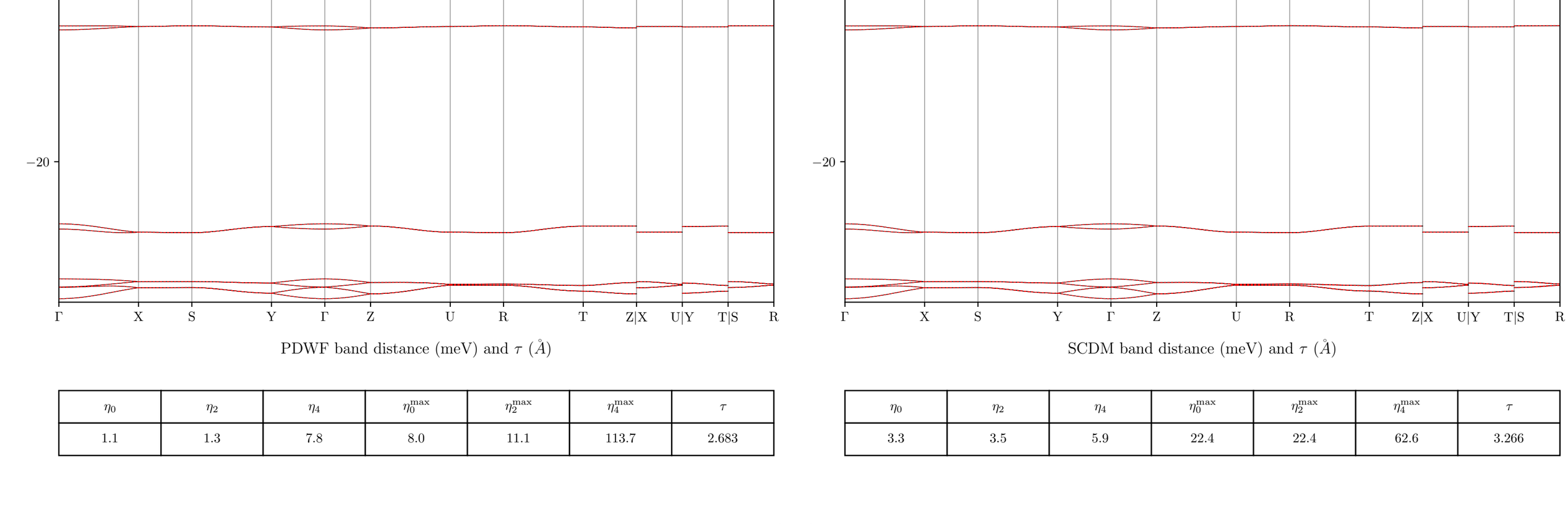
Cs4O4 **INCLUDE** semicore
PW=57eb31c9-3e55-4aca-acd2-e333a26caba3
W90=42cf498c-bac8-427b-a94b-c69d9877566e



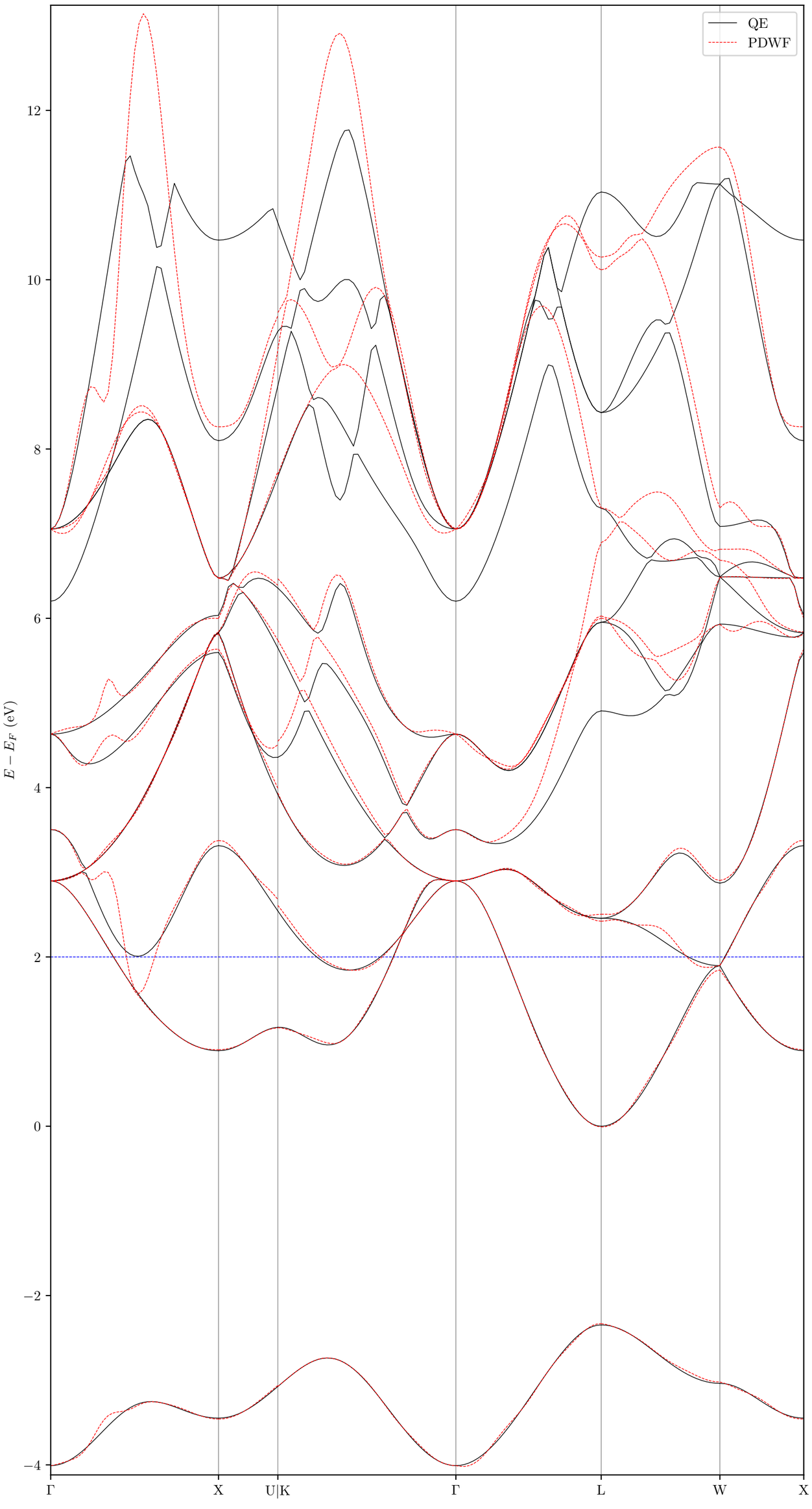

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.3 | 3.5 | 5.9 | 22.4 | 22.4 | 62.6 | 3.266 |

Hamiltonian decay



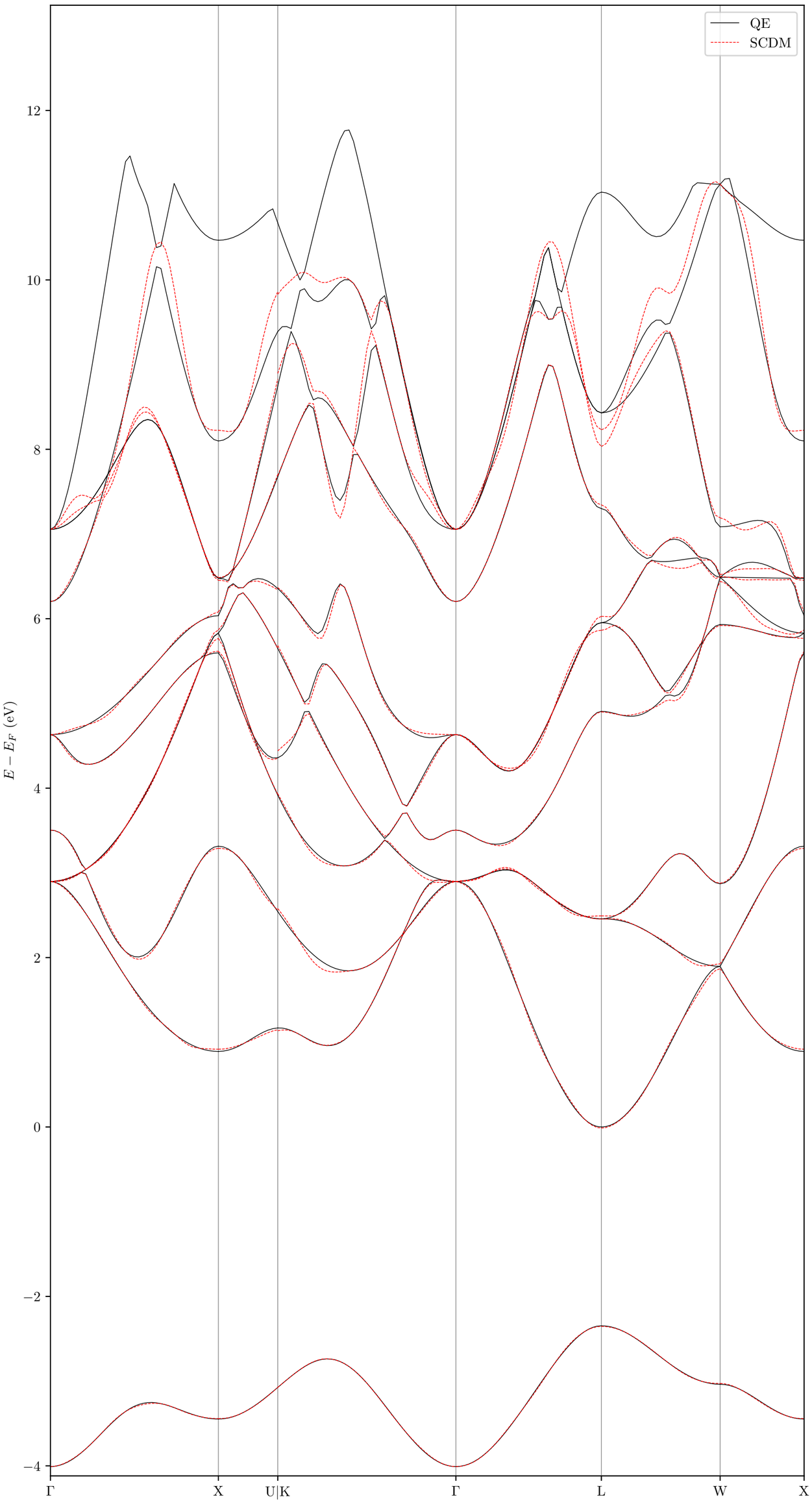
CsH exclude semicore
PW=b5e6db94-5f33-4085-b660-75f303c35bc2
W90=40662ede-e028-4207-820a-725f97be86a6




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 22.7 | 20.6 | 65.8 | 121.4 | 121.4 | 617.0 | 2.821 |

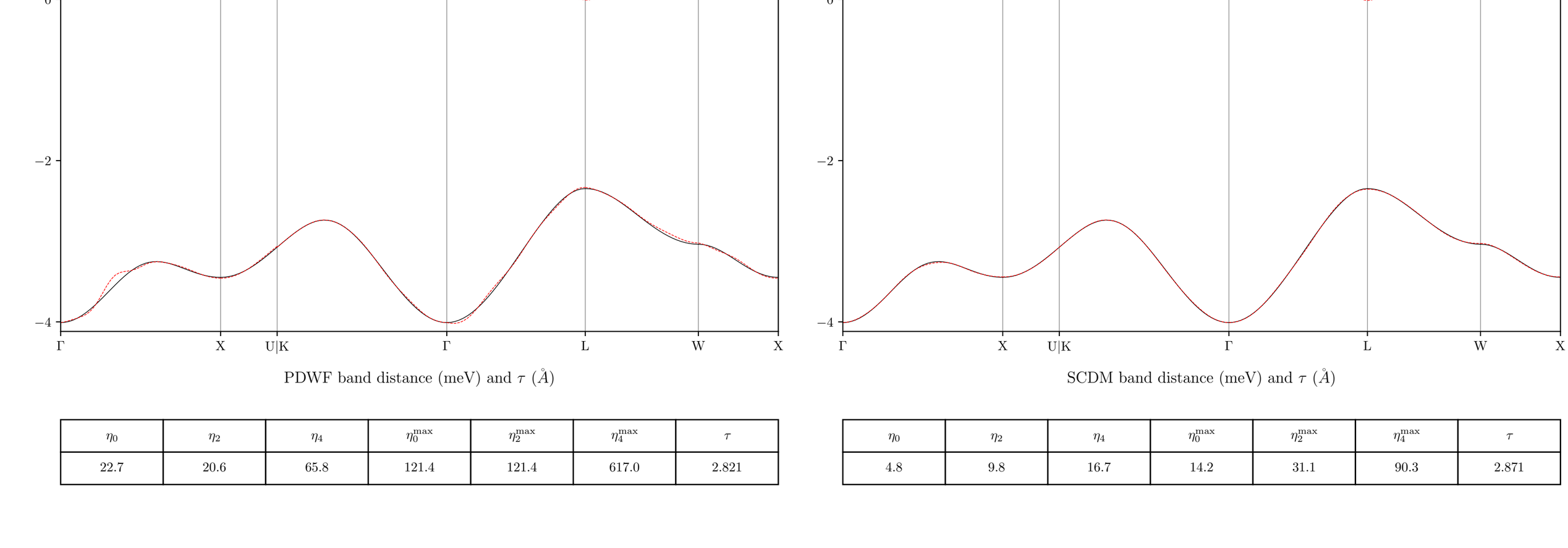
CsH exclude semicore
PW=b5e6db94-5f33-4085-b660-75f303c35bc2
W90=e719dee4-0a70-473e-97ea-7d29e16c1a9d



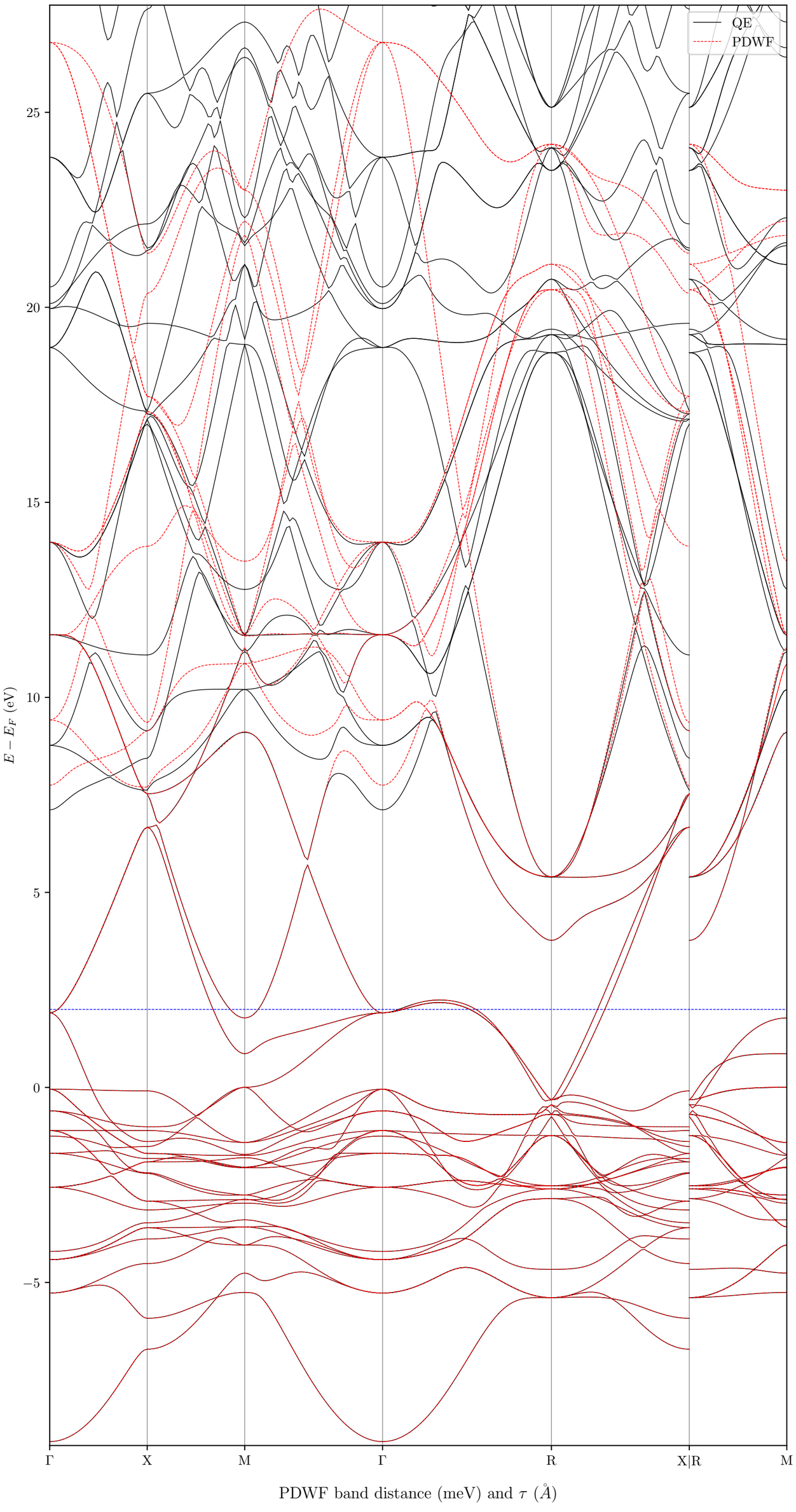

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.8 | 9.8 | 16.7 | 14.2 | 31.1 | 90.3 | 2.871 |

Hamiltonian decay



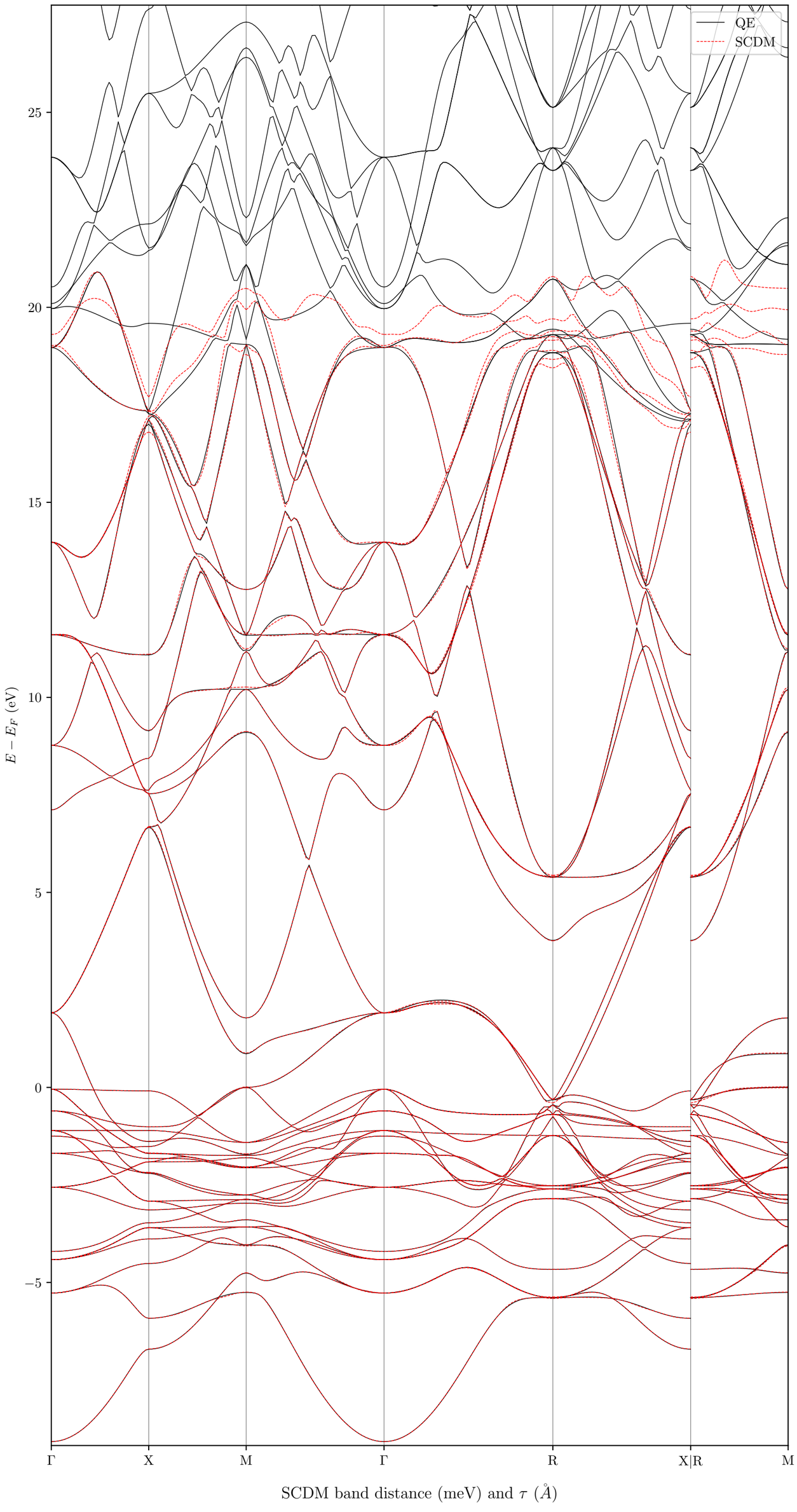
Cu3Pt exclude semicore
PW=75d73ae9-776e-4861-9eb7-dfd6efd11633
W90=196090c9-3e66-4623-9e52-e17f828c215a




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.9 | 1.1 | 1.2 | 8.8 | 8.8 | 10.5 | 2.058 |

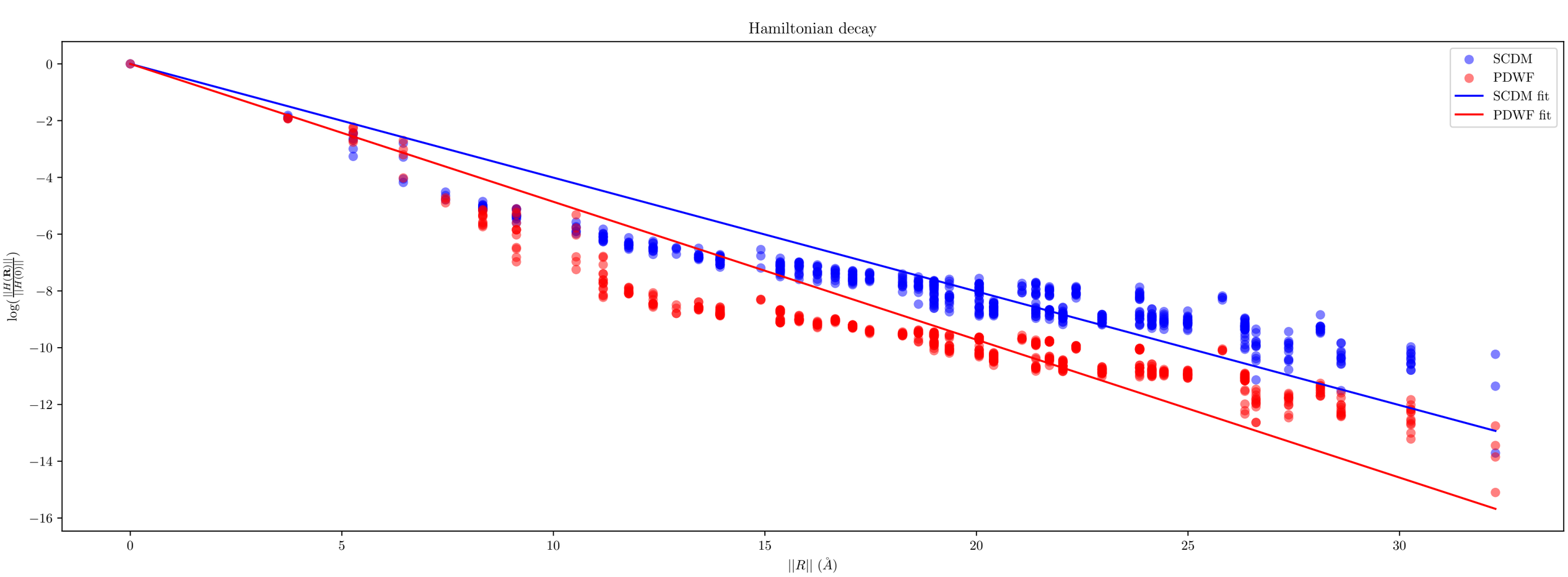
Cu3Pt exclude semicore
PW=75d73ae9-776e-4861-9eb7-dfd6efd11633
W90=4c8ceb31-7ff4-47bc-a998-9eb173d4436b



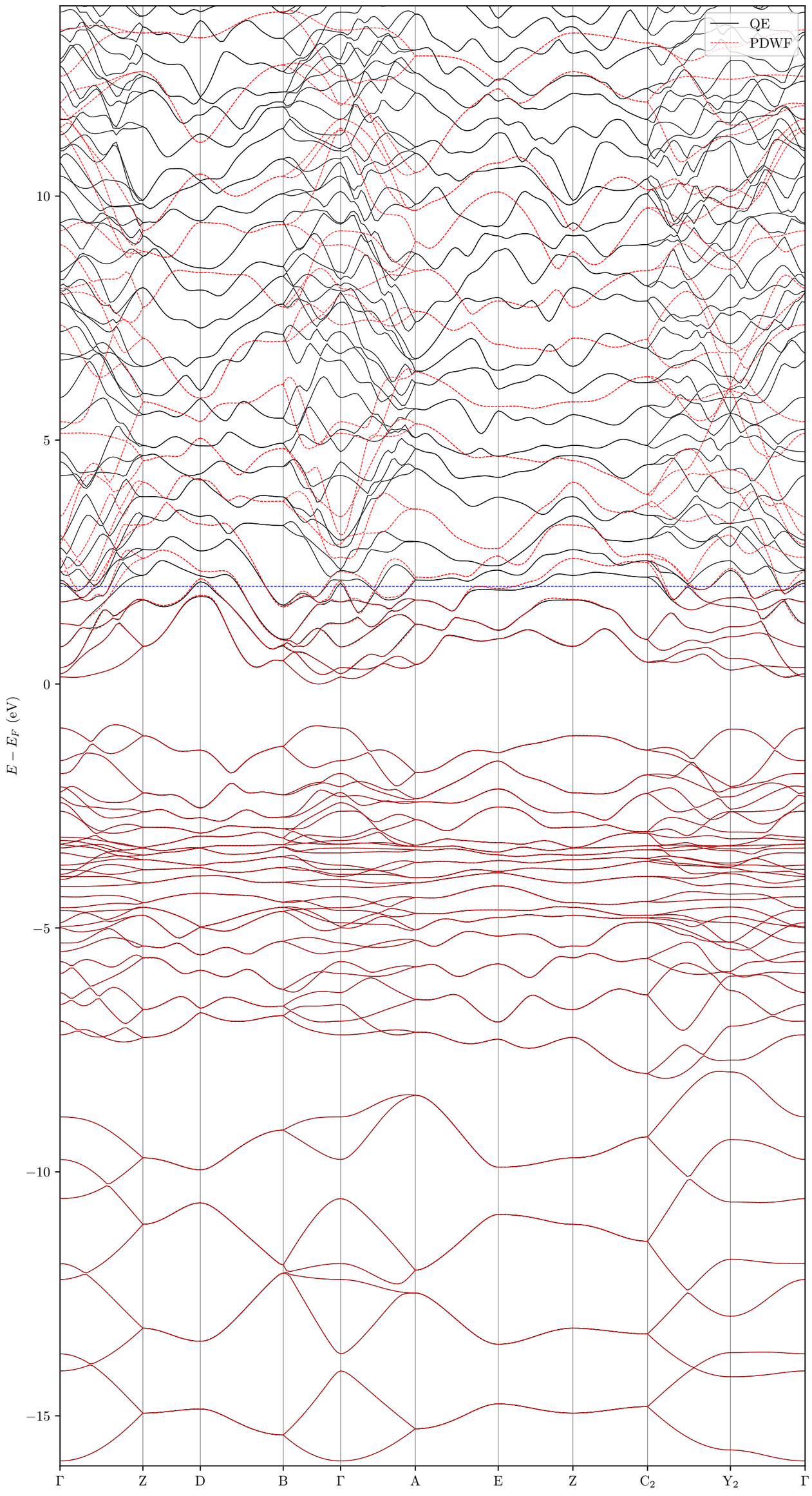

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.1 | 5.5 | 5.8 | 82.3 | 84.7 | 84.7 | 2.495 |

Hamiltonian decay



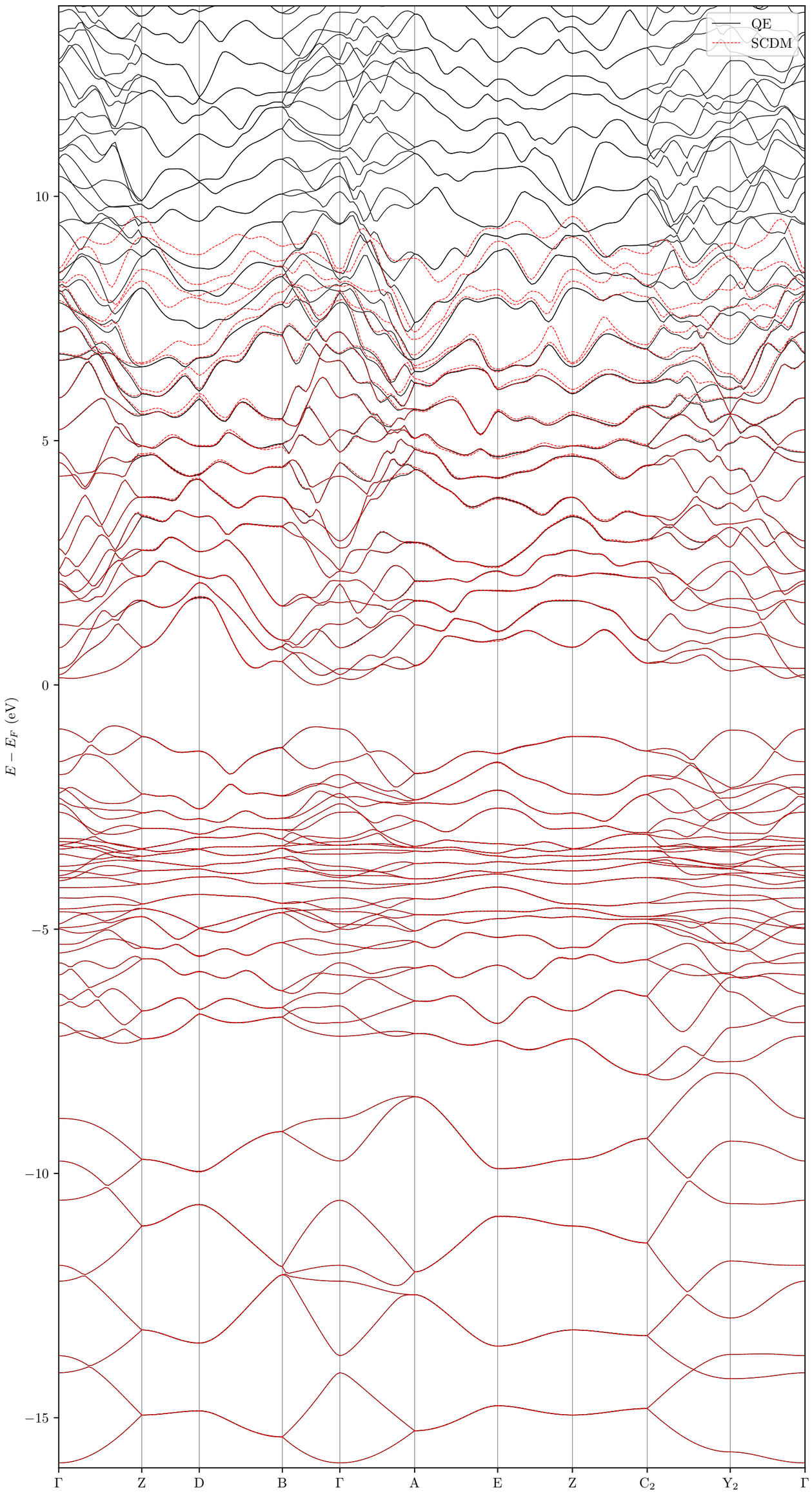
Cu4P8 exclude semicore
PW=be09ac4e-e658-4591-a1bb-fa918849f9d2
W90=b4eafccd-902c-435a-98f6-dd14d4003e71




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.4 | 4.0 | 112.0 | 8.9 | 47.3 | 684.3 | 2.682 |

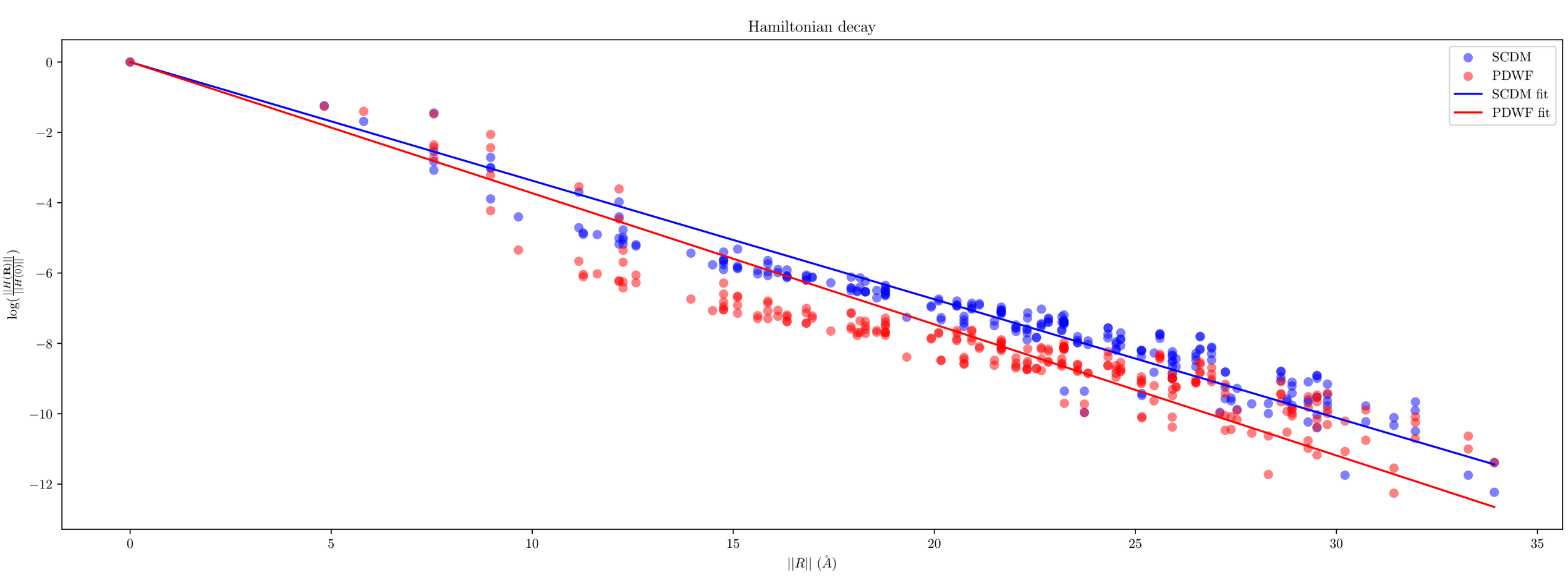
Cu4P8 exclude semicore
PW=be09ac4e-e658-4591-a1bb-fa918849f9d2
W90=3a9f2cc6-8000-40e6-9bb2-8ac5475061aa



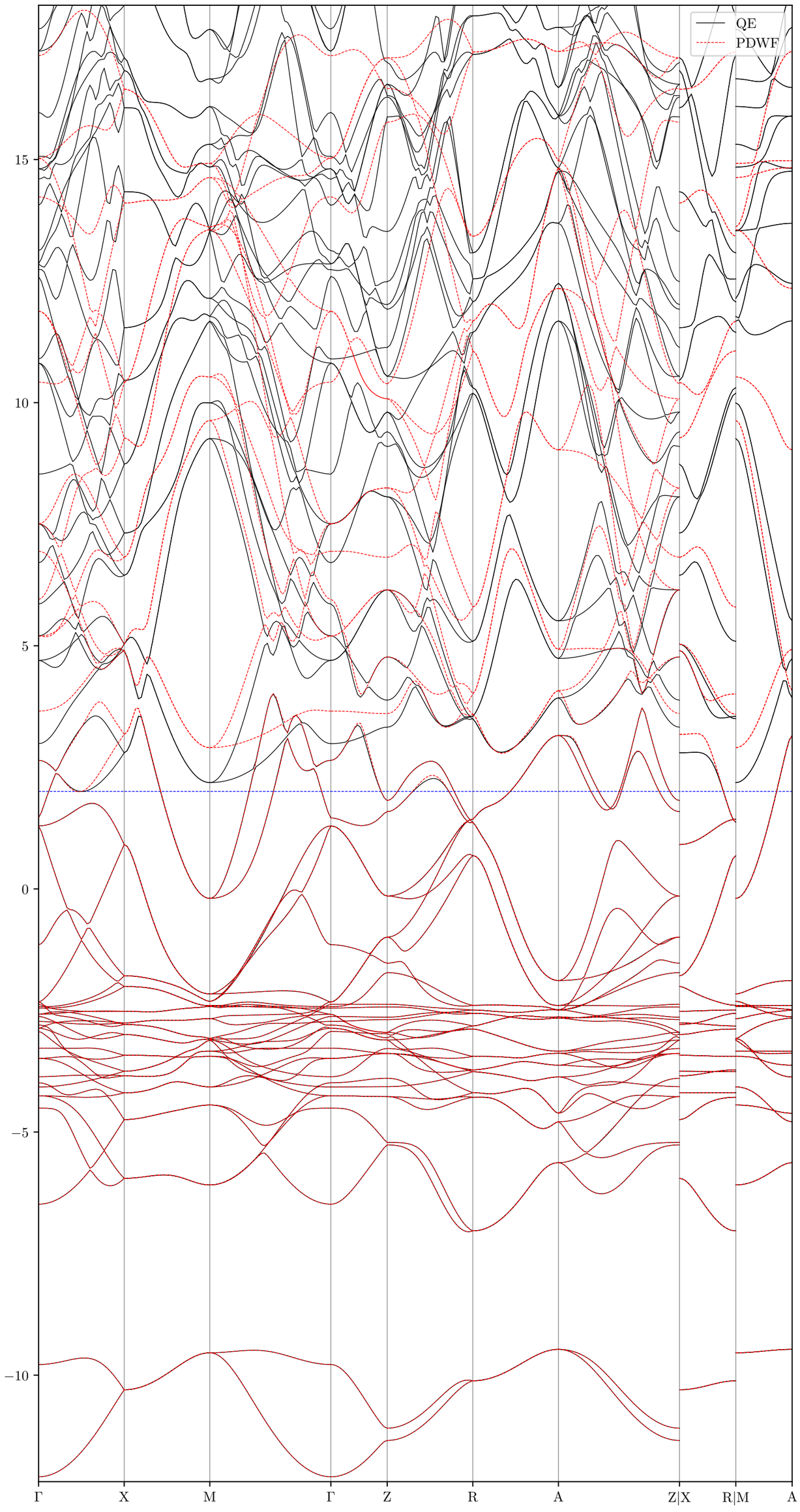

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.5 | 3.0 | 4.2 | 14.4 | 29.8 | 30.5 | 2.965 |

Hamiltonian decay



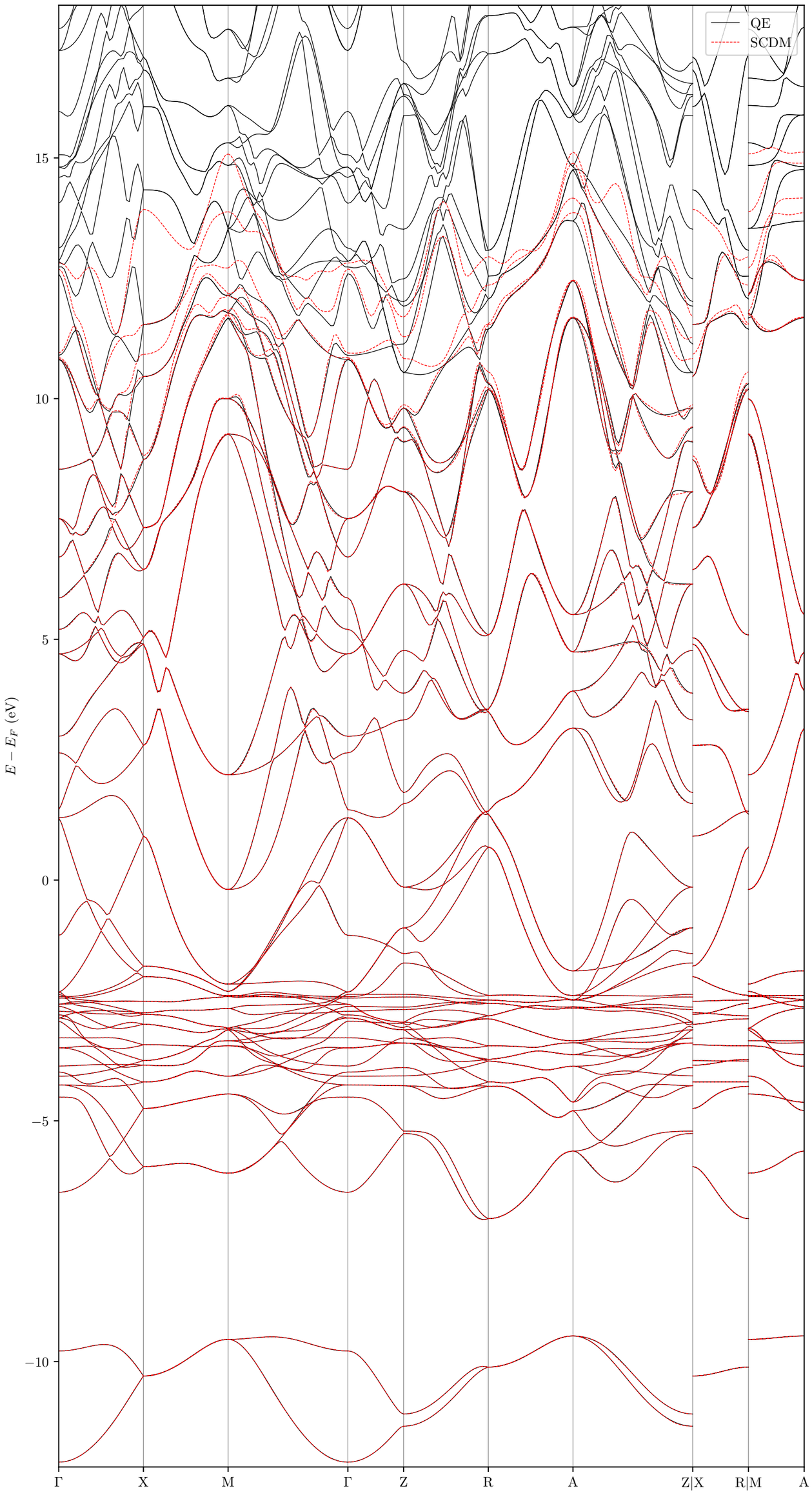
Cu4Sb2 exclude semicore
PW=b7ba5d05-75d3-46fd-b003-a754123188a3
W90=d75a8a21-3543-4770-99b3-040634a070a1




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.3 | 3.5 | 91.9 | 22.6 | 23.7 | 751.8 | 2.282 |

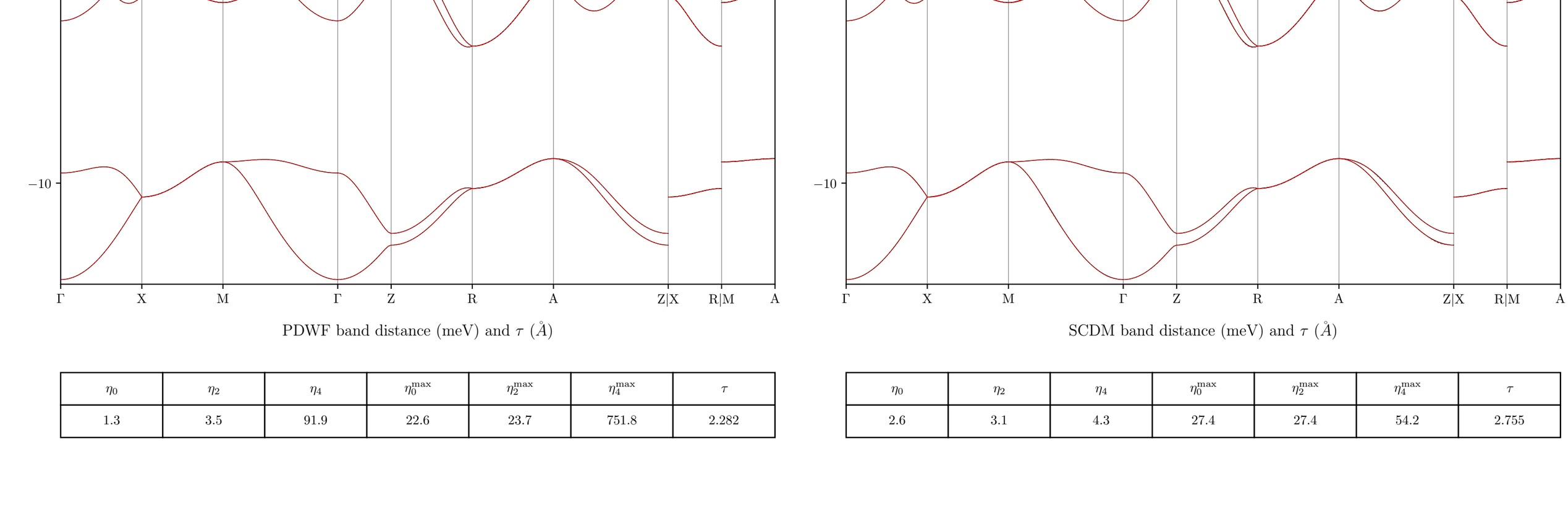
Cu4Sb2 exclude semicore
PW=b7ba5d05-75d3-46fd-b003-a754123188a3
W90=d4b20d7f-dd04-45c4-af48-7f3429874428

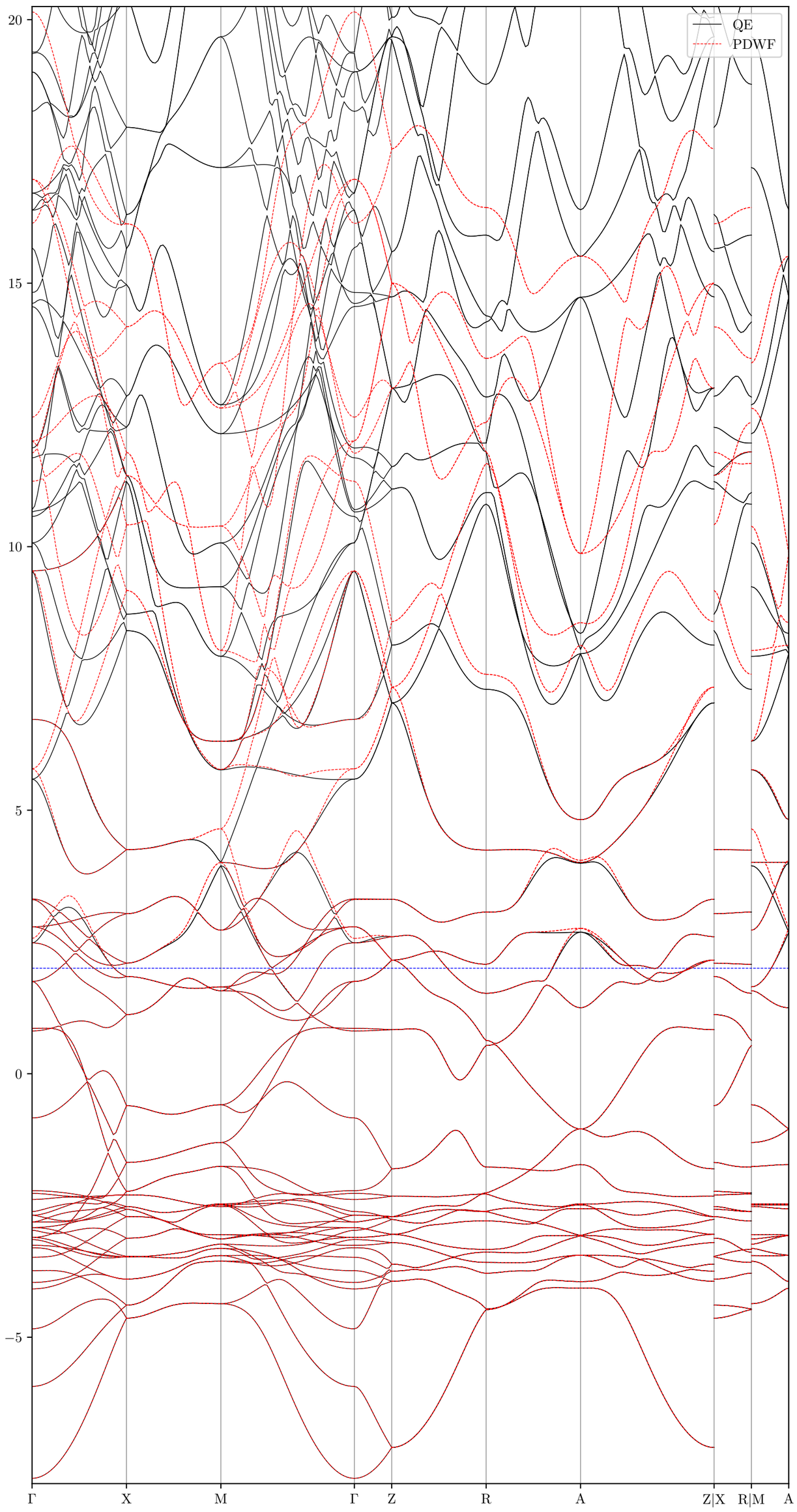



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.6 | 3.1 | 4.3 | 27.4 | 27.4 | 54.2 | 2.755 |

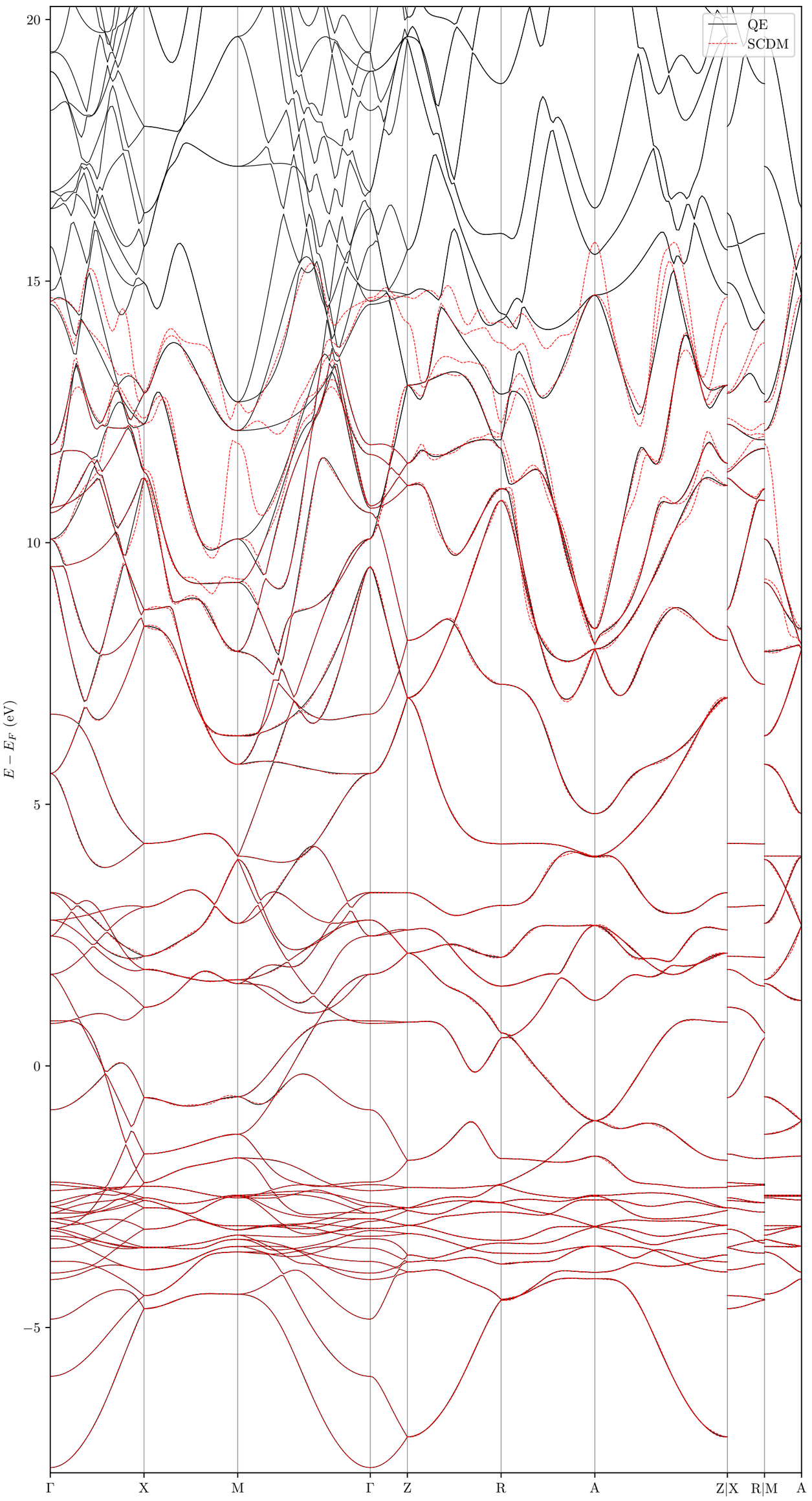
Hamiltonian decay





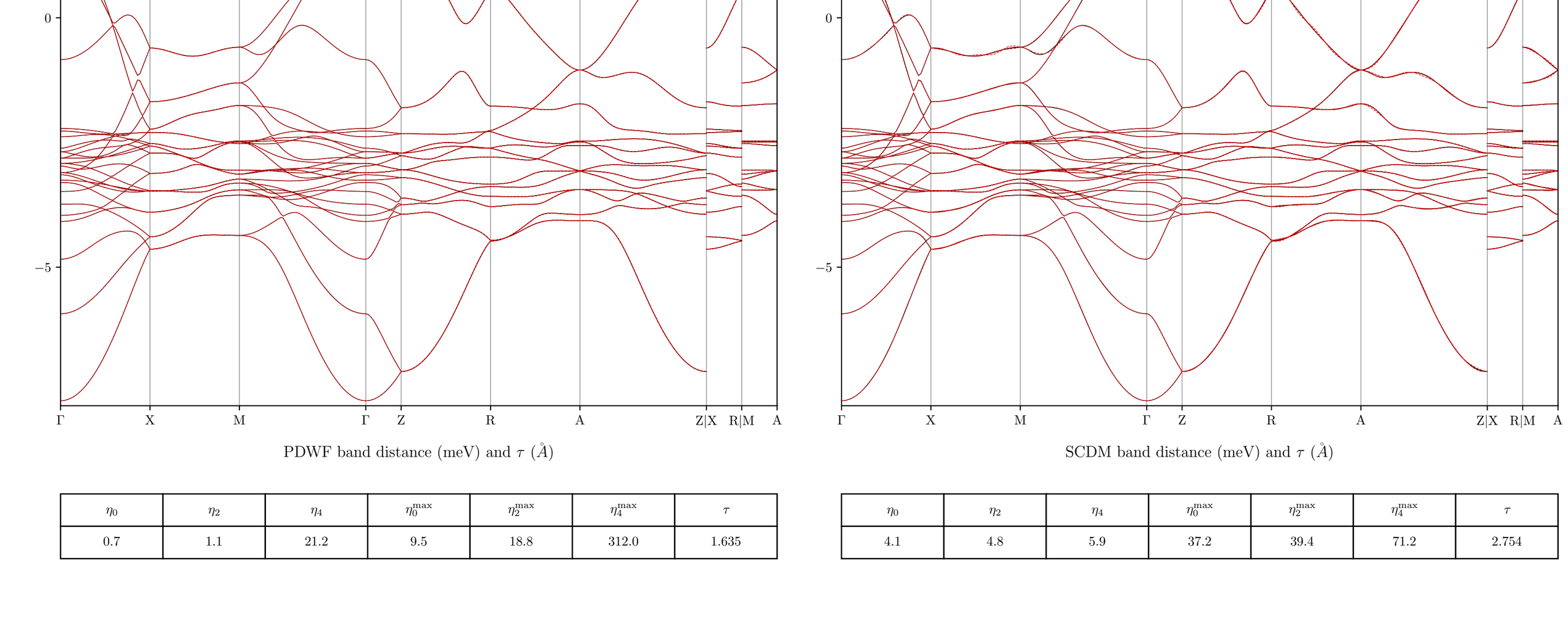

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

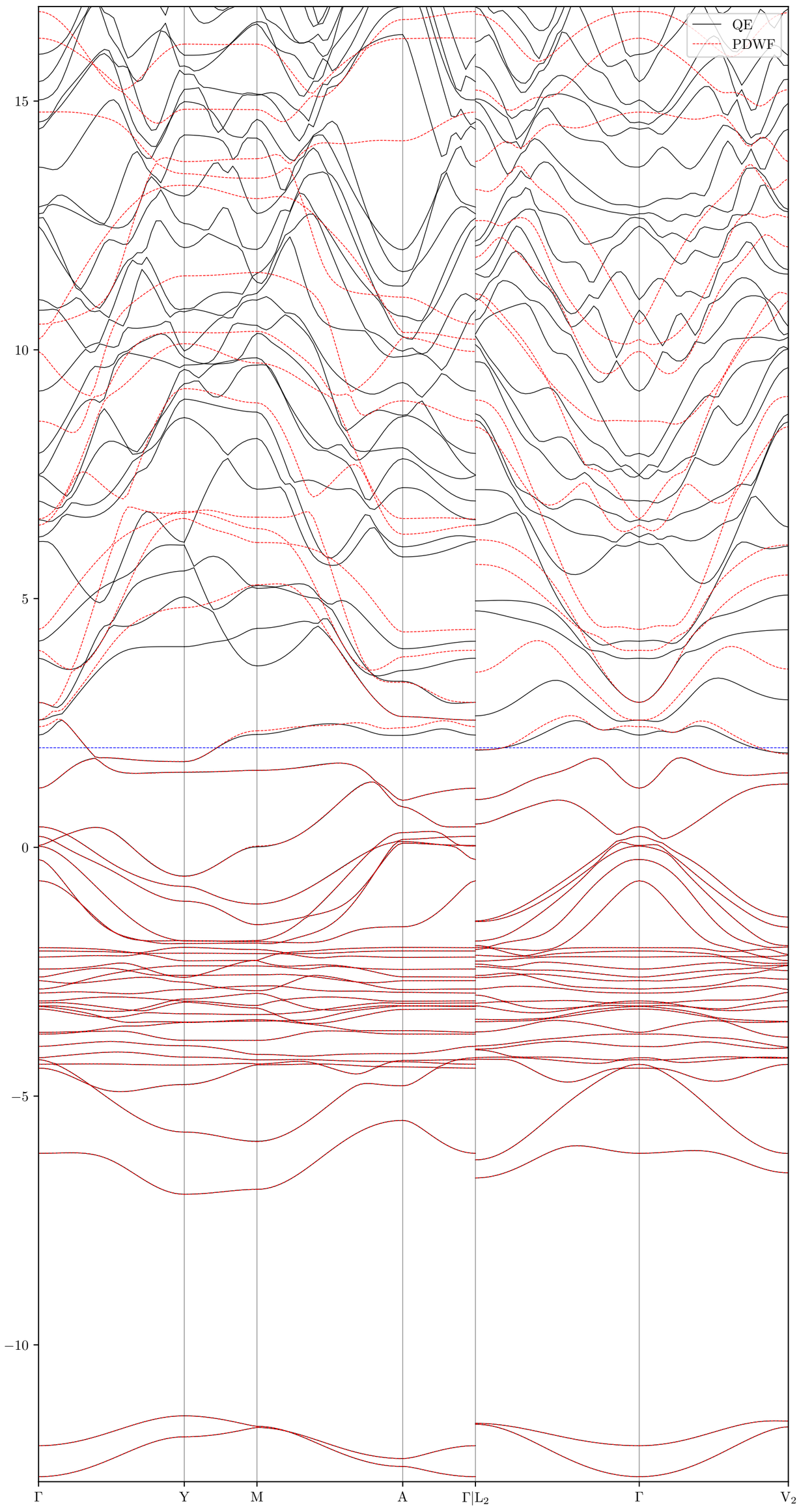
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 1.1 | 21.2 | 9.5 | 18.8 | 312.0 | 1.635 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

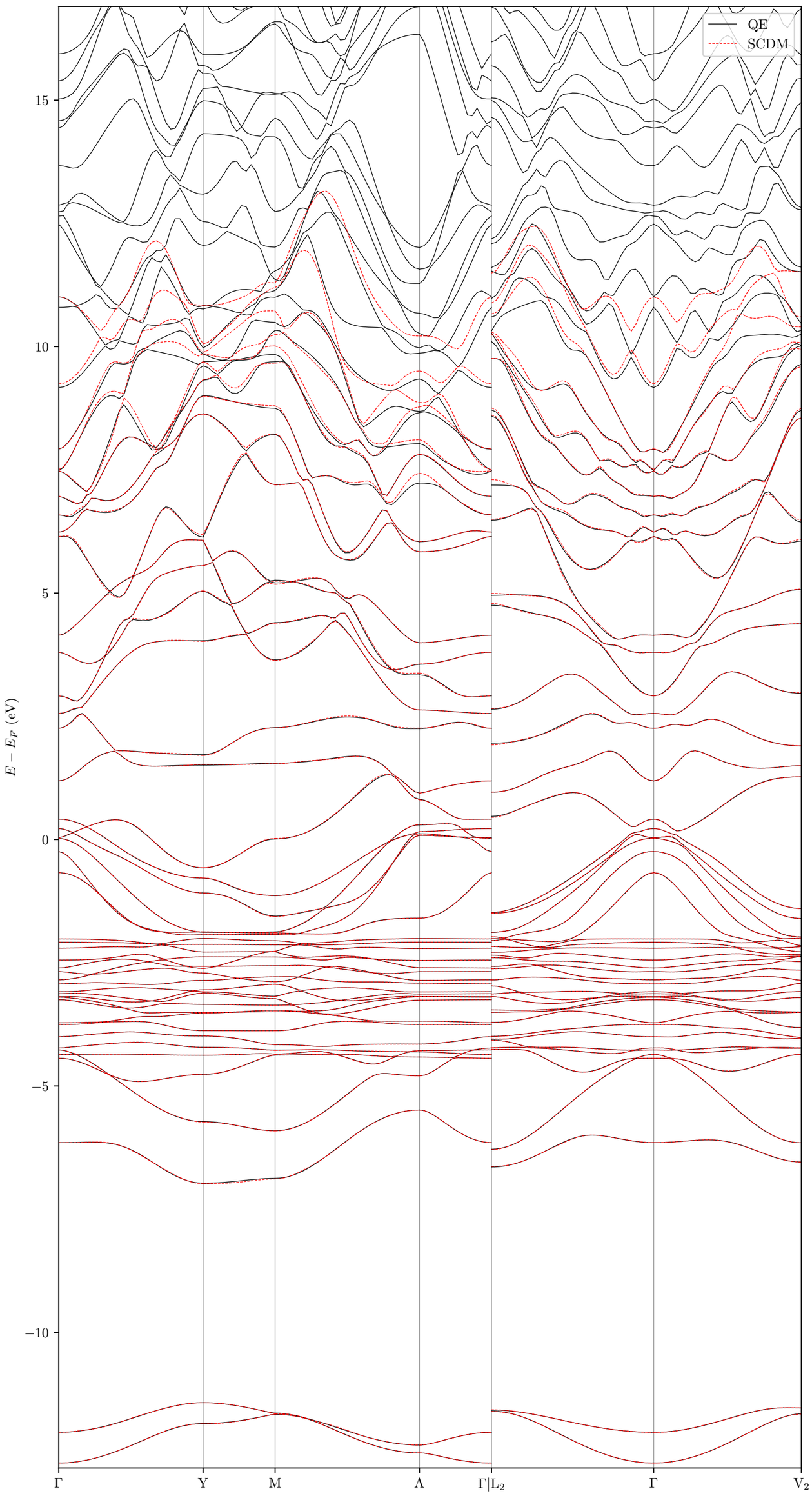
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.1 | 4.8 | 5.9 | 37.2 | 39.4 | 71.2 | 2.754 |





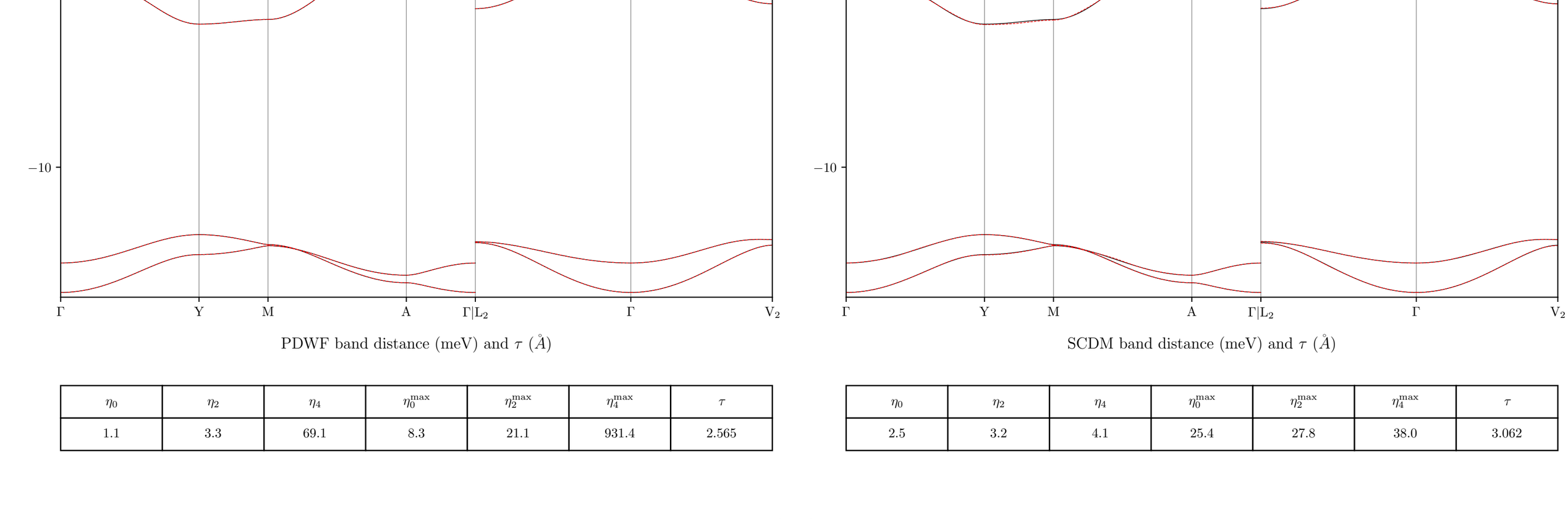

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 3.3 | 69.1 | 8.3 | 21.1 | 931.4 | 2.565 |

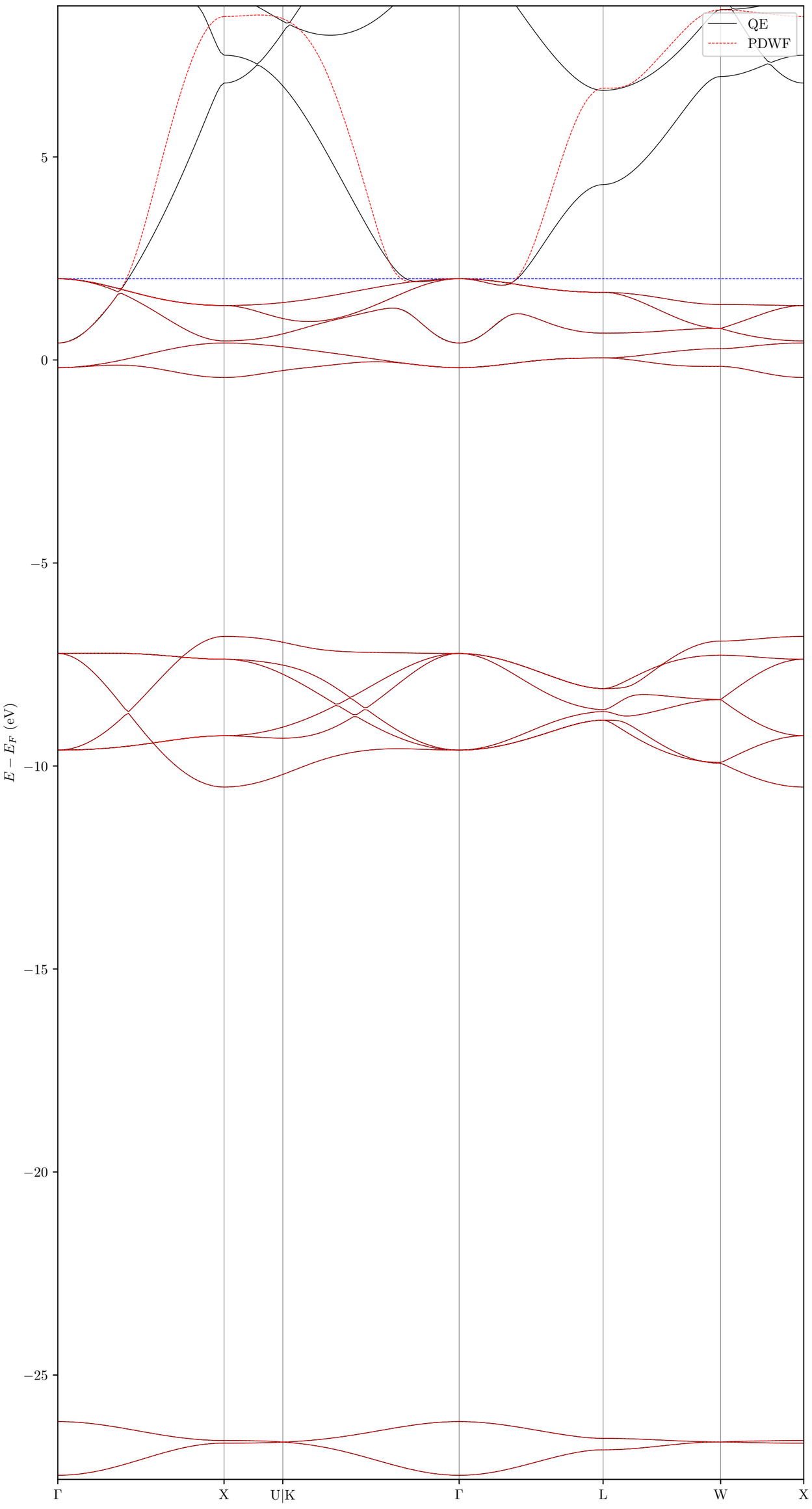



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.5 | 3.2 | 4.1 | 25.4 | 27.8 | 38.0 | 3.062 |



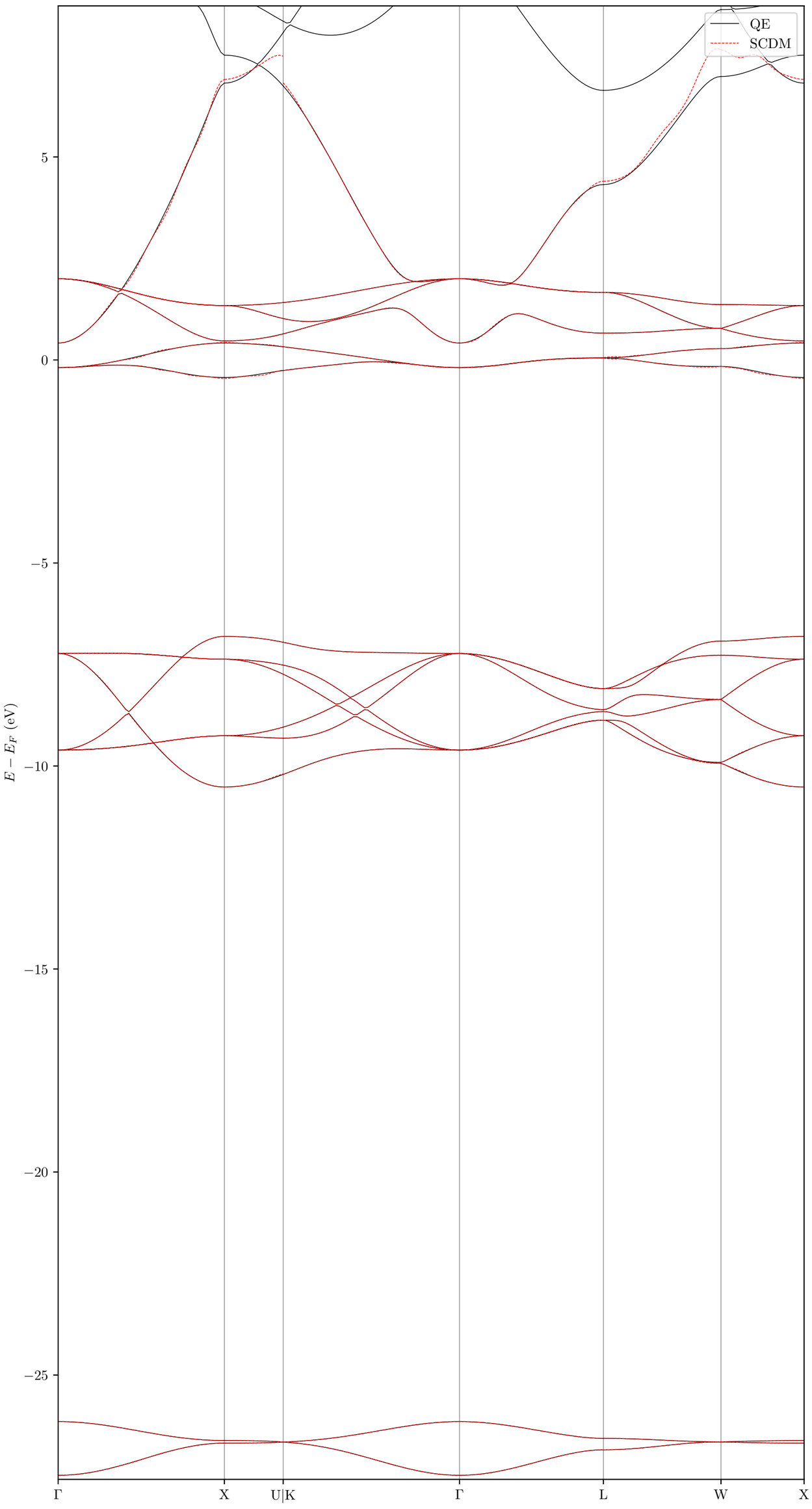
F2Ti exclude semicore
PW=4d19128a-0610-4a0e-8f99-a0498261c54e
W90=855338dd-82e9-4af7-8891-2cd46a87b9ea




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 3.0 | 47.8 | 1.3 | 34.3 | 820.7 | 1.779 |

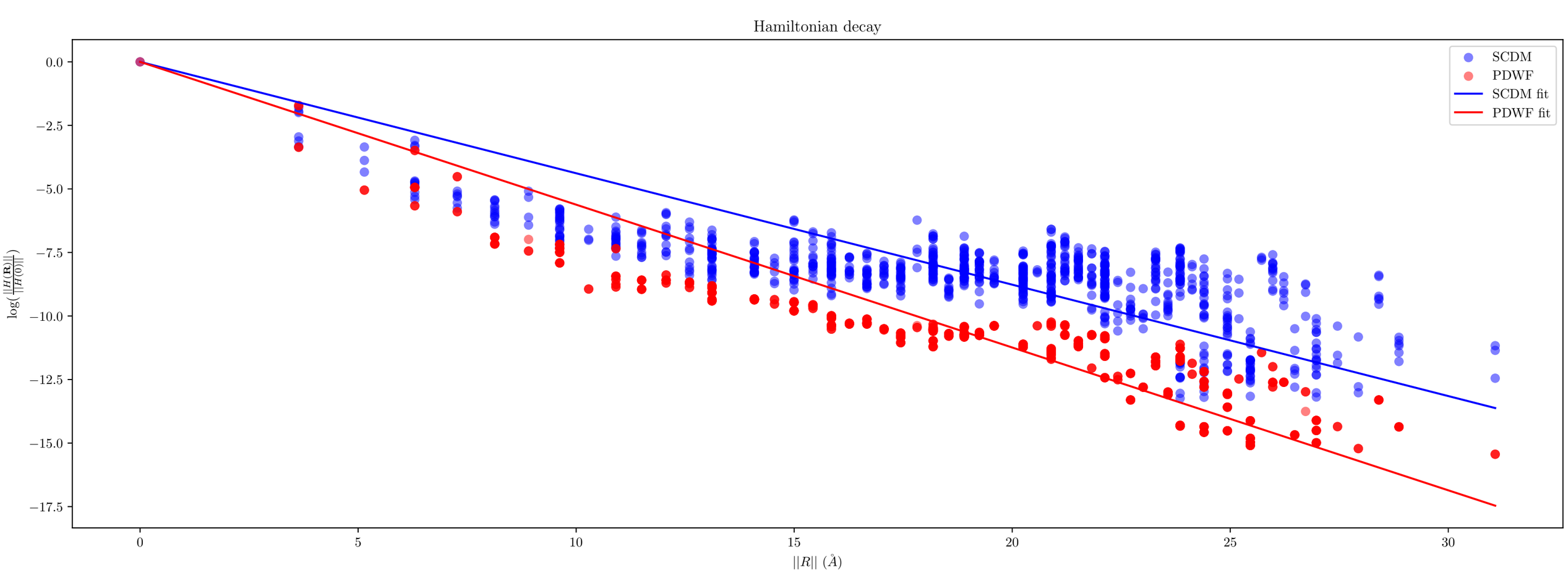
F2Ti exclude semicore
PW=4d19128a-0610-4a0e-8f99-a0498261c54e
W90=0a9b5a45-b2b8-4816-aa18-fa4ba9903cab



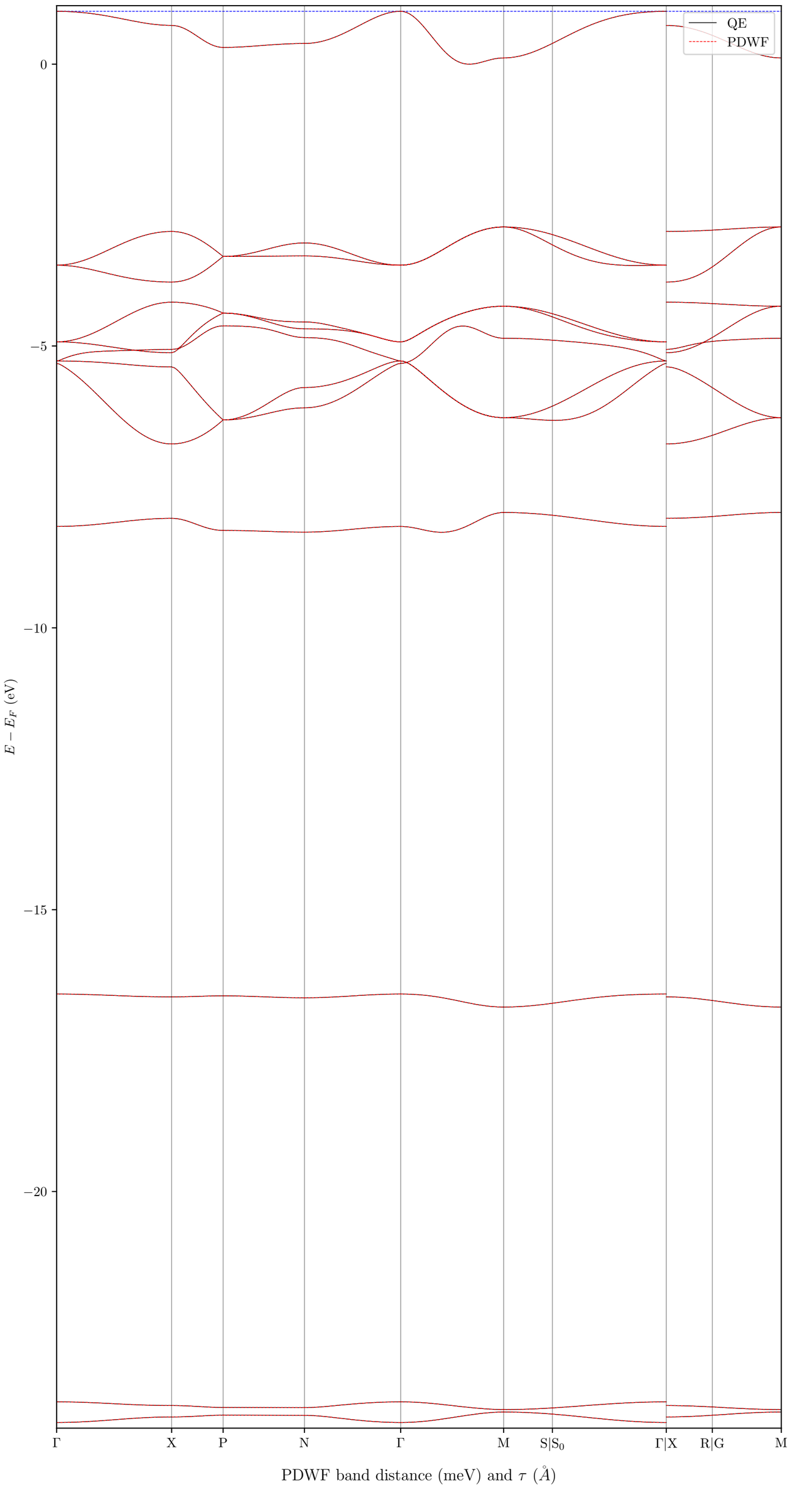

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.0 | 4.4 | 5.6 | 35.6 | 36.6 | 82.6 | 2.281 |

Hamiltonian decay



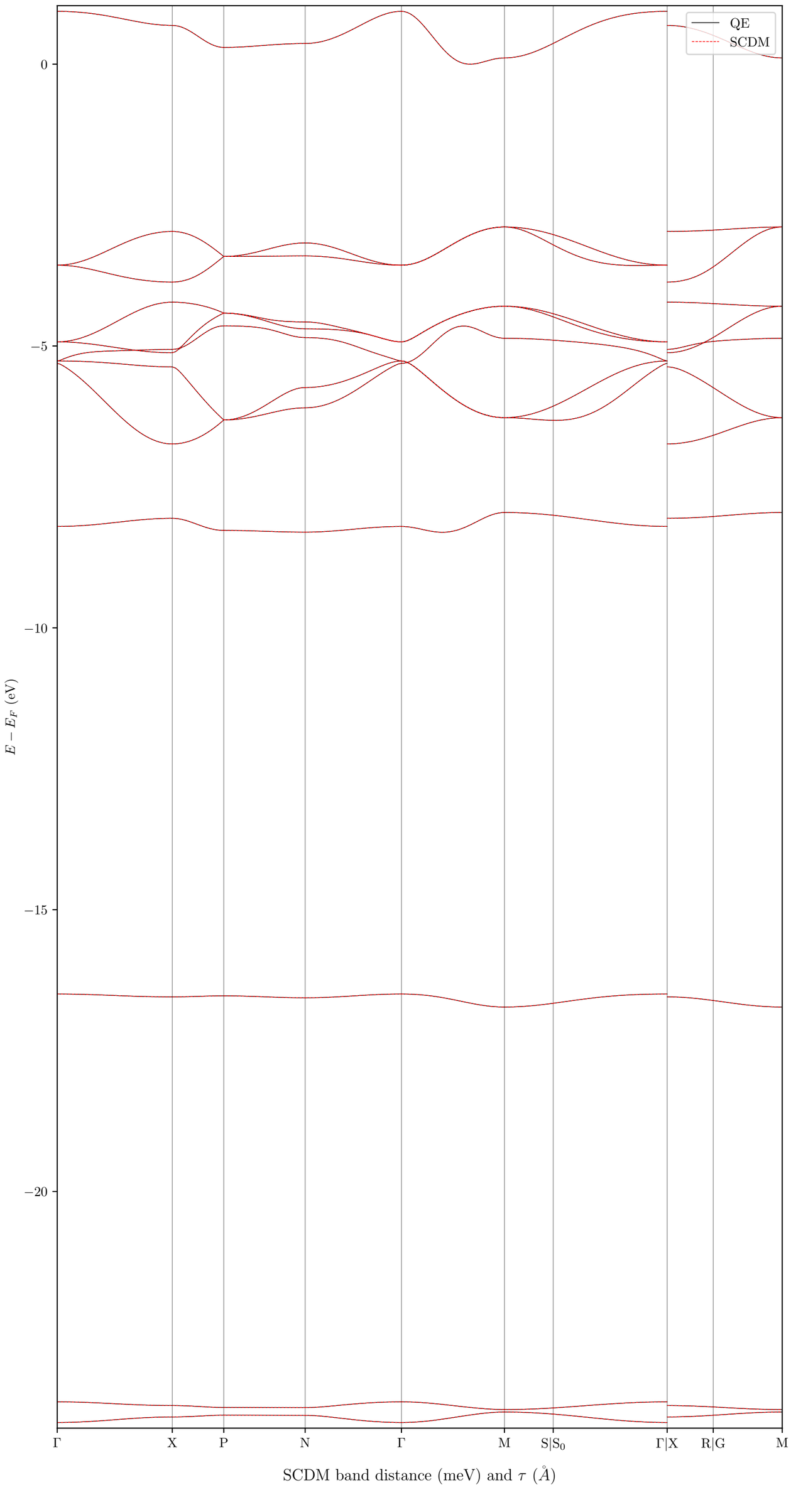
F2Xe exclude semicore
PW=1f759faa-5f2d-46b9-9e4a-d0e84379a658
W90=3cf45ec8-d767-4dea-8ba0-e6333a71187e




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 1.461 |

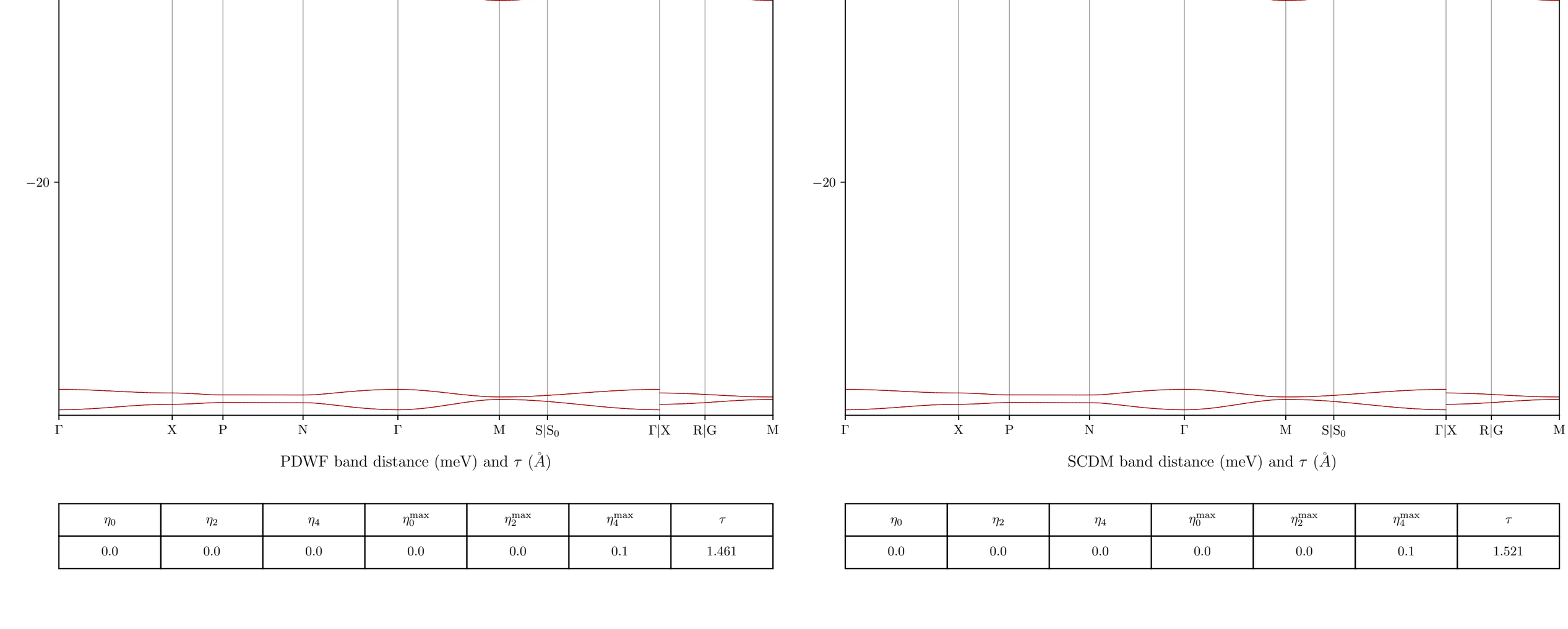
F2Xe exclude semicore
PW=1f759faa-5f2d-46b9-9e4a-d0e84379a658
W90=67e8fb44-cdc0-45e4-99b9-83d841d37847



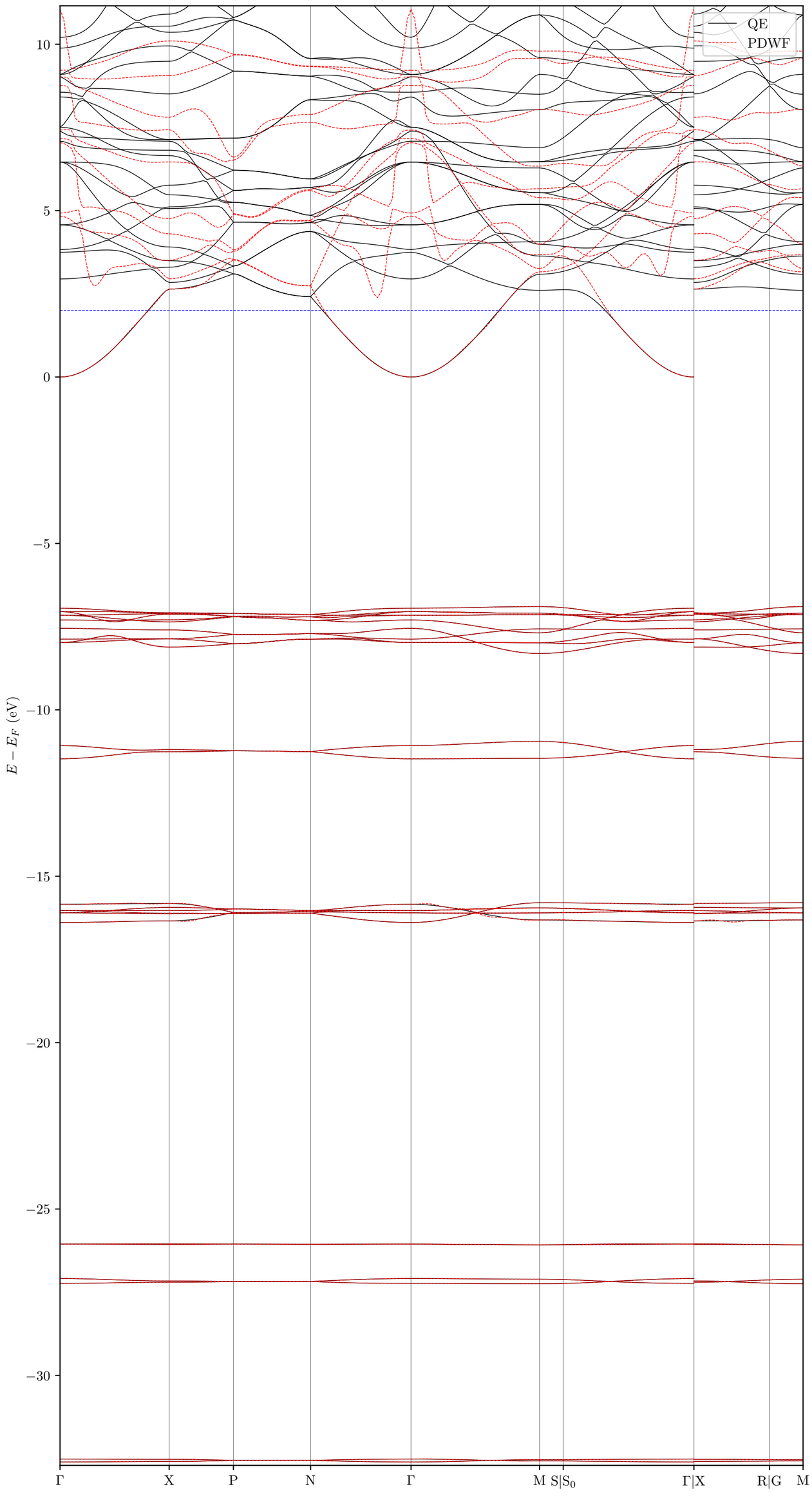

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 1.521 |

Hamiltonian decay



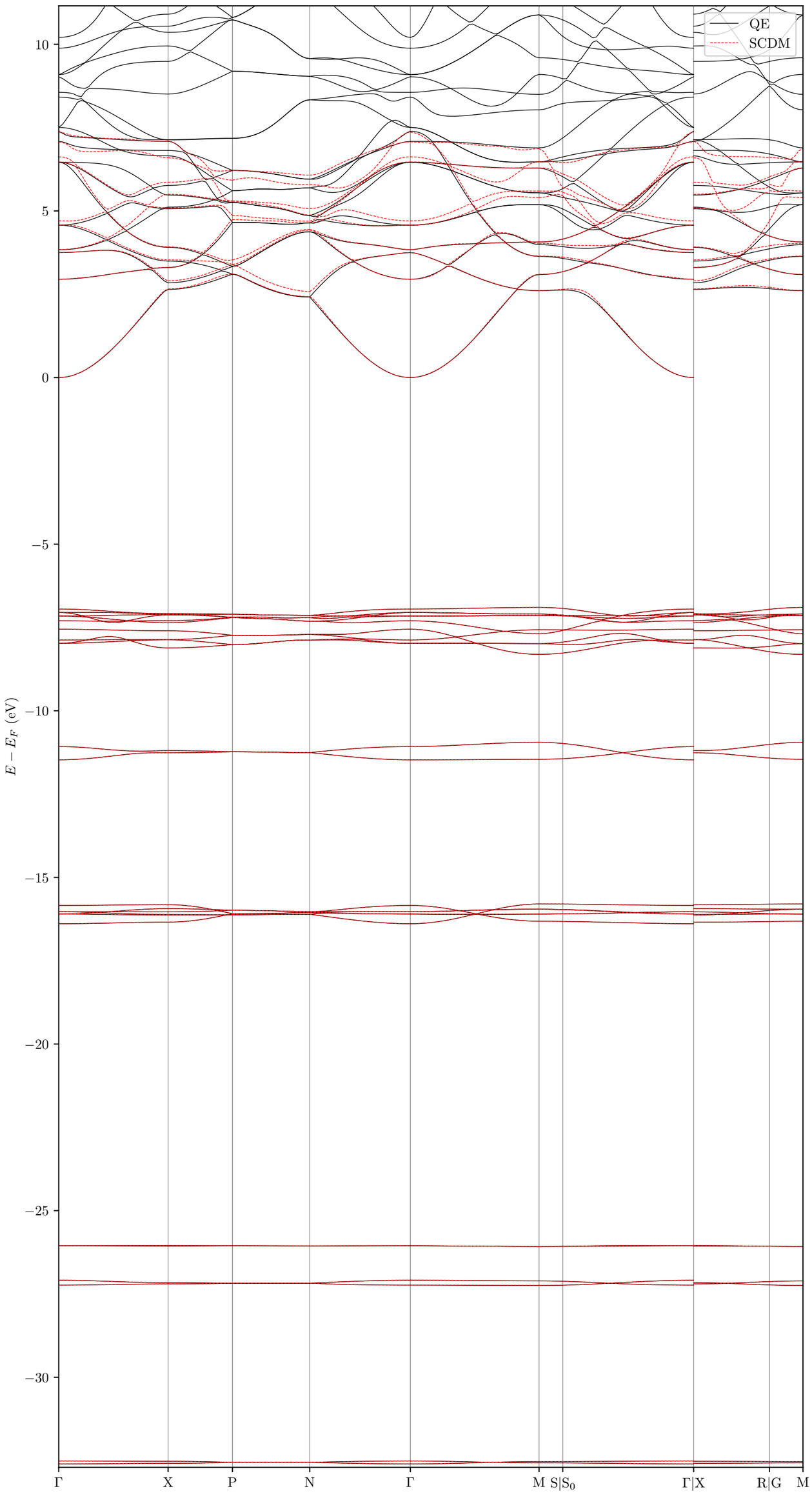
F4H2K2 **INCLUDE** semicore
PW=eed97ba0-21c3-4769-aa94-e6069ca79411
W90=bb379938-fb68-4cfa-ab8e-a0cda8c5605e




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.0 | 3.0 | 3.0 | 52.3 | 52.3 | 52.3 | 2.773 |

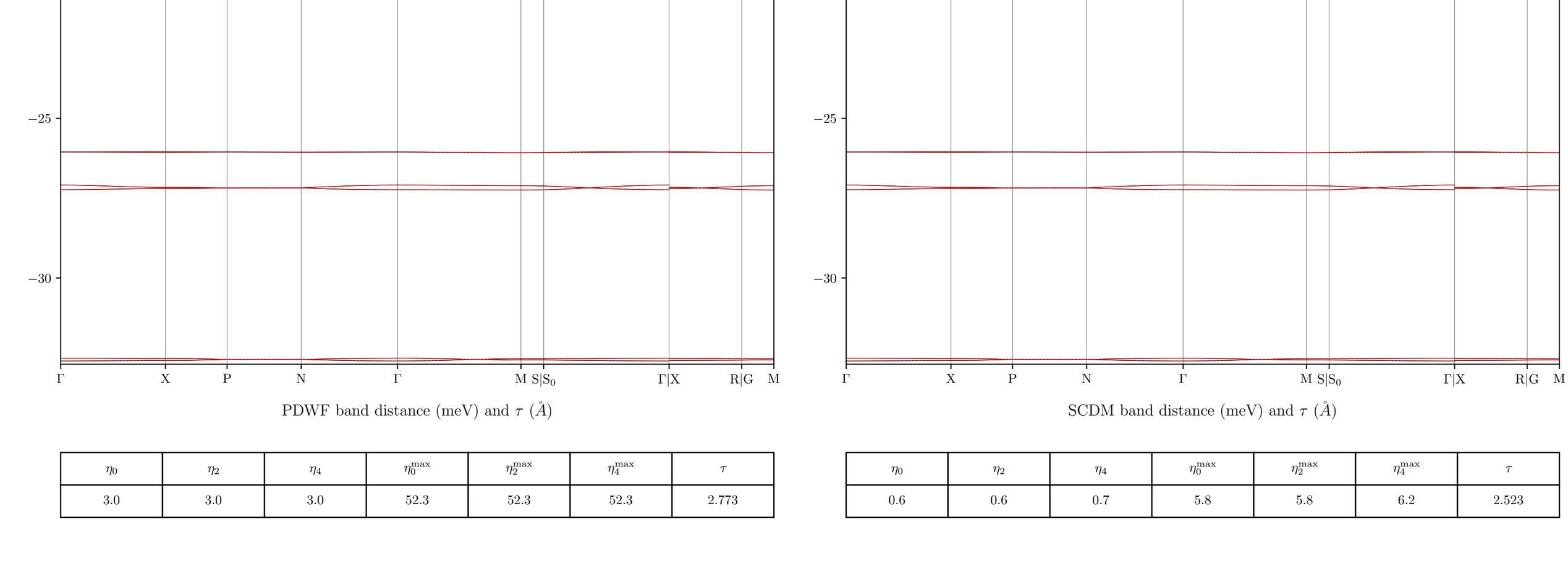
F4H2K2 **INCLUDE** semicore
PW=eed97ba0-21c3-4769-aa94-e6069ca79411
W90=afa80ddd-472c-4eaa-a648-6fedda6f784b



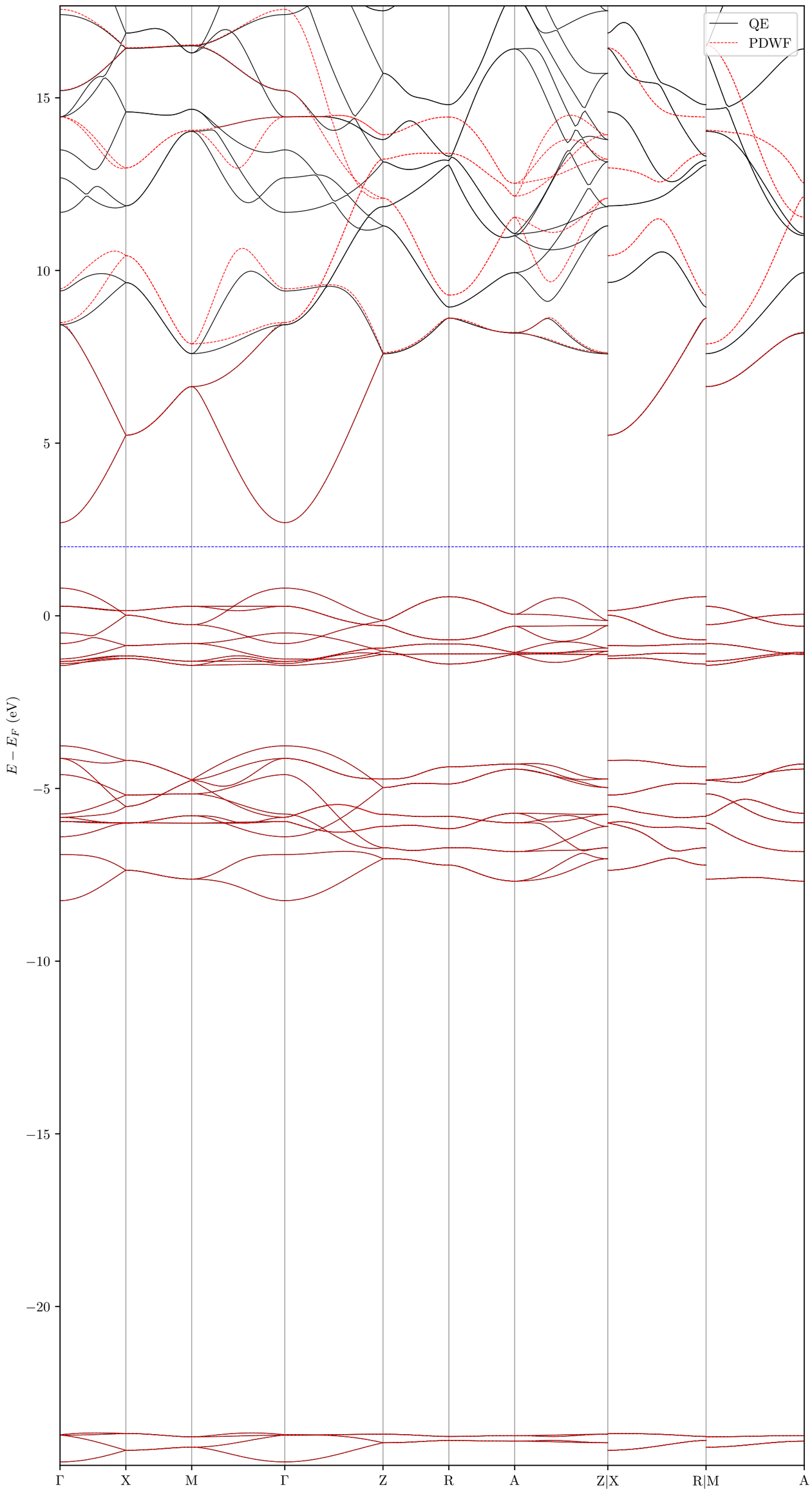

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 0.7 | 5.8 | 5.8 | 6.2 | 2.523 |

Hamiltonian decay



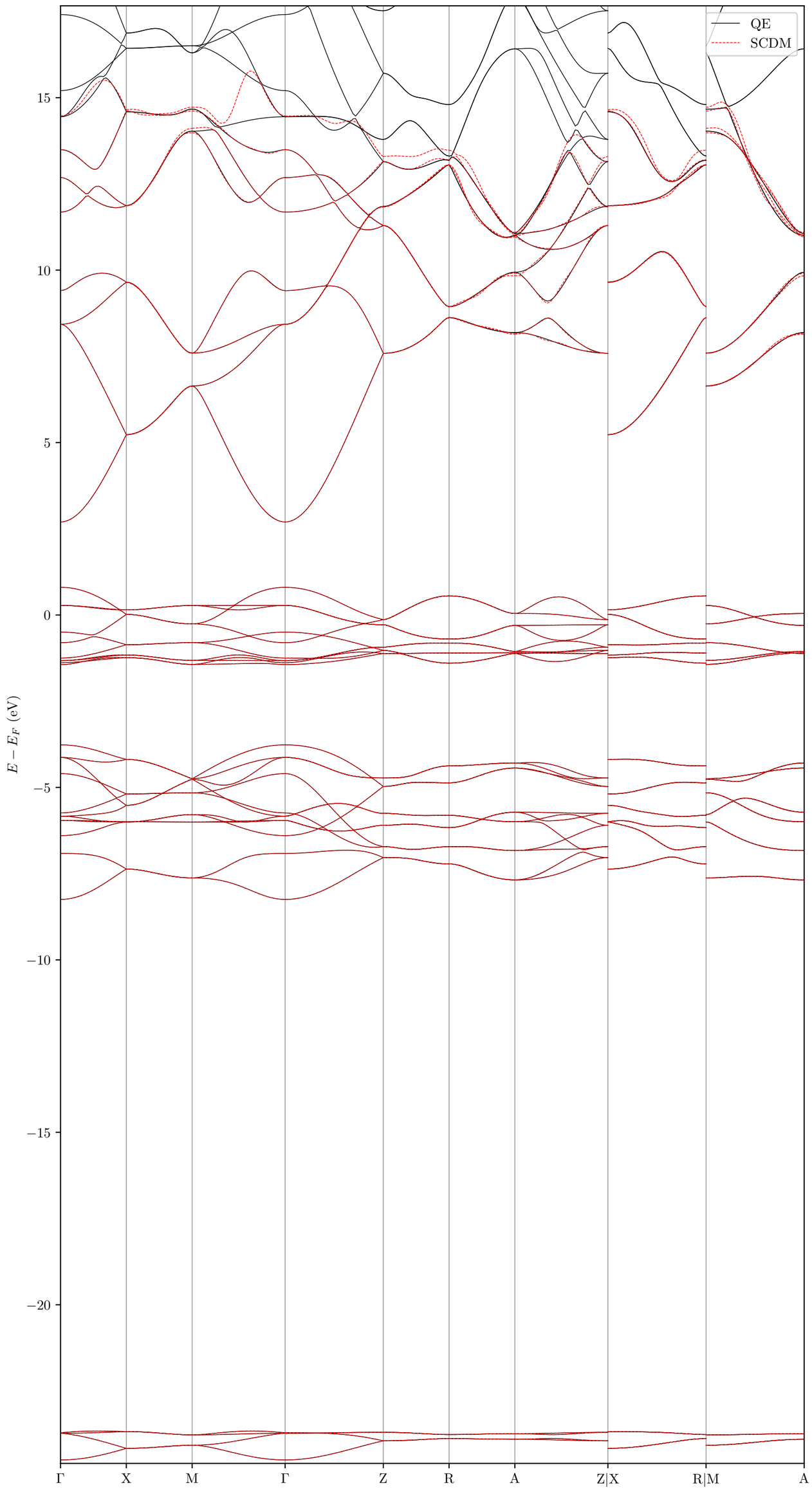
F4Ni2 exclude semicore
PW=7850d076-391a-41db-aaae-d7fce79e2740
W90=27bce679-b1eb-494d-9c2f-b6995d176a86




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 0.3 | 2.4 | 2.4 | 2.4 | 2.026 |

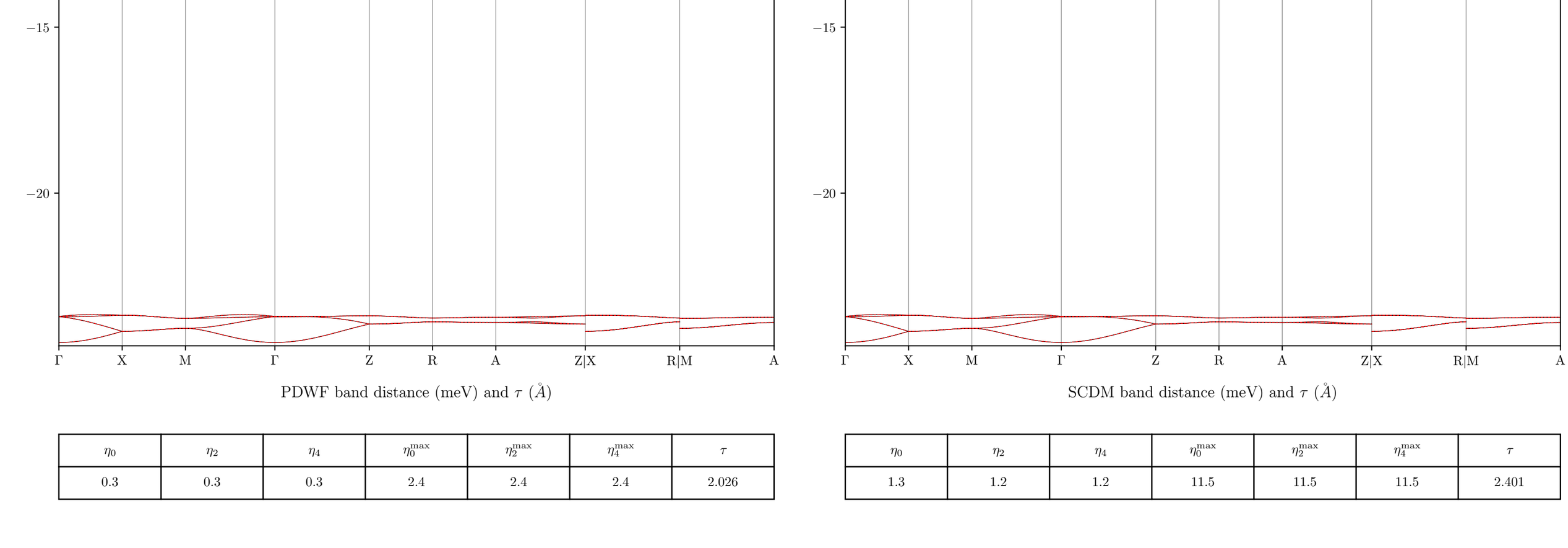
F4Ni2 exclude semicore
PW=7850d076-391a-41db-aaae-d7fce79e2740
W90=ff0c3a99-f9d0-4fad-ad1b-b5e1fbc4011e



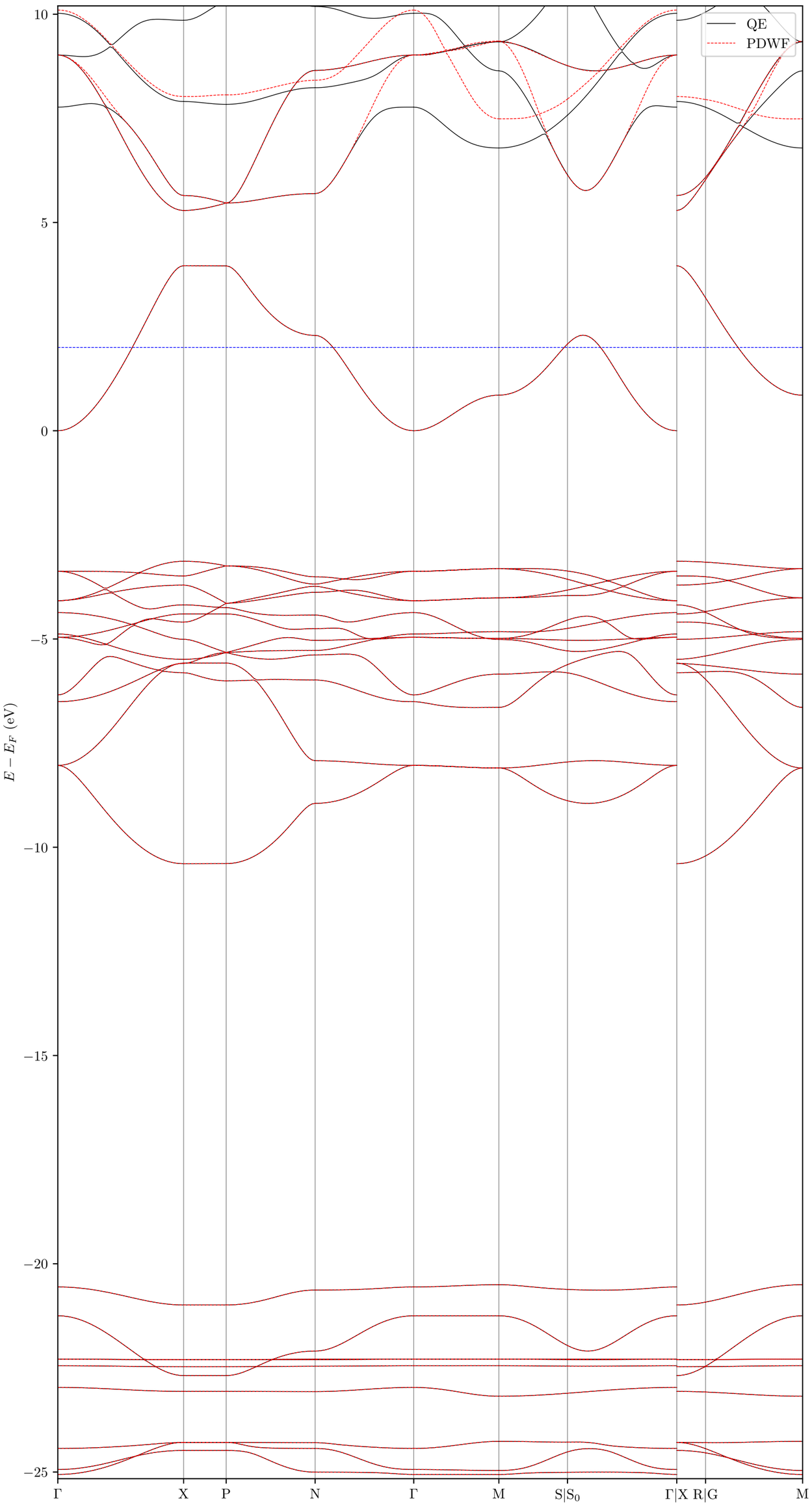

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.3 | 1.2 | 1.2 | 11.5 | 11.5 | 11.5 | 2.401 |

Hamiltonian decay



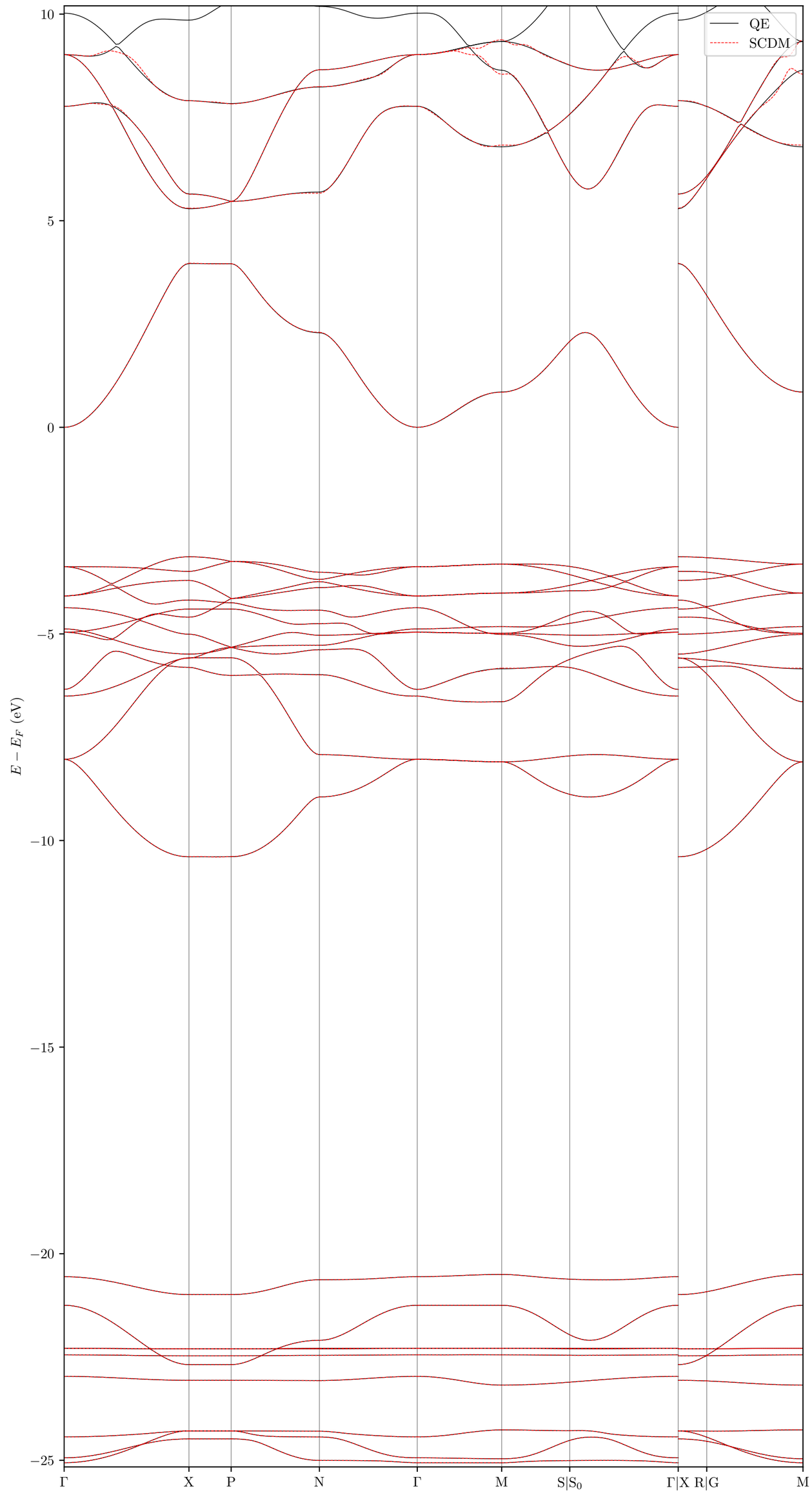
F4Sn **INCLUDE** semicore
PW=db800bcb-8295-45b6-b643-ec59829e8a85
W90=31815379-86a8-471c-8d6c-bfa8666ab1a6




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.4 | 0.4 | 0.4 | 2.7 | 2.7 | 3.8 | 2.328 |

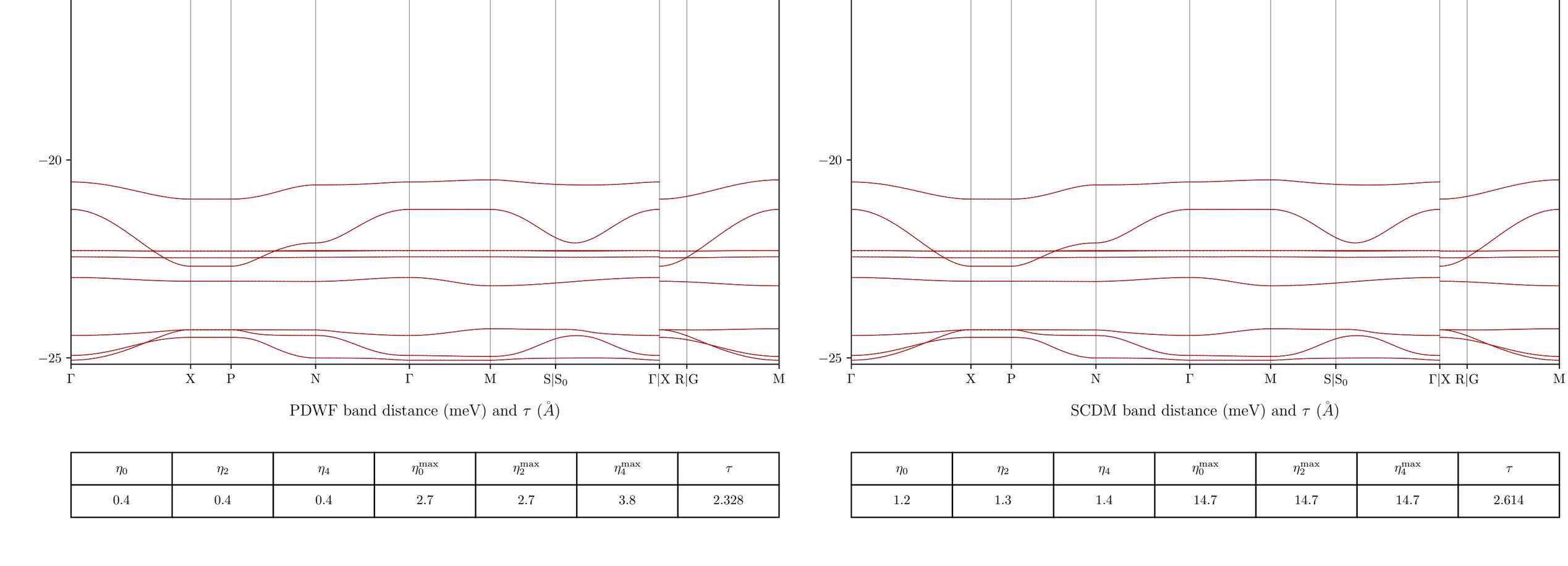
F4Sn **INCLUDE** semicore
PW=db800bcb-8295-45b6-b643-ec59829e8a85
W90=9a8504a8-0688-49e3-b491-78a5cb454e20



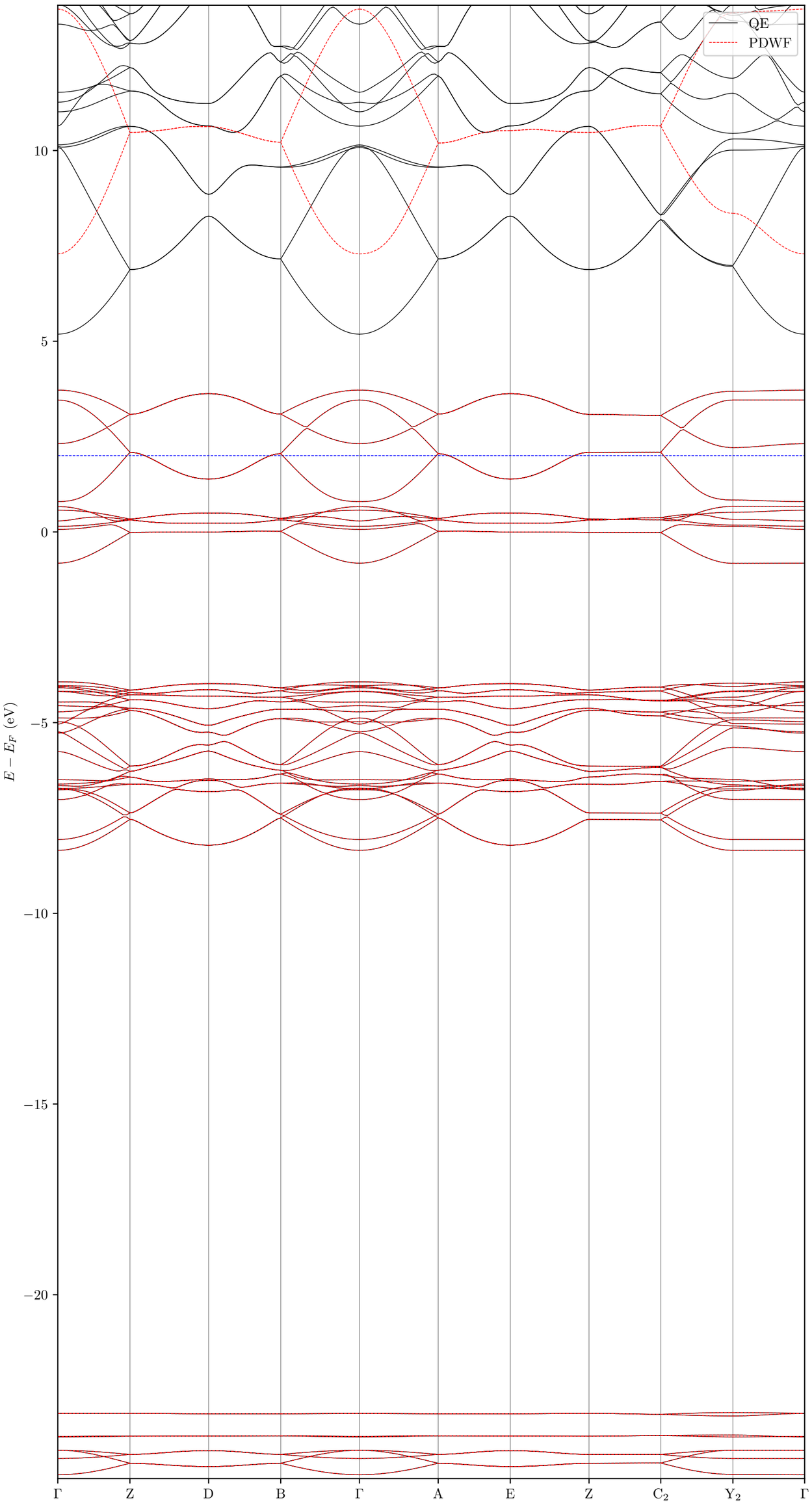

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.3 | 1.4 | 14.7 | 14.7 | 14.7 | 2.614 |

Hamiltonian decay



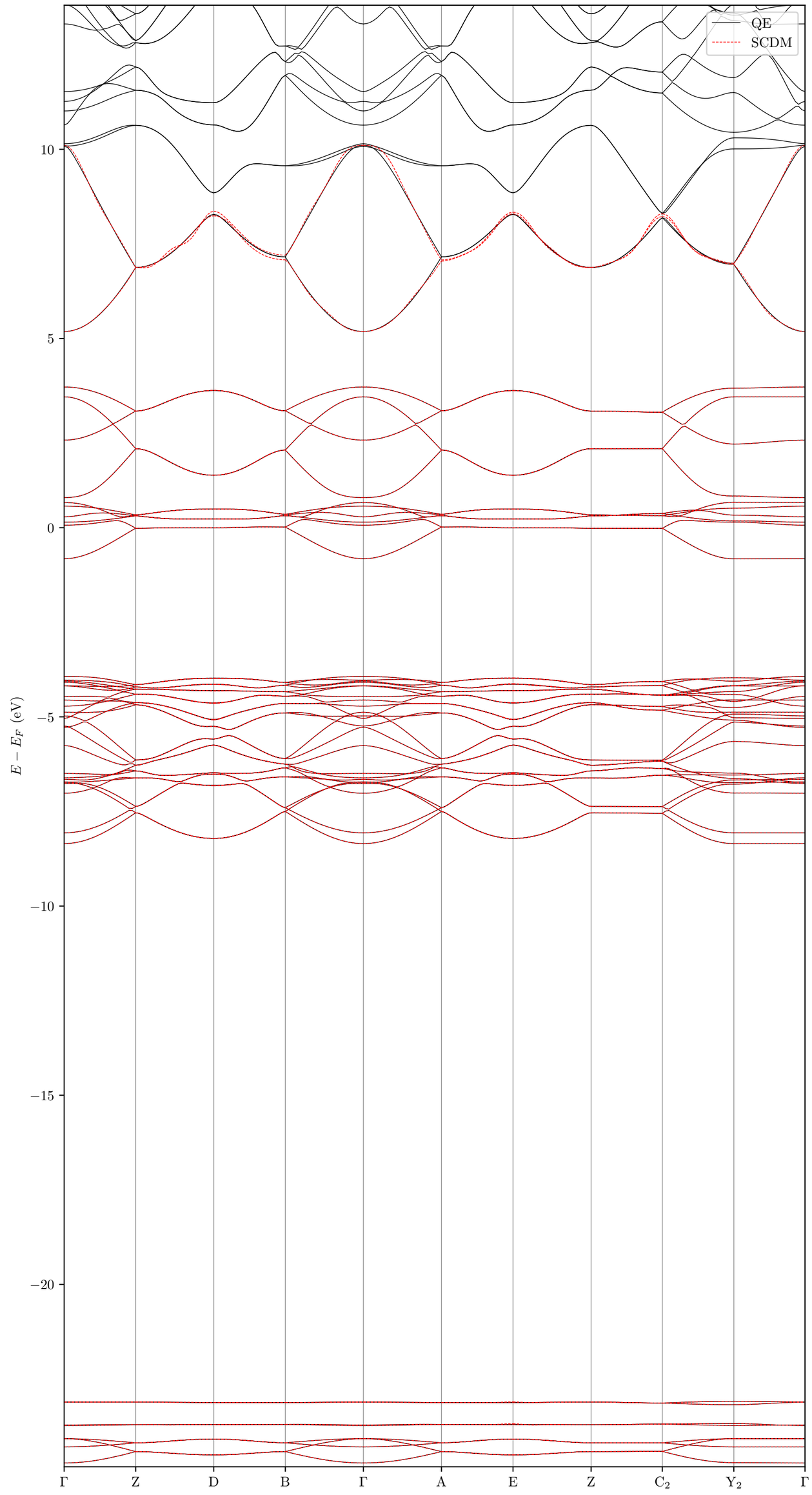
F8V2 exclude semicore
PW=3381d759-0afc-4a03-8553-1555cf74bcd9
W90=b09aca9d-1366-47ad-96ea-b722db6d50eb




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.3 | 0.3 | 0.3 | 1.914 |

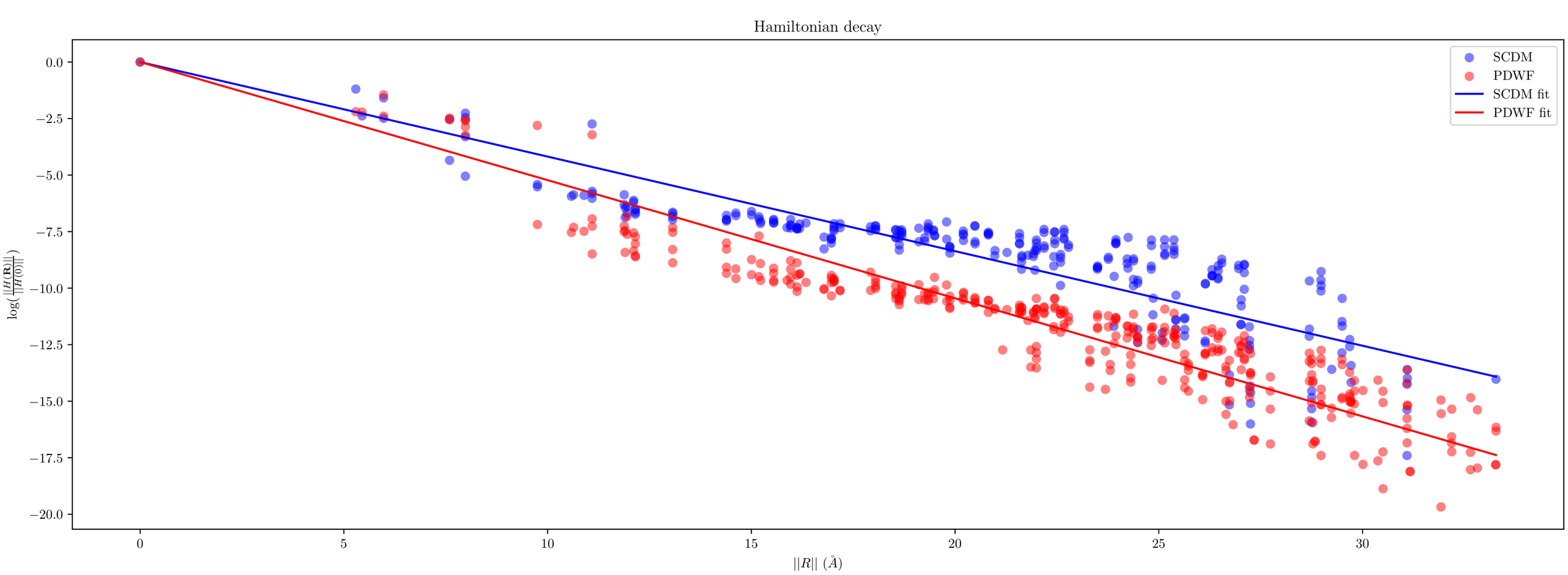
F8V2 exclude semicore
PW=3381d759-0afc-4a03-8553-1555cf74bcd9
W90=cdef1780-ad45-47f0-85de-118bbbcae1c0

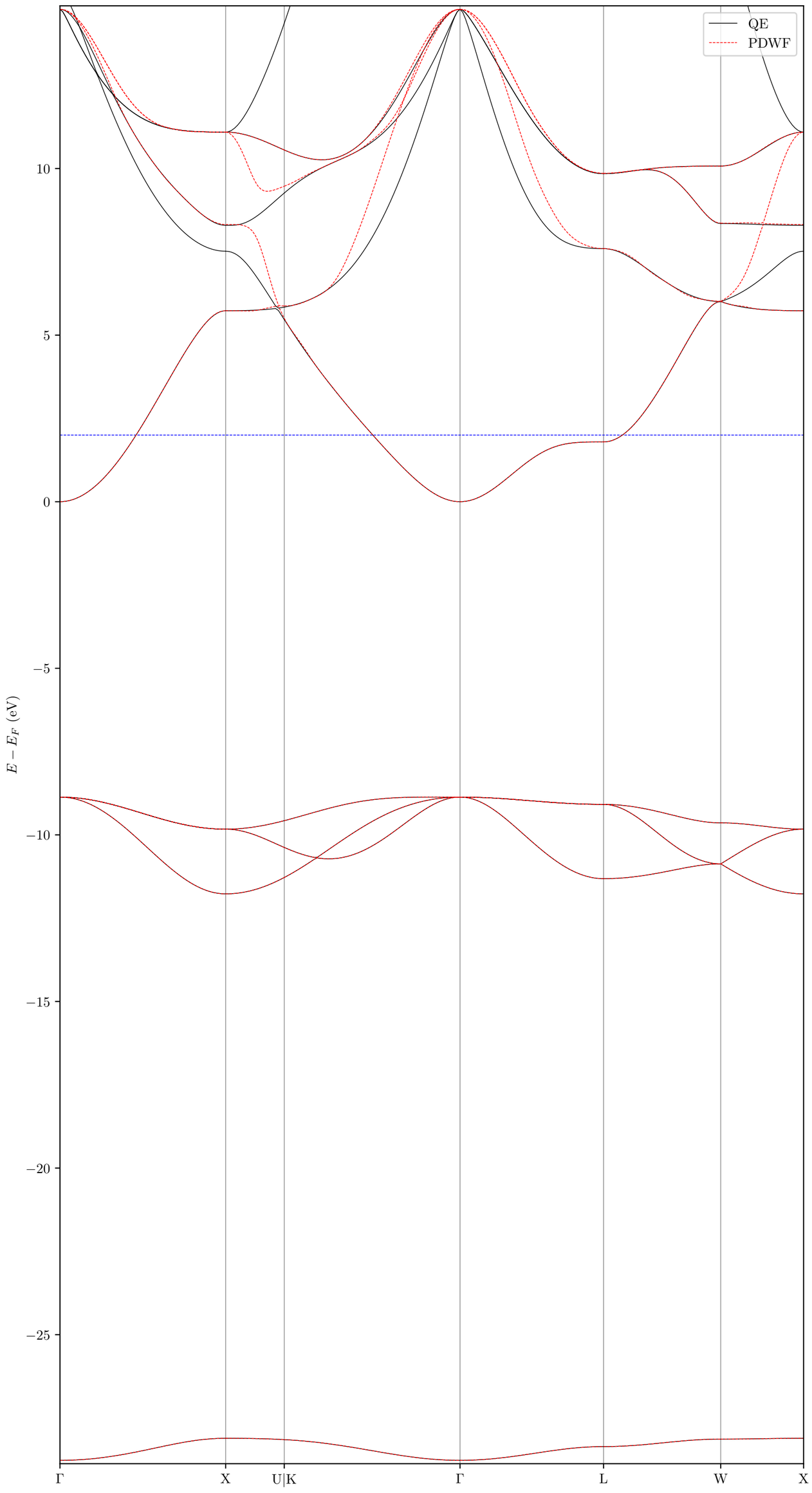



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.8 | 1.6 | 1.6 | 26.1 | 26.1 | 26.1 | 2.391 |

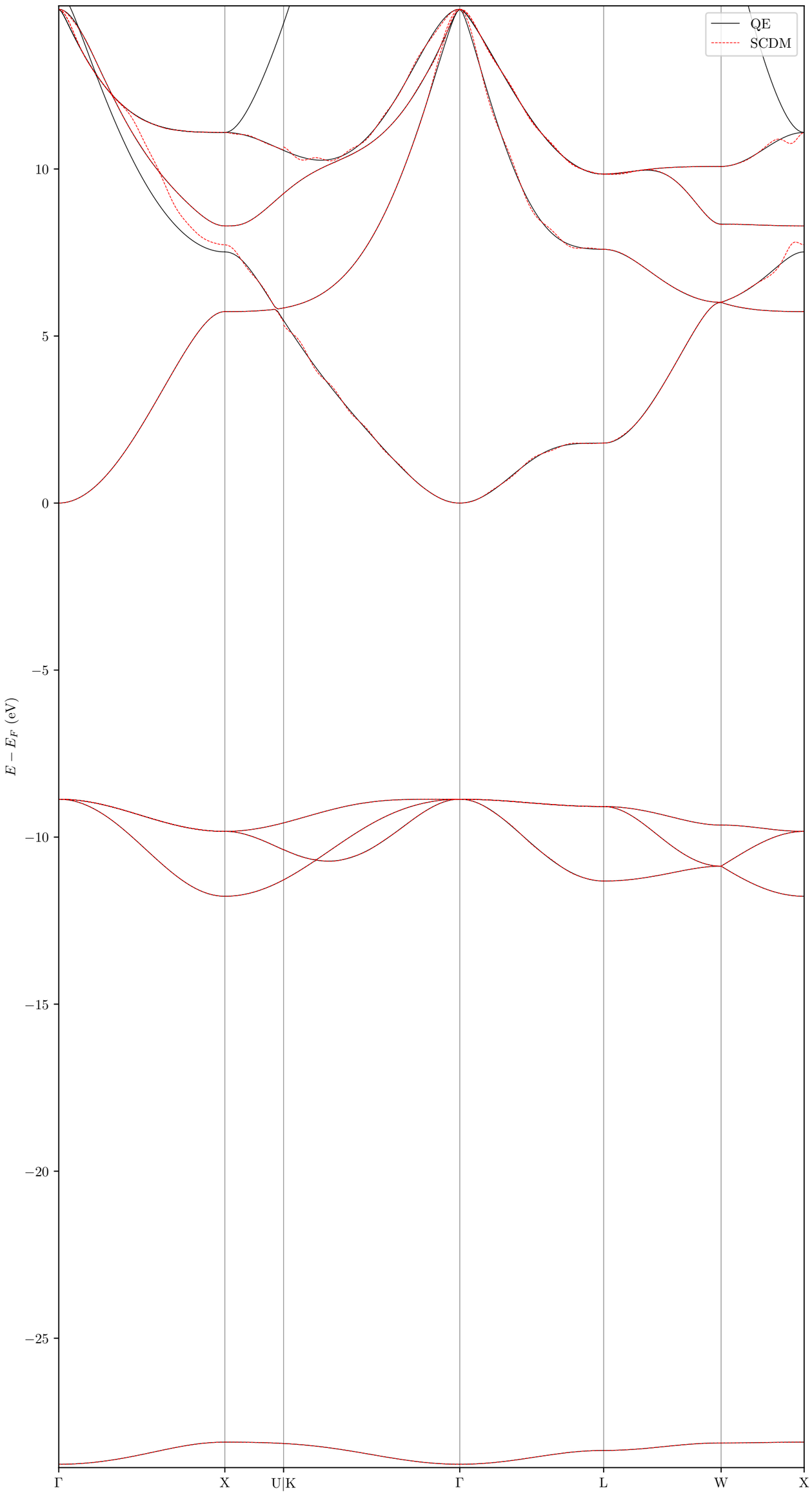
Hamiltonian decay





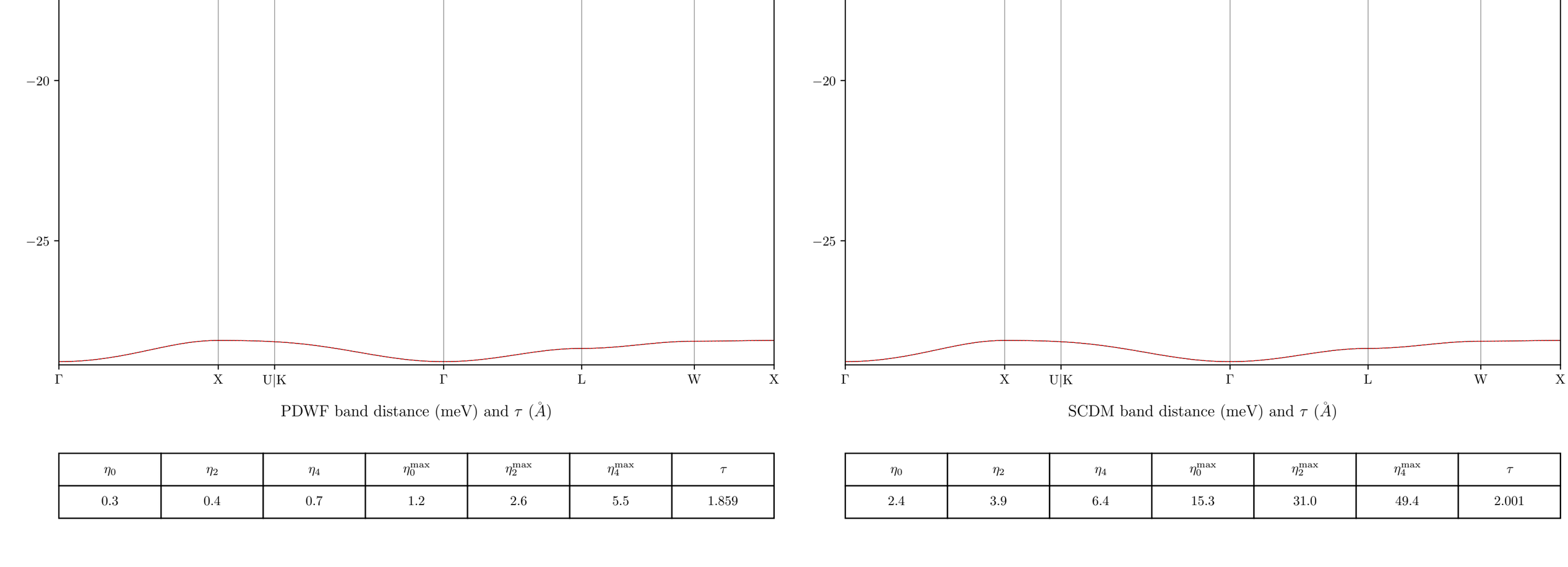

PDWF band distance (meV) and $\tau$ ($\AA$)

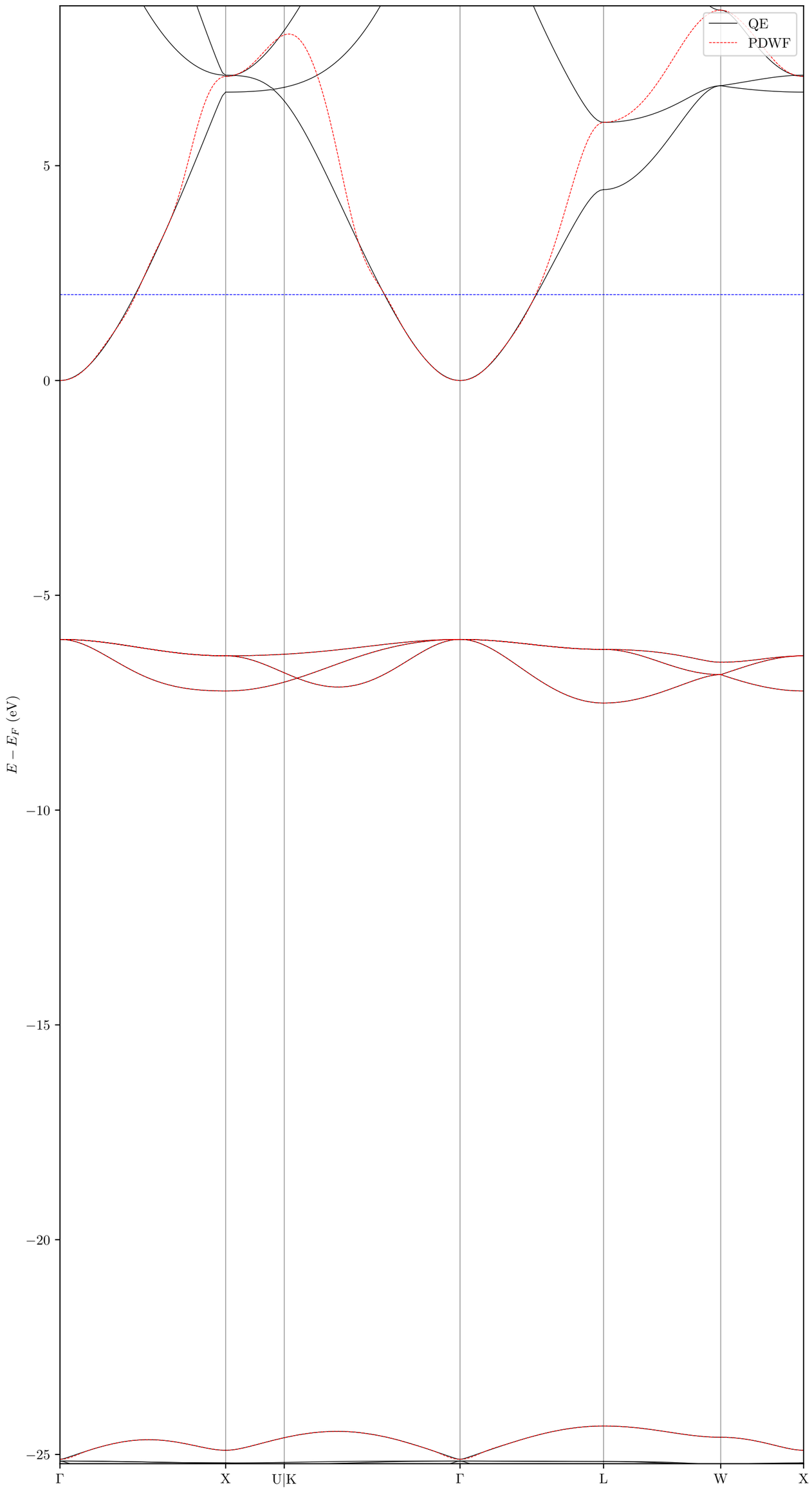
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.4 | 0.7 | 1.2 | 2.6 | 5.5 | 1.859 |




SCDM band distance (meV) and $\tau$ ($\AA$)

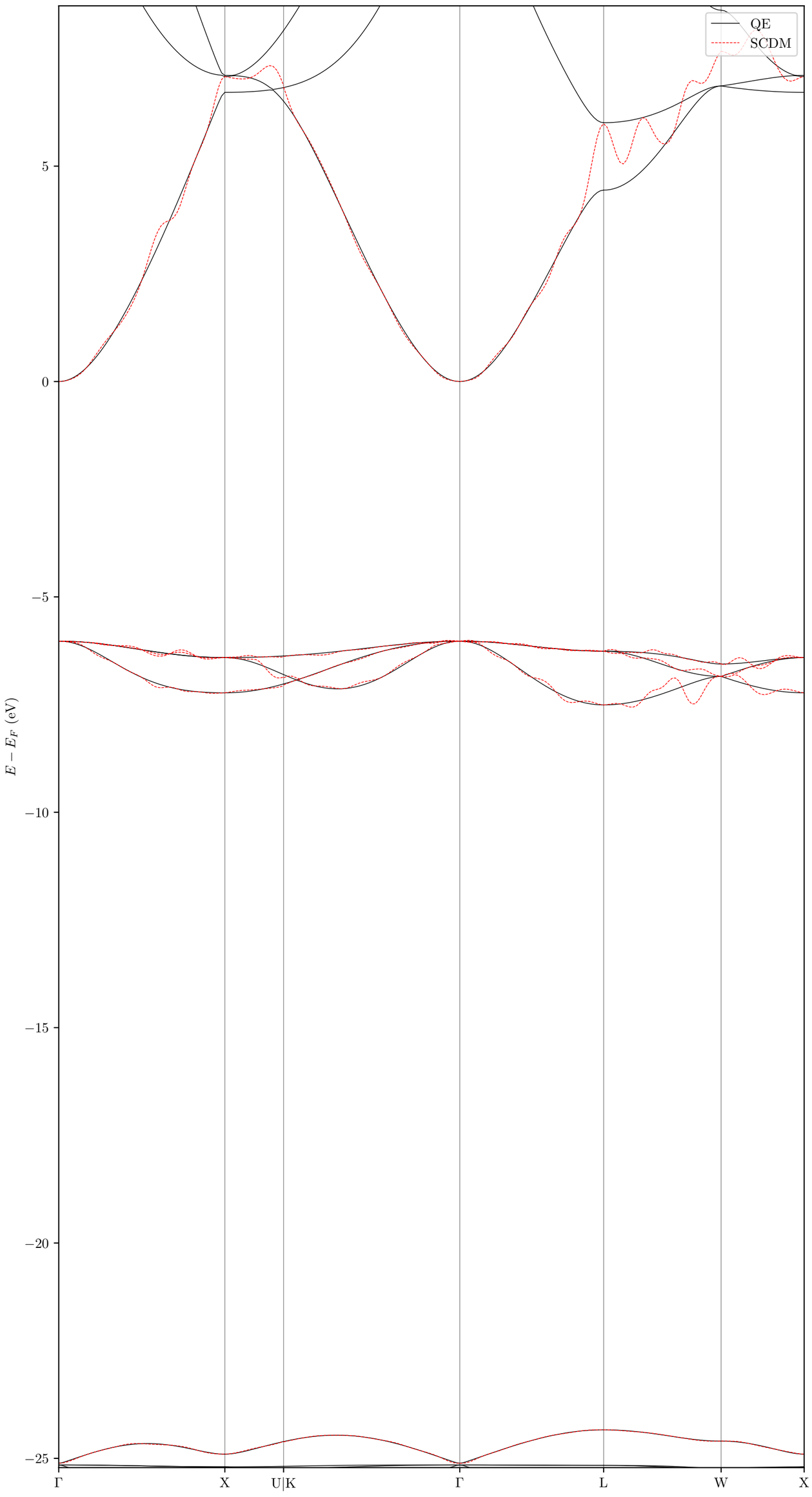
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.4 | 3.9 | 6.4 | 15.3 | 31.0 | 49.4 | 2.001 |





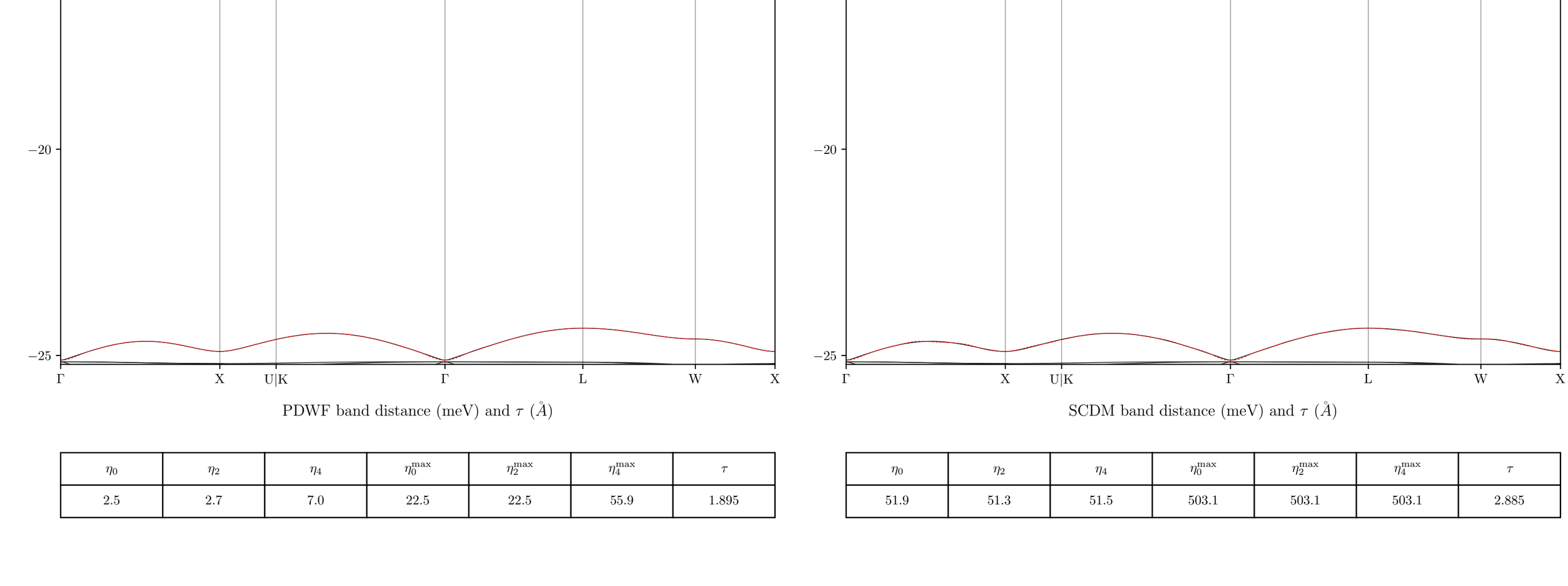

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.5 | 2.7 | 7.0 | 22.5 | 22.5 | 55.9 | 1.895 |

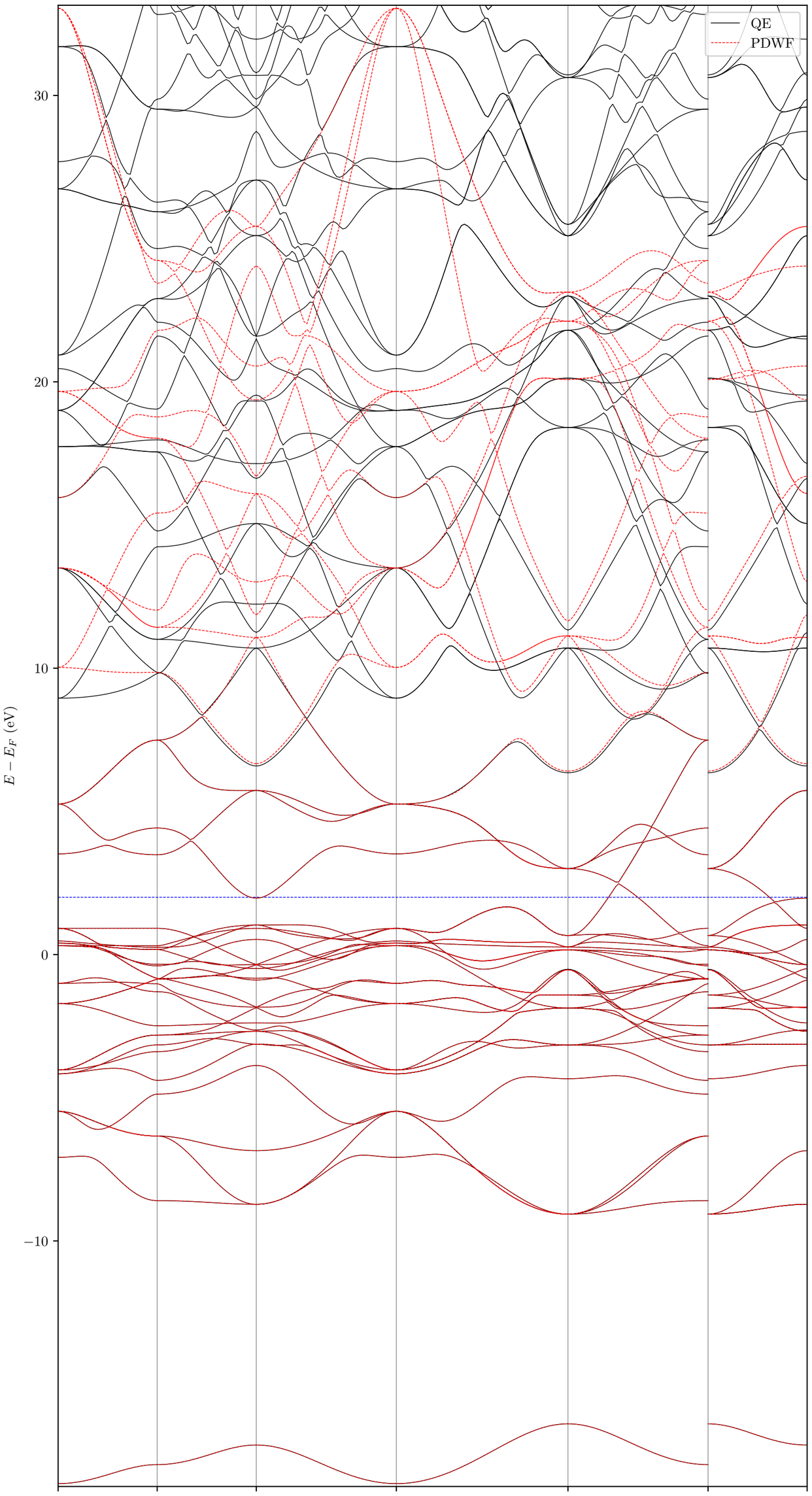



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 51.9 | 51.3 | 51.5 | 503.1 | 503.1 | 503.1 | 2.885 |



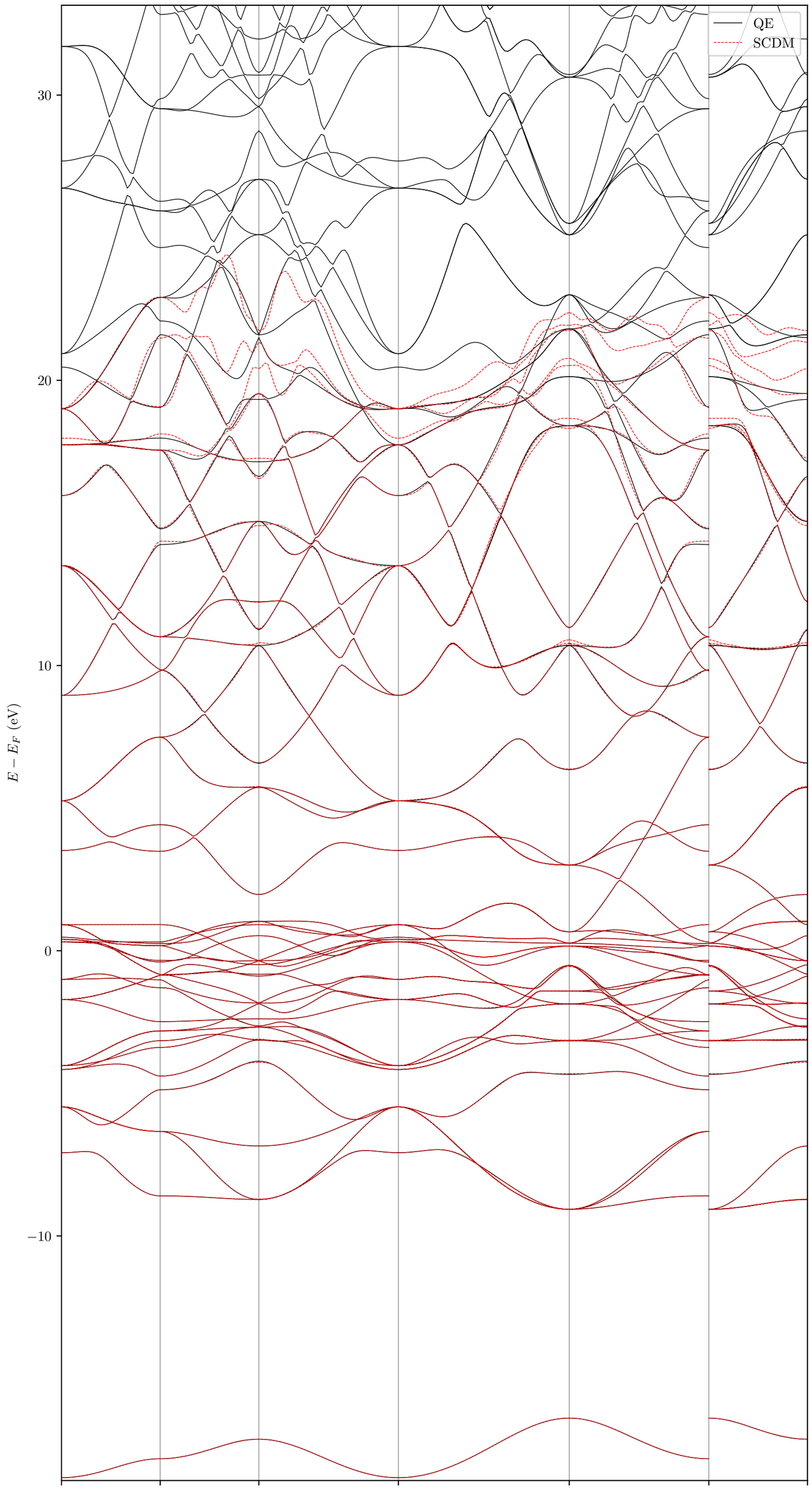
Fe4N exclude semicore
PW=6a91be56-9ee7-4bc6-b3c8-c21def59b2f3
W90=819b7f98-ef7a-45f8-a4d9-af20ec3615c9




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.7 | 1.5 | 1.6 | 18.9 | 19.0 | 19.0 | 1.928 |

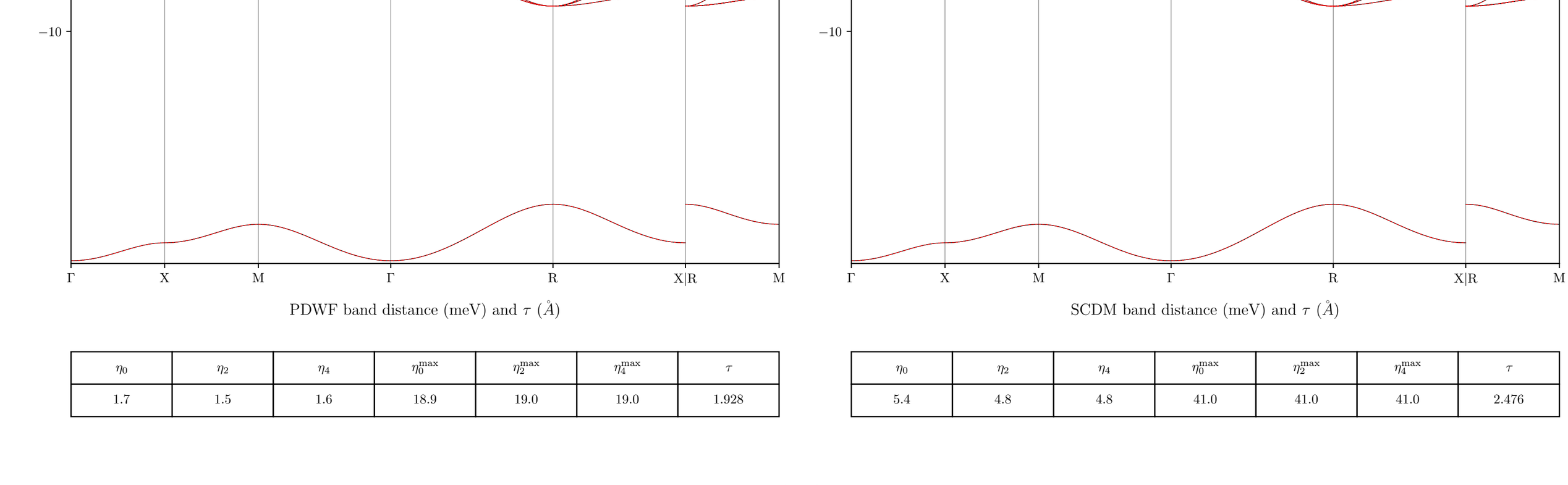
Fe4N exclude semicore
PW=6a91be56-9ee7-4bc6-b3c8-c21def59b2f3
W90=68f3d2cc-5d0d-415e-af72-310af59ec2be

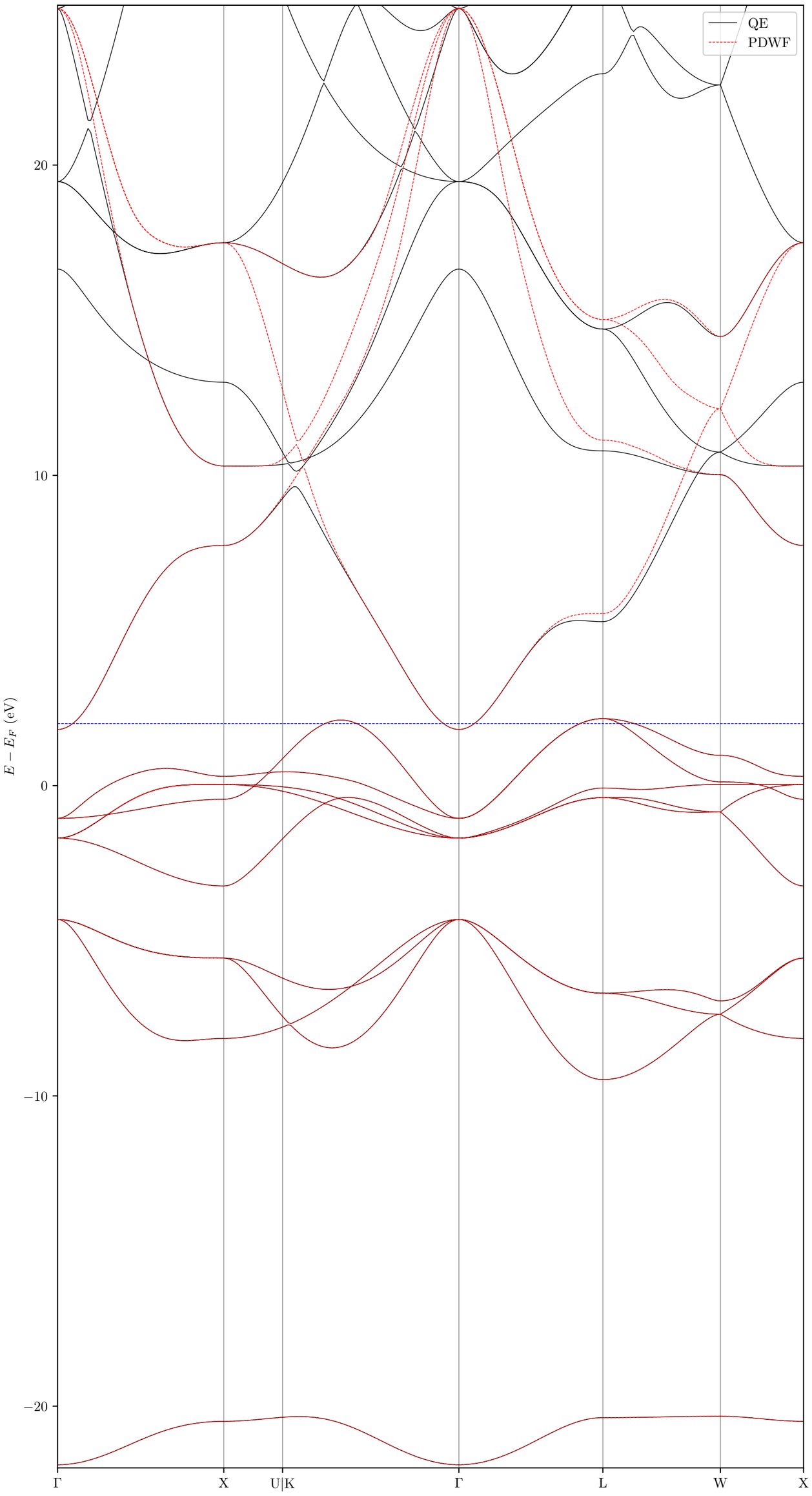



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.4 | 4.8 | 4.8 | 41.0 | 41.0 | 41.0 | 2.476 |

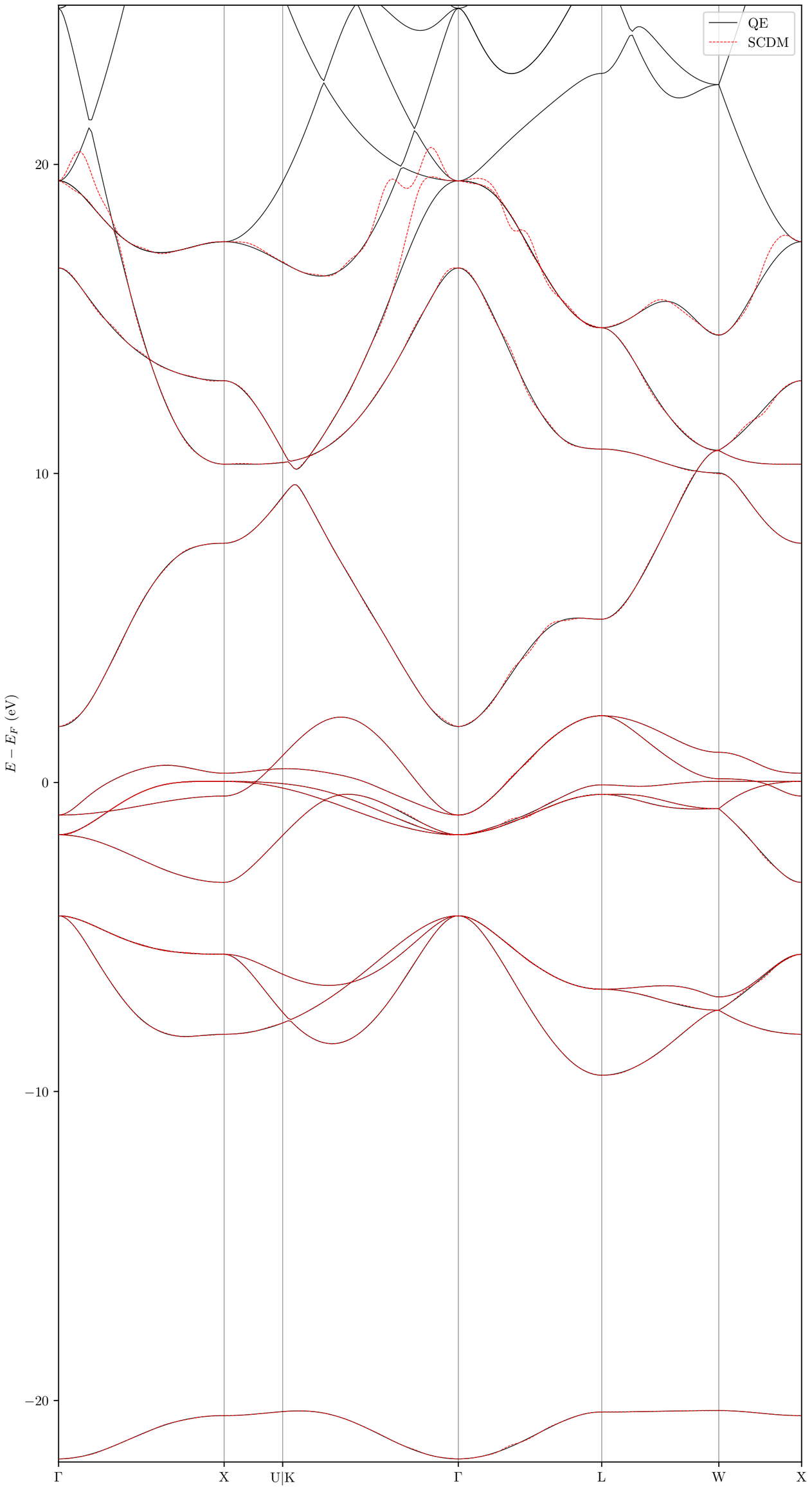
Hamiltonian decay





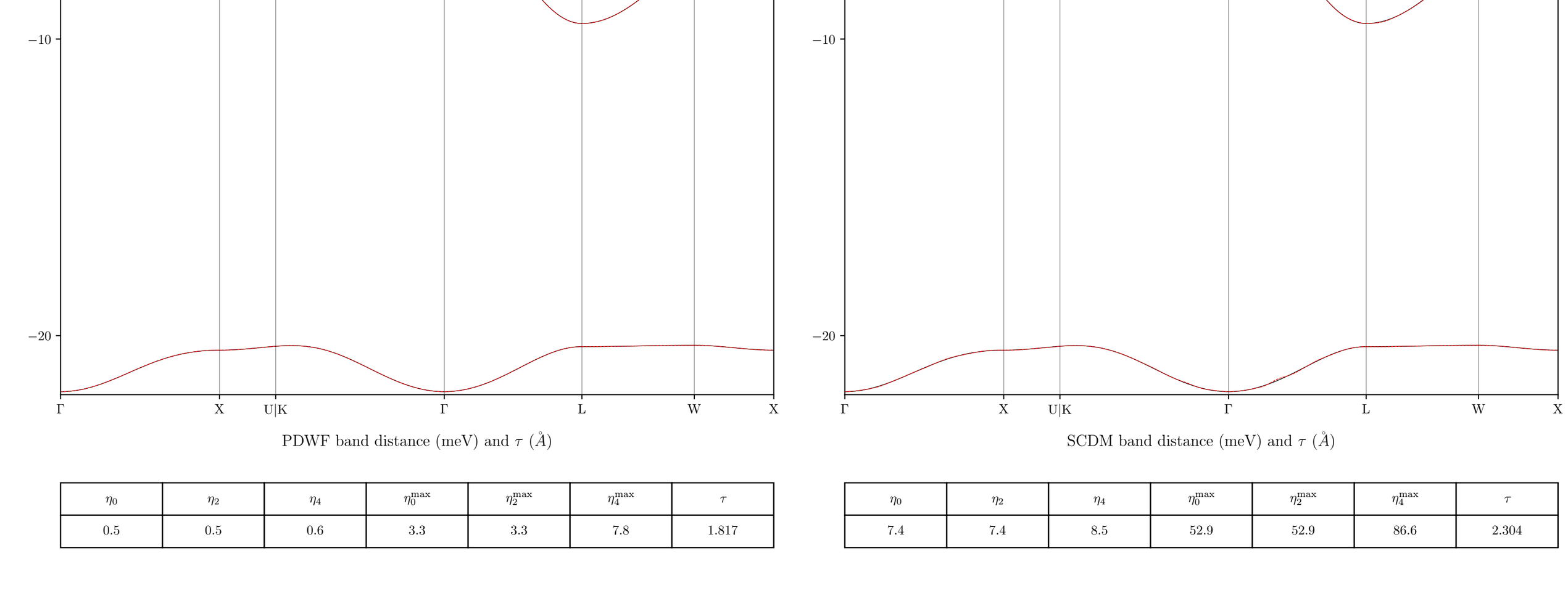

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

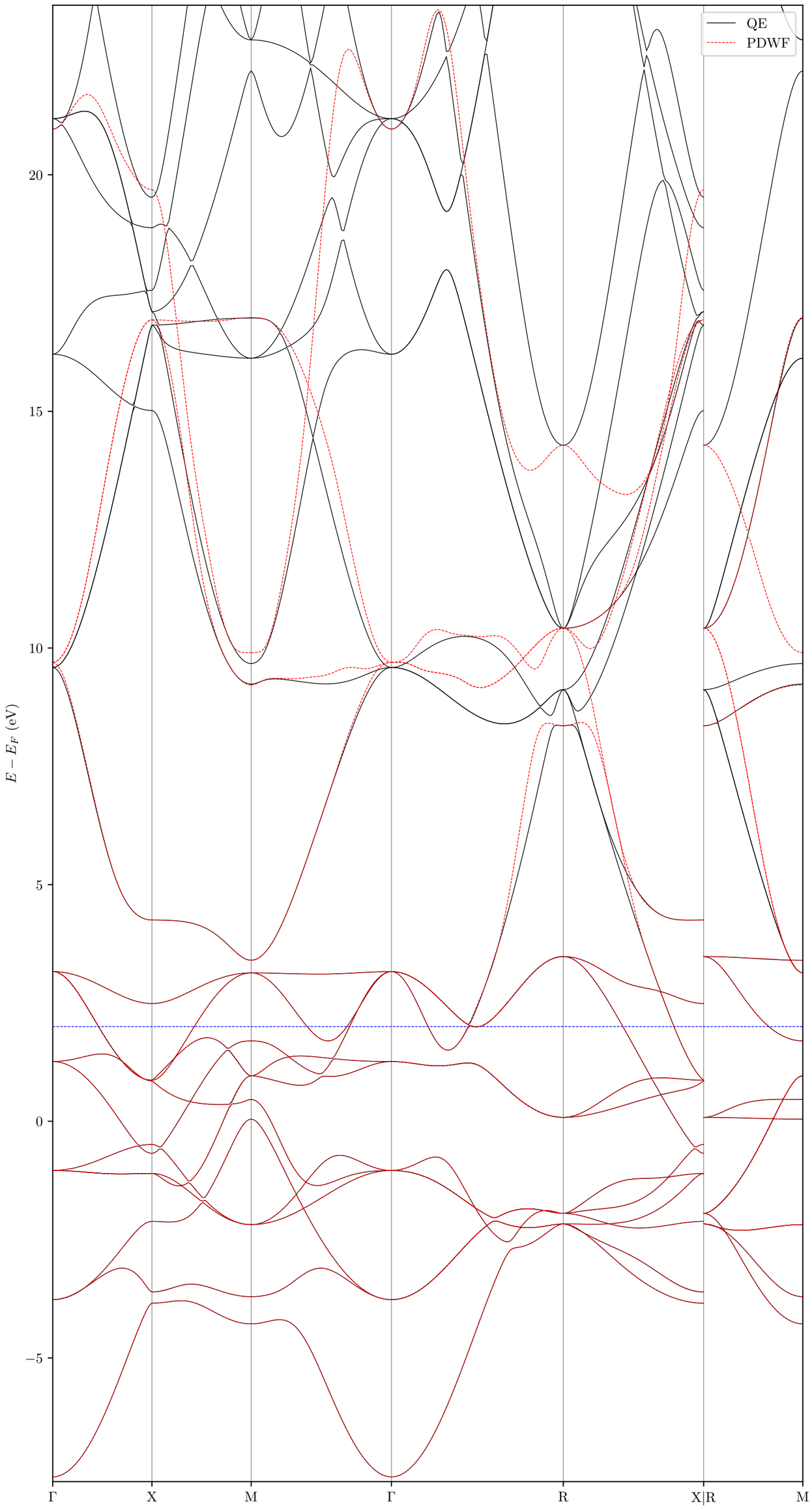
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.5 | 0.6 | 3.3 | 3.3 | 7.8 | 1.817 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

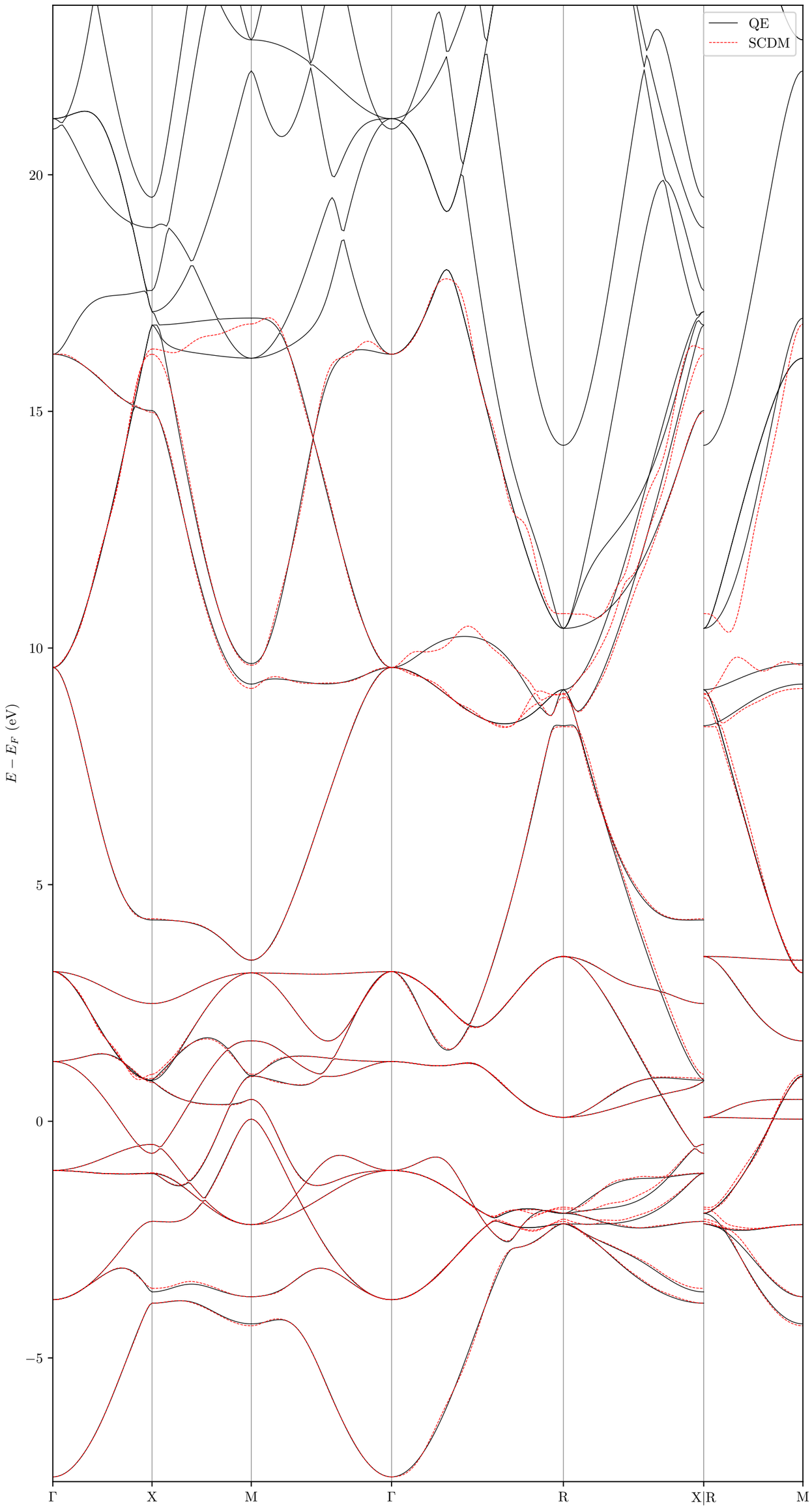
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.4 | 7.4 | 8.5 | 52.9 | 52.9 | 86.6 | 2.304 |





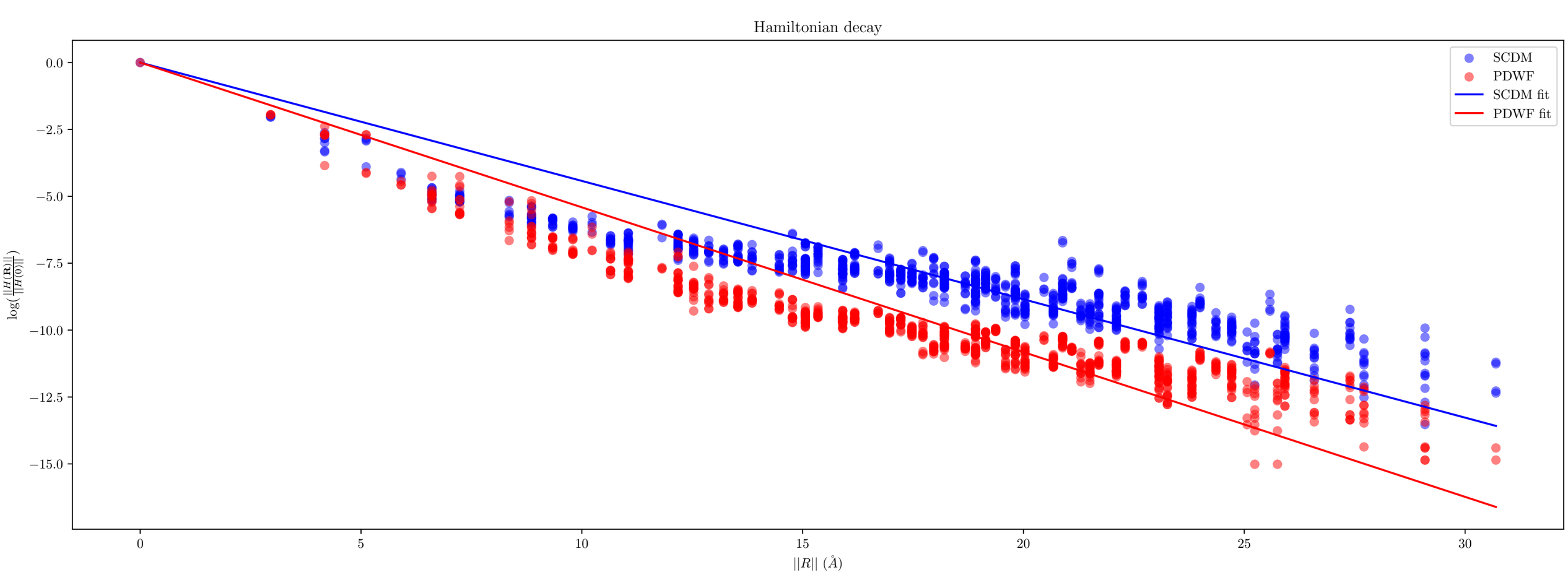

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

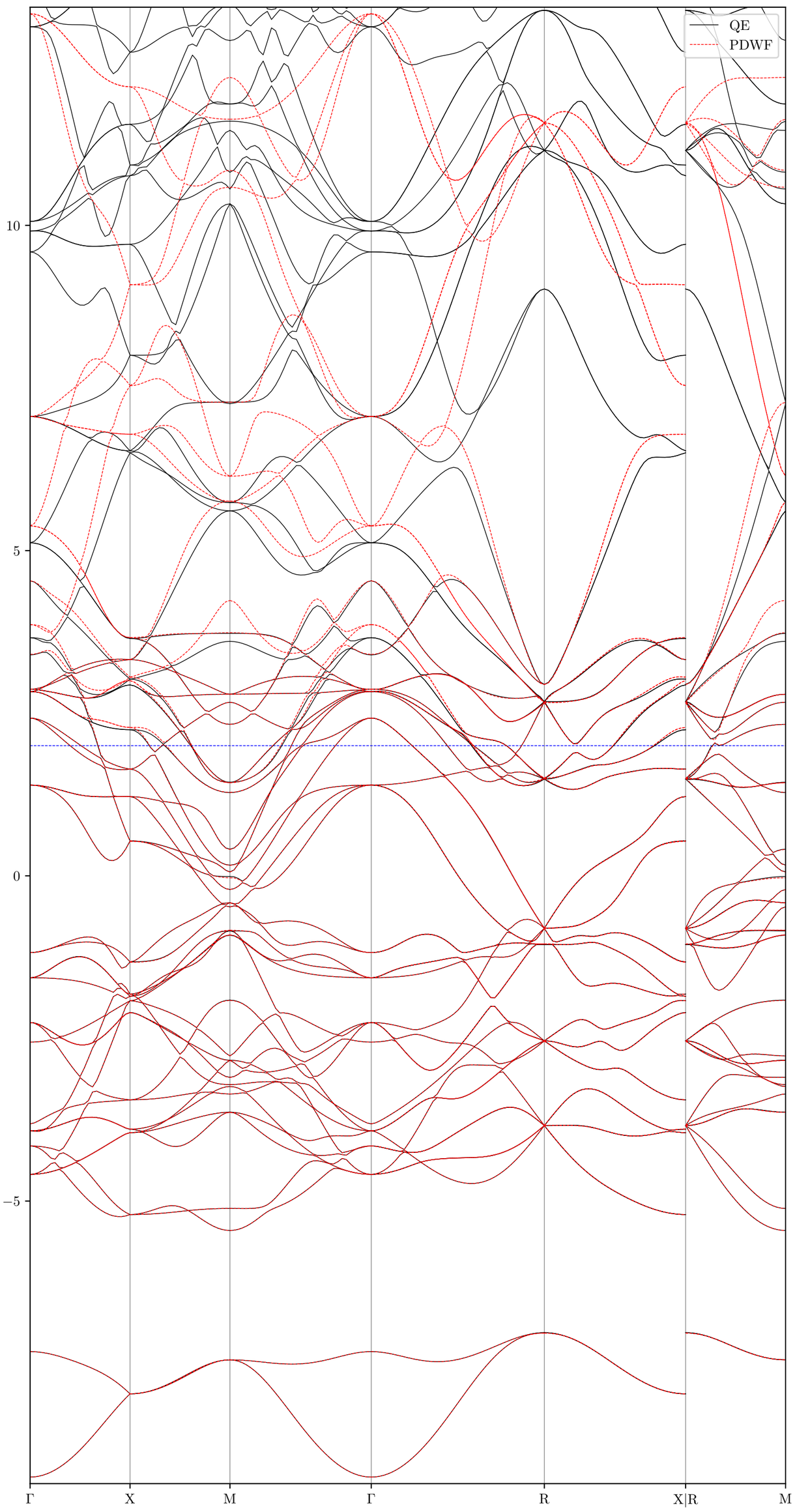
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.4 | 1.8 | 3.1 | 7.7 | 19.7 | 34.9 | 1.848 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

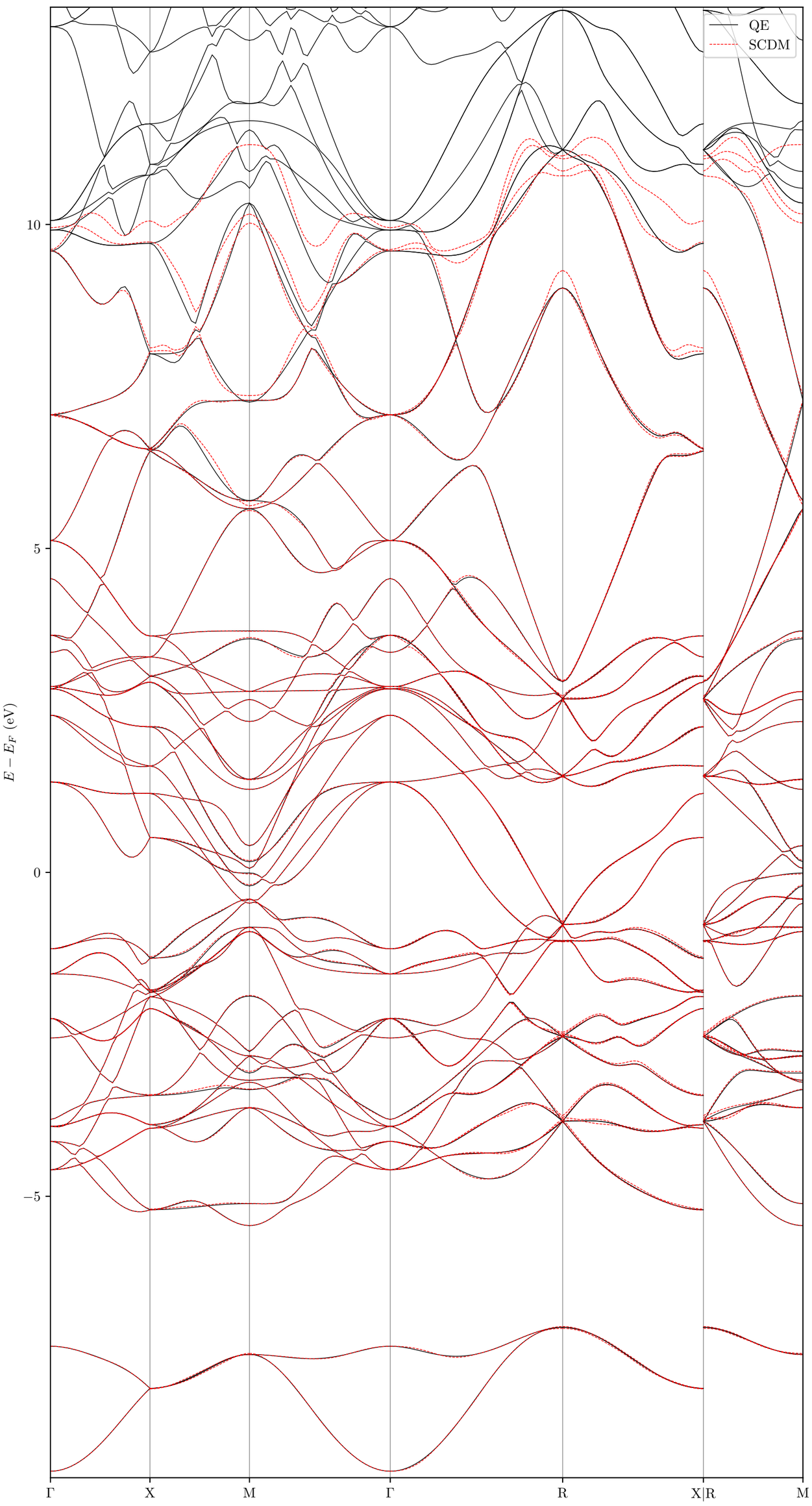
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 31.8 | 29.4 | 28.6 | 160.1 | 160.1 | 160.1 | 2.261 |





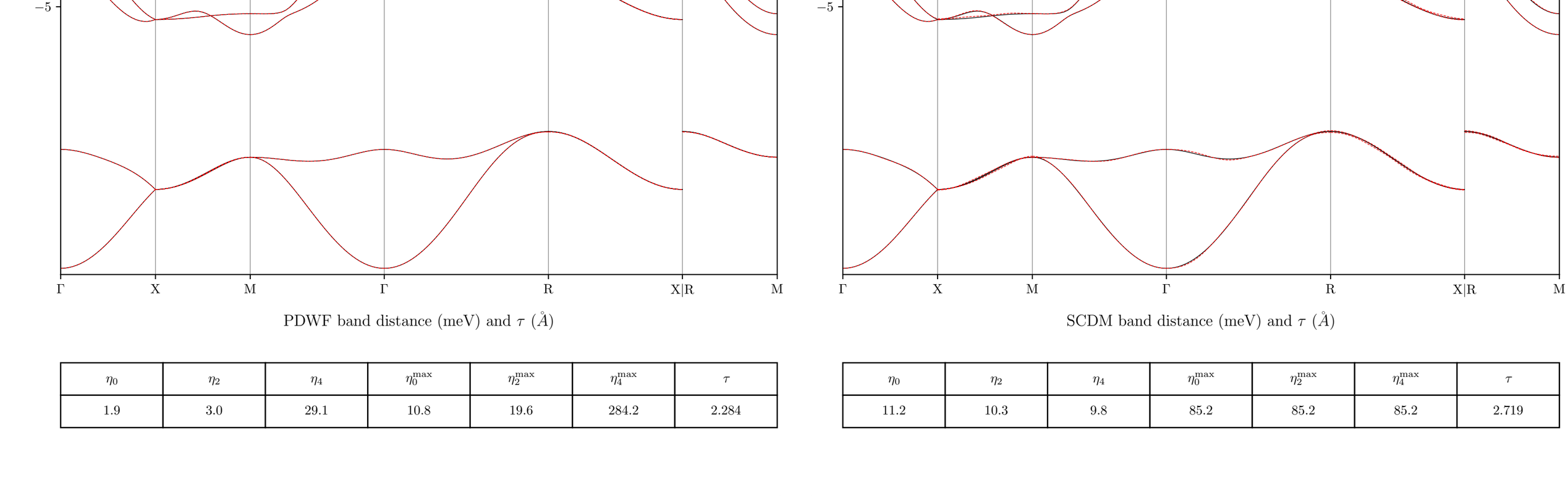

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.9 | 3.0 | 29.1 | 10.8 | 19.6 | 284.2 | 2.284 |

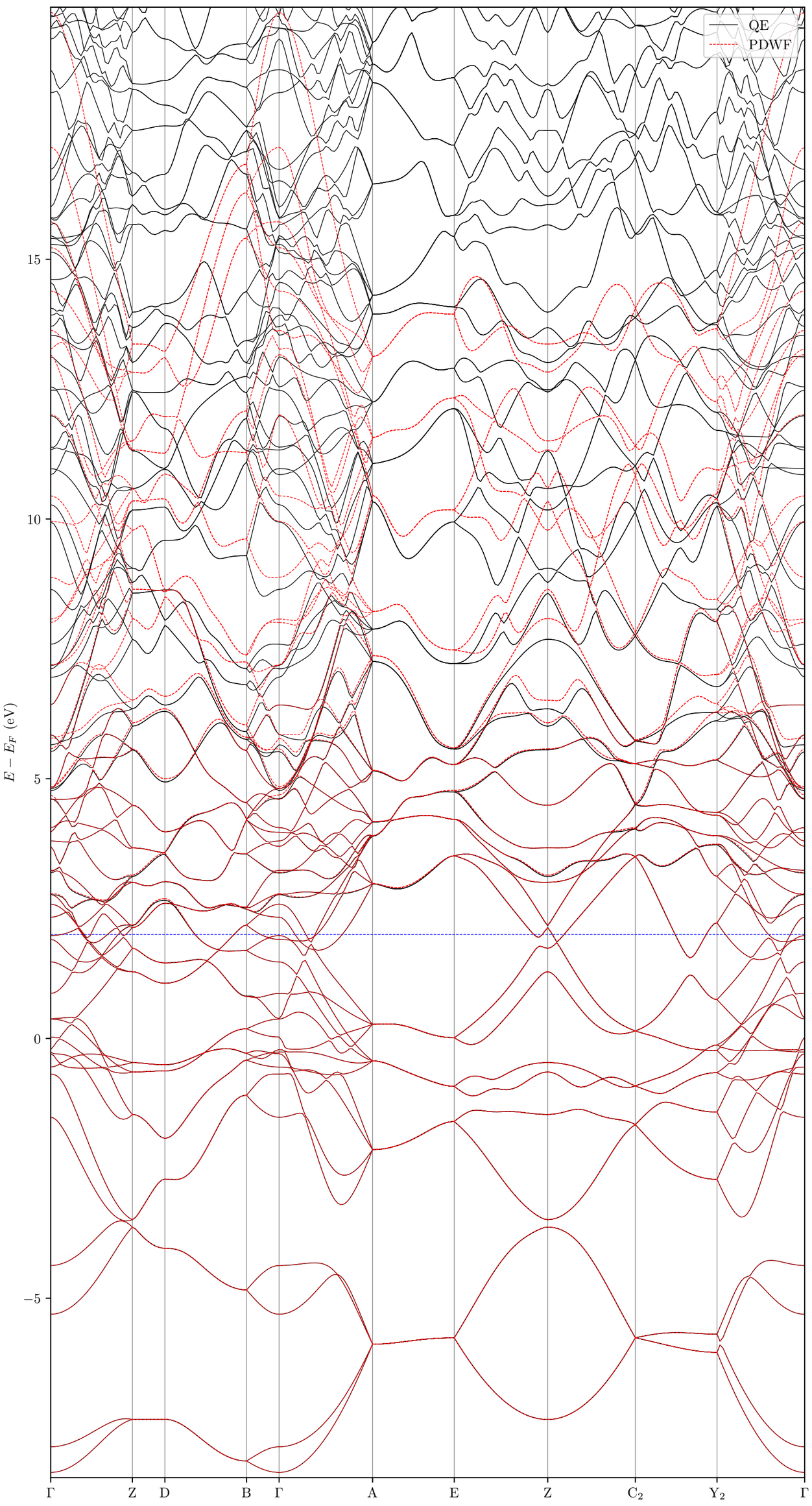



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 11.2 | 10.3 | 9.8 | 85.2 | 85.2 | 85.2 | 2.719 |



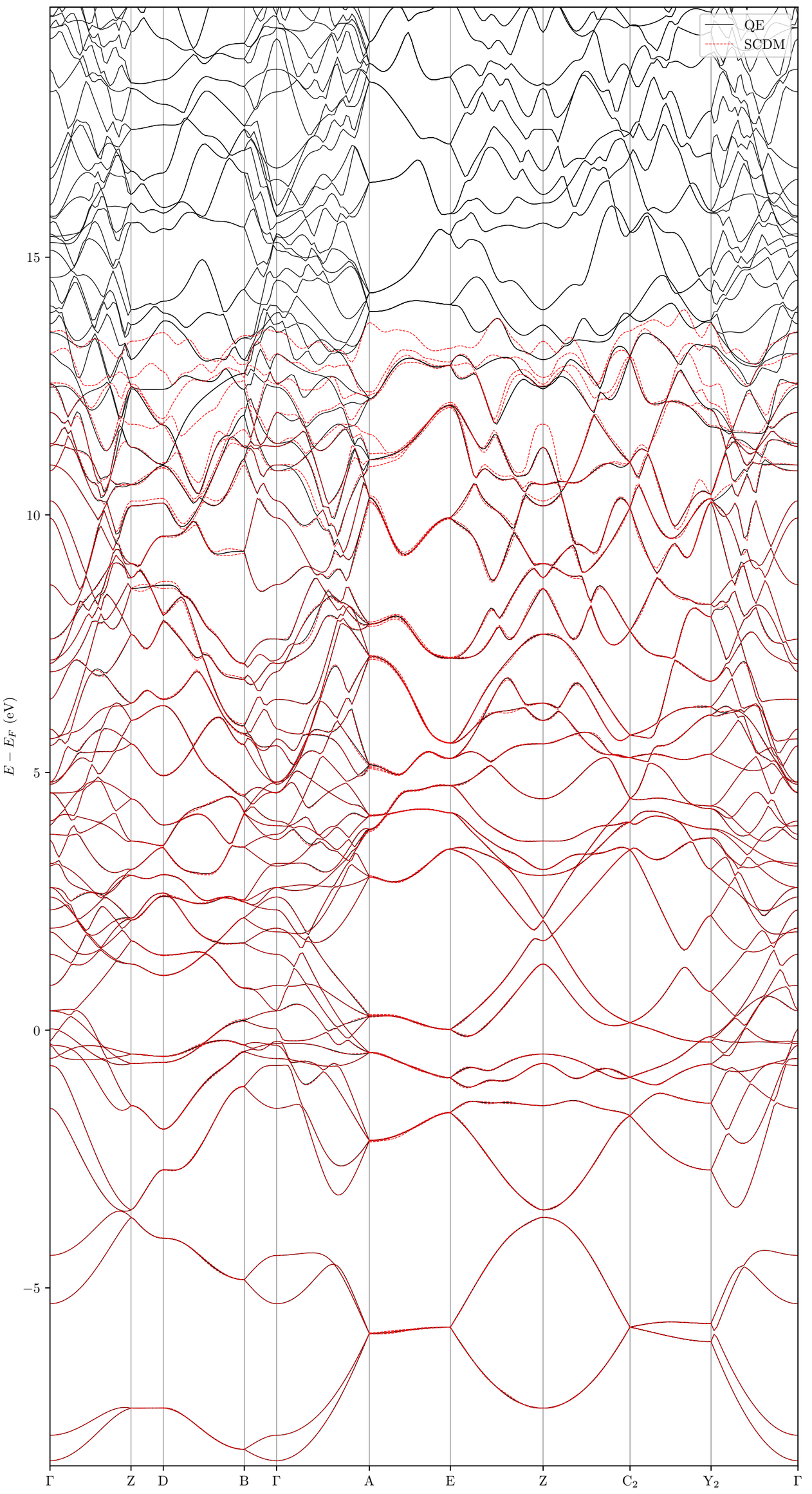
Ga4Y4 exclude semicore
PW=3e9111e3-9583-4773-b753-c4abe04acb91
W90=452e801d-f6f0-4d46-ba97-7f5dcc173e55




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.0 | 1.3 | 5.5 | 5.5 | 8.7 | 33.0 | 2.480 |

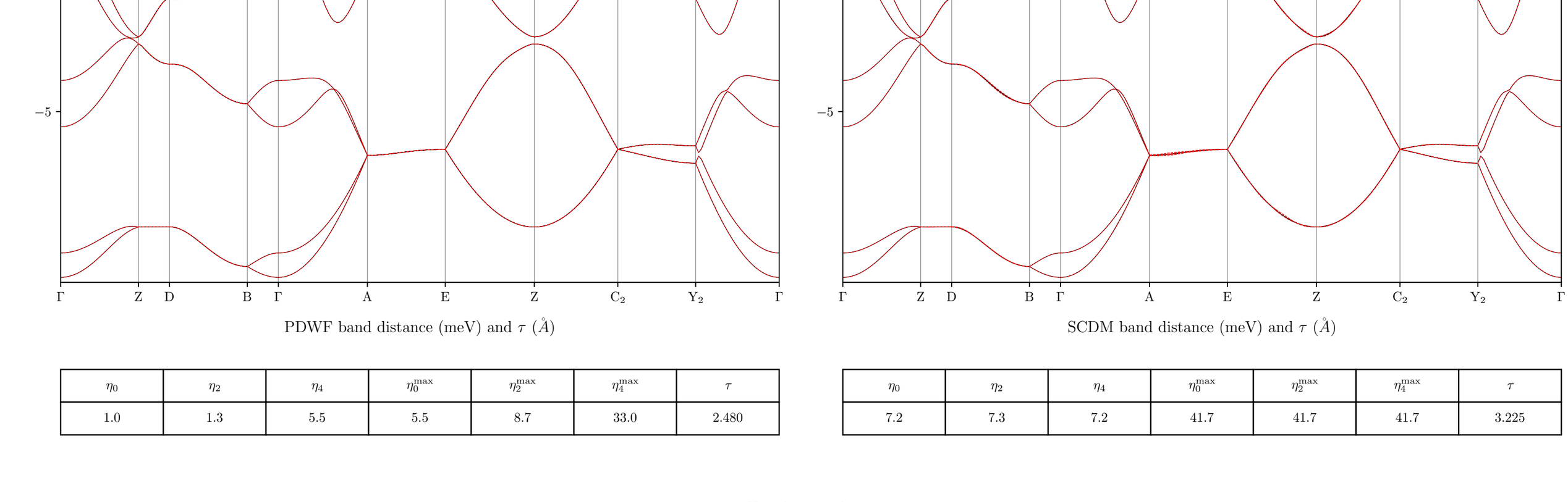
Ga4Y4 exclude semicore
PW=3e9111e3-9583-4773-b753-c4abe04acb91
W90=1f11ee3f-3977-432e-9949-b8e40dd50823



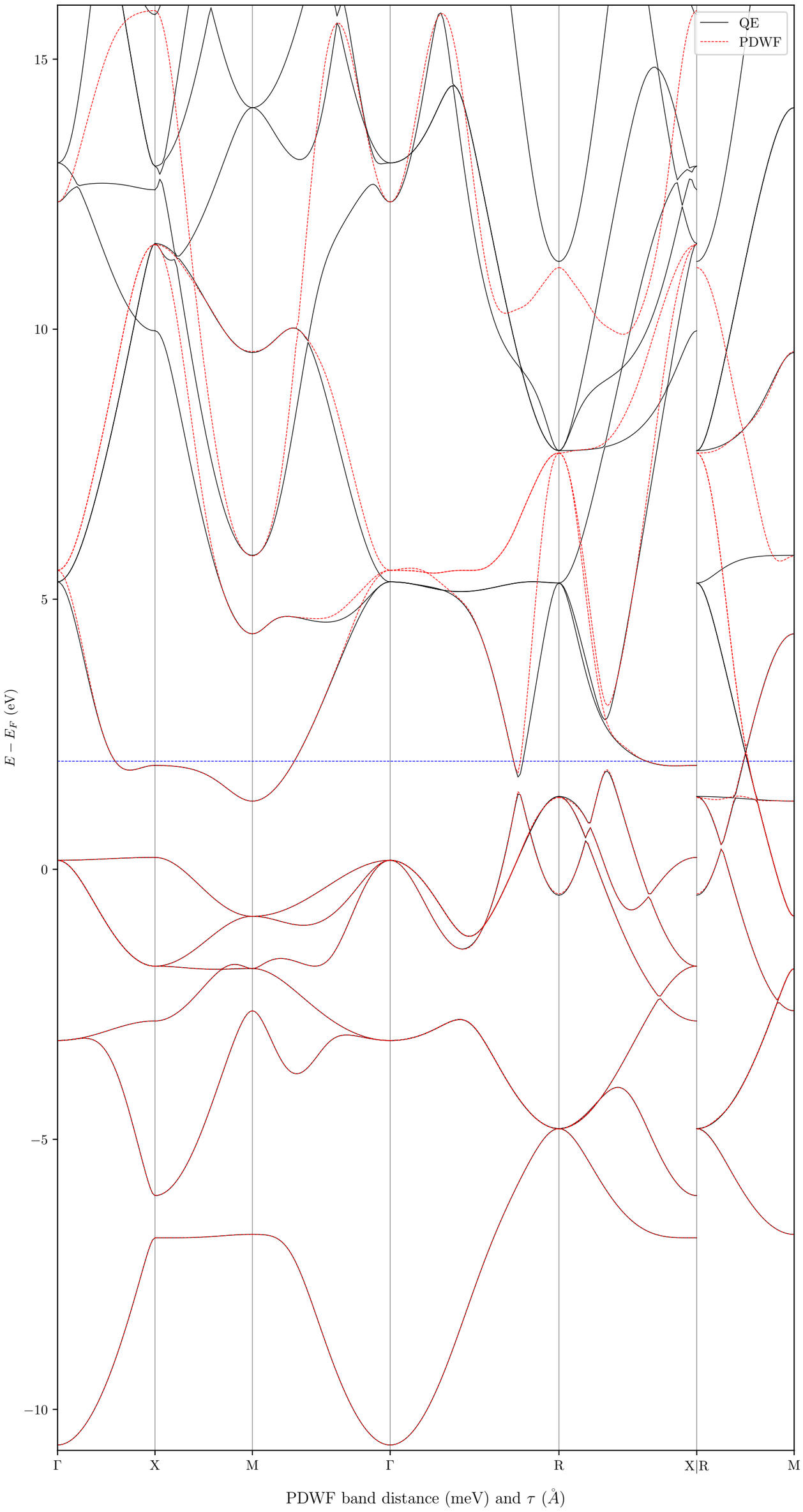

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.2 | 7.3 | 7.2 | 41.7 | 41.7 | 41.7 | 3.225 |

Hamiltonian decay



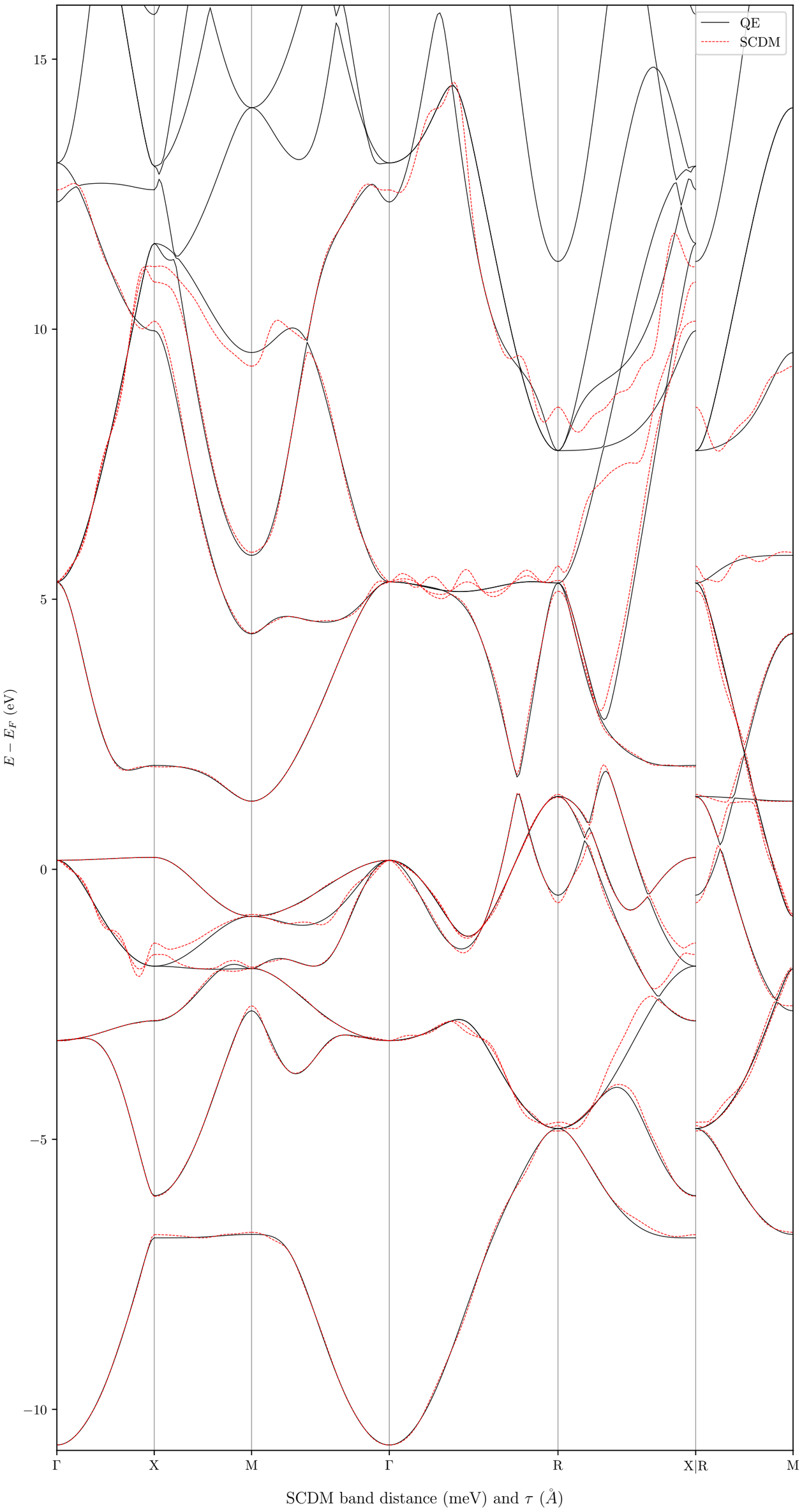
GaRu exclude semicore
PW=6f51fb08-c6fc-4dba-a8b8-673127557708
W90=ab08d256-f3a5-4544-bc92-1e9007271e5b




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.5 | 9.1 | 66.7 | 25.4 | 158.9 | 979.2 | 1.940 |

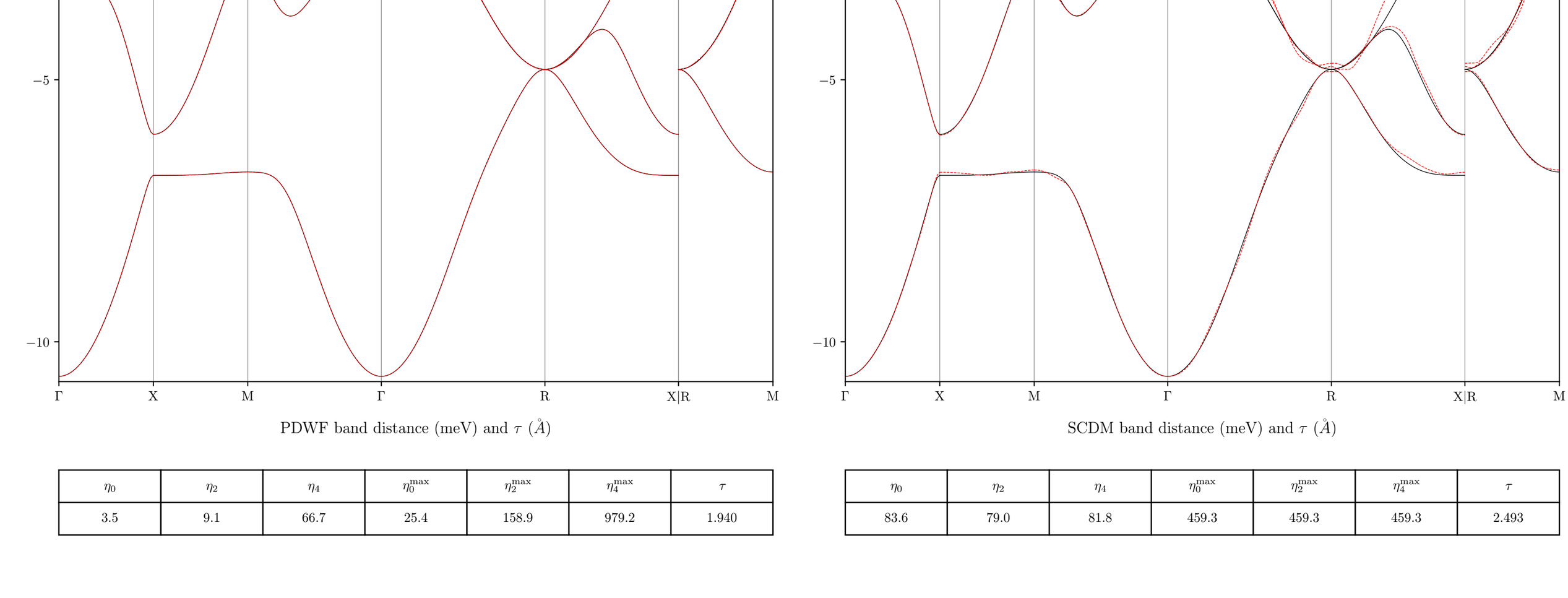
GaRu exclude semicore
PW=6f51fb08-c6fc-4dba-a8b8-673127557708
W90=540e3850-5649-41b4-bfb4-0a54a6fba830



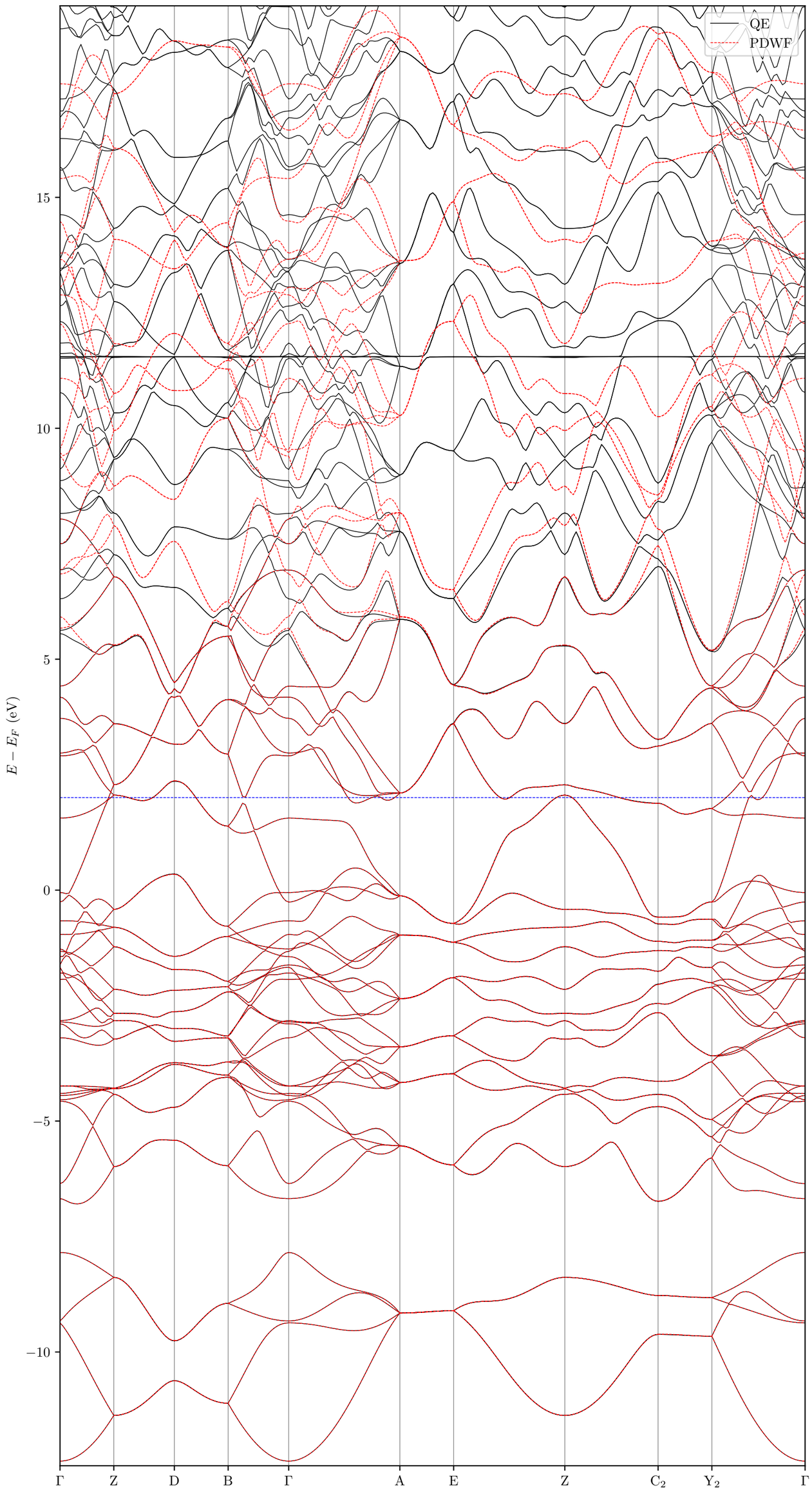

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 83.6 | 79.0 | 81.8 | 459.3 | 459.3 | 459.3 | 2.493 |

Hamiltonian decay



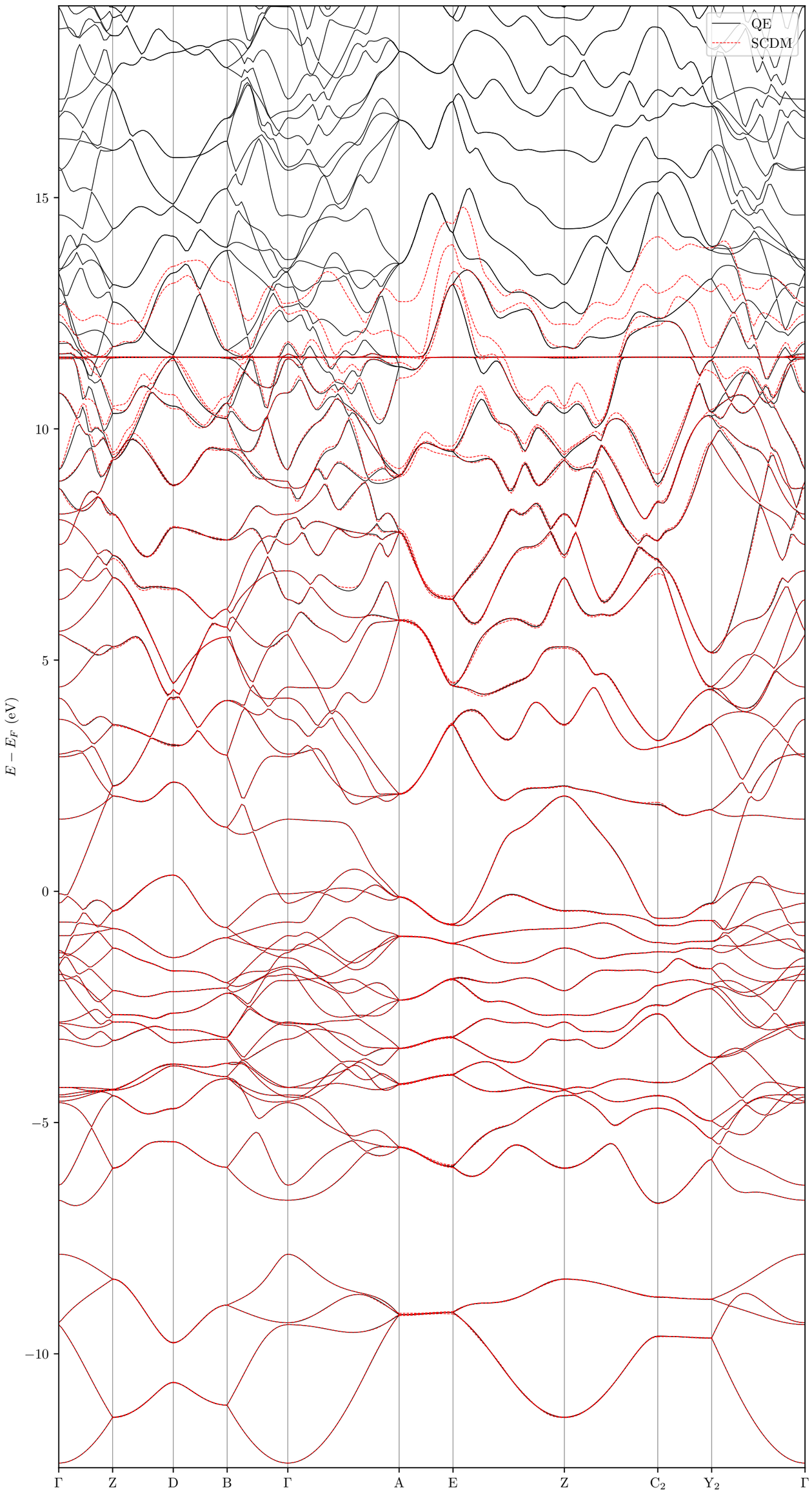
Ge4Ir4 exclude semicore
PW=4a63fb97-1d03-48b7-9541-d22202a678ff
W90=3f9fd84e-9a73-4928-be83-912731a6f3d2




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.7 | 1.7 | 2.0 | 9.9 | 9.9 | 12.3 | 2.274 |

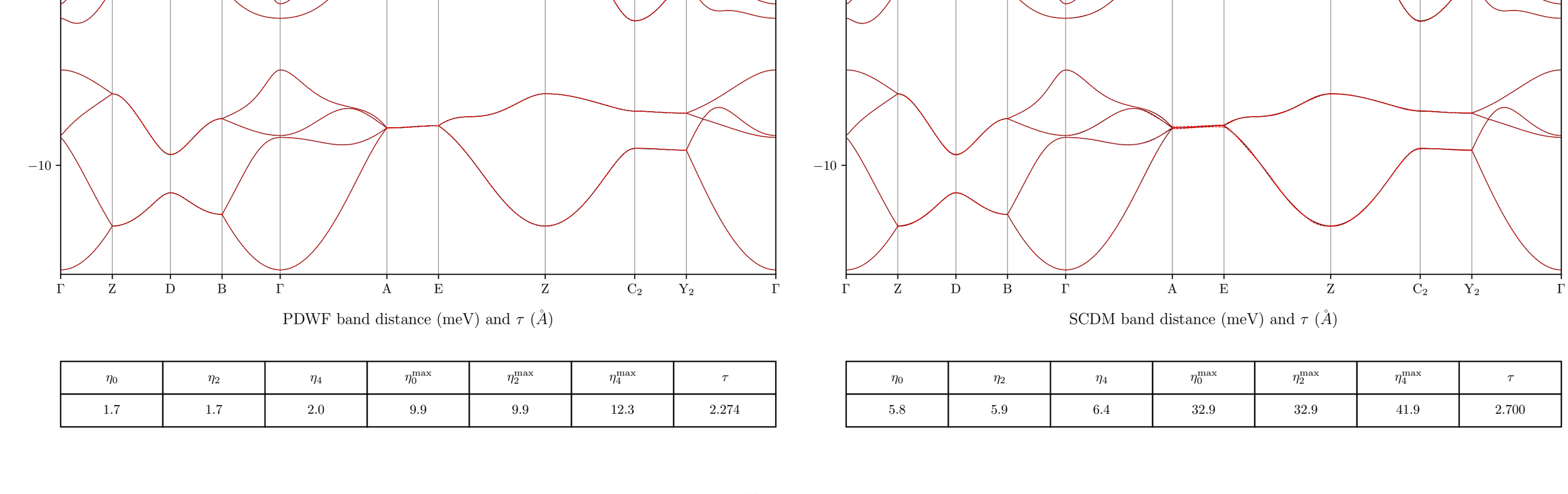
Ge4Ir4 exclude semicore
PW=4a63fb97-1d03-48b7-9541-d22202a678ff
W90=8d73e8f0-9431-4e42-88dd-d0c54ca3c68b



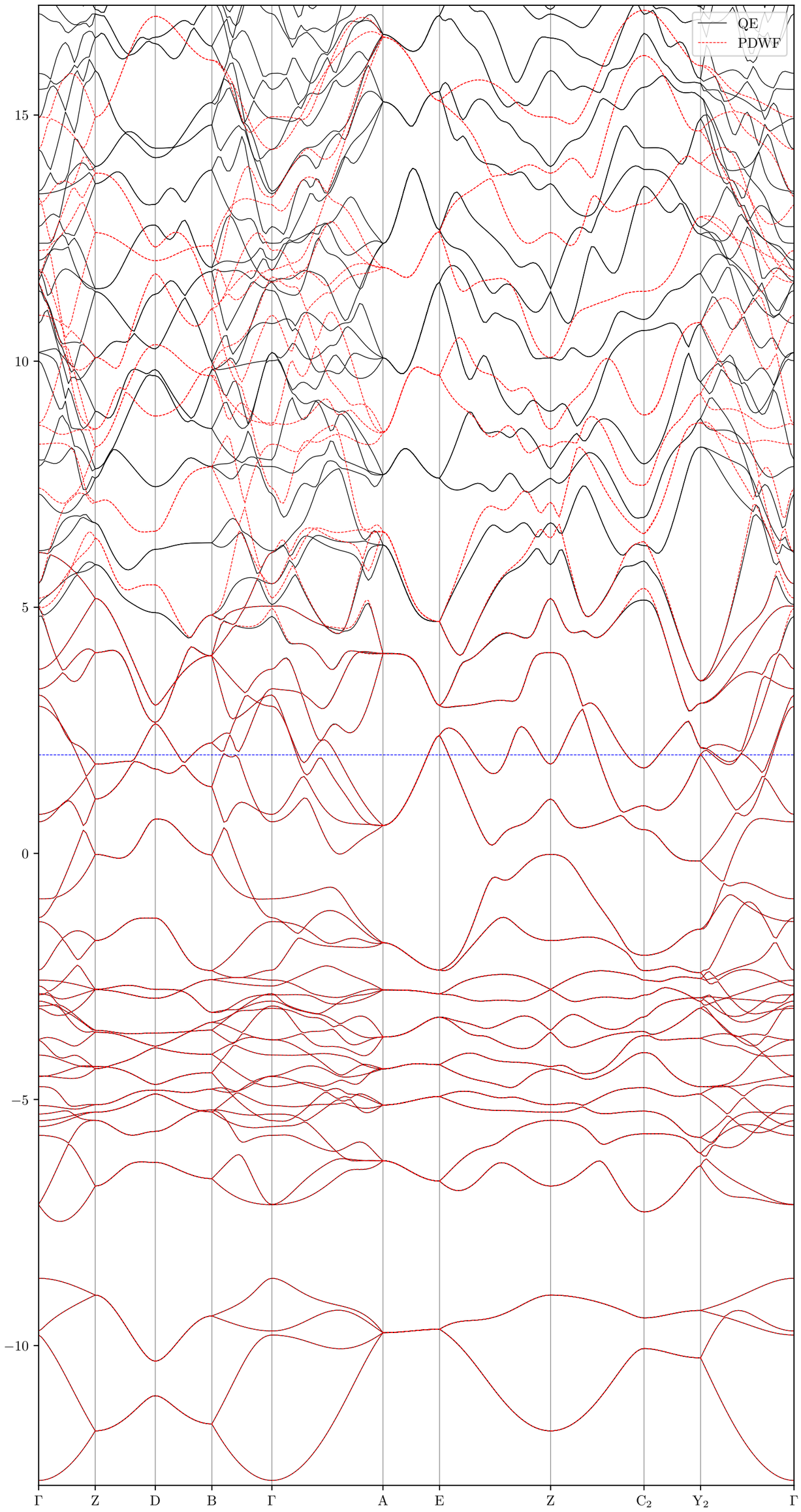

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.8 | 5.9 | 6.4 | 32.9 | 32.9 | 41.9 | 2.700 |

Hamiltonian decay



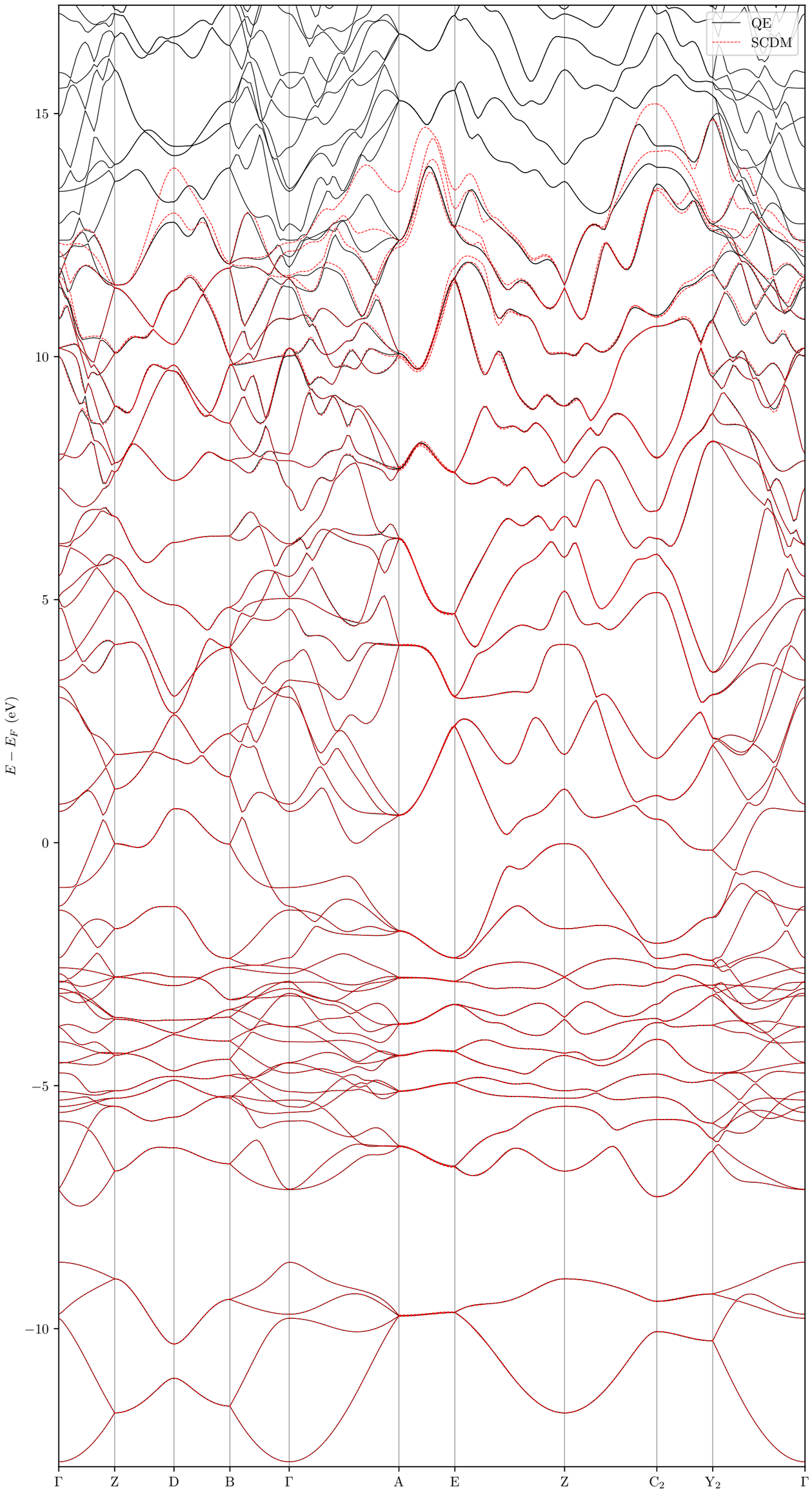
Ge4Pt4 exclude semicore
PW=cf7cf41a-cdd0-4413-b297-8fa3e86941bf
W90=6ffa2784-b697-4ca1-a398-ab5e3e13ef6e




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.2 | 1.6 | 6.5 | 7.1 | 13.6 | 2.372 |

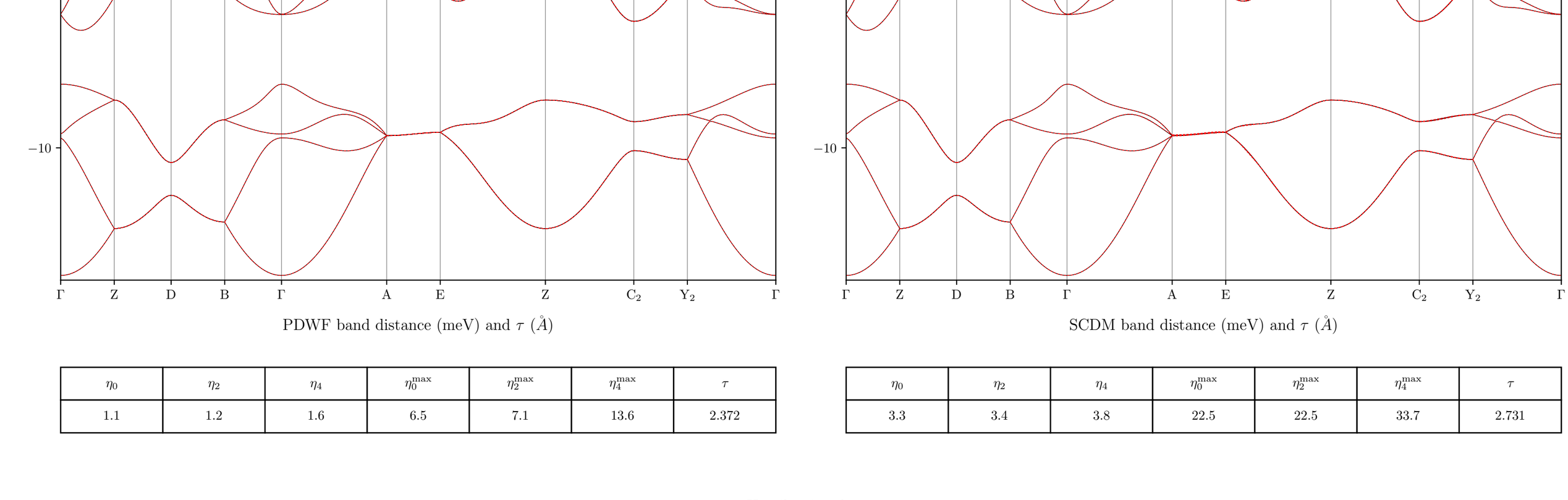
Ge4Pt4 exclude semicore
PW=cf7cf41a-cdd0-4413-b297-8fa3e86941bf
W90=6a7a4da9-0eed-49fa-b296-55b3f313ee3e



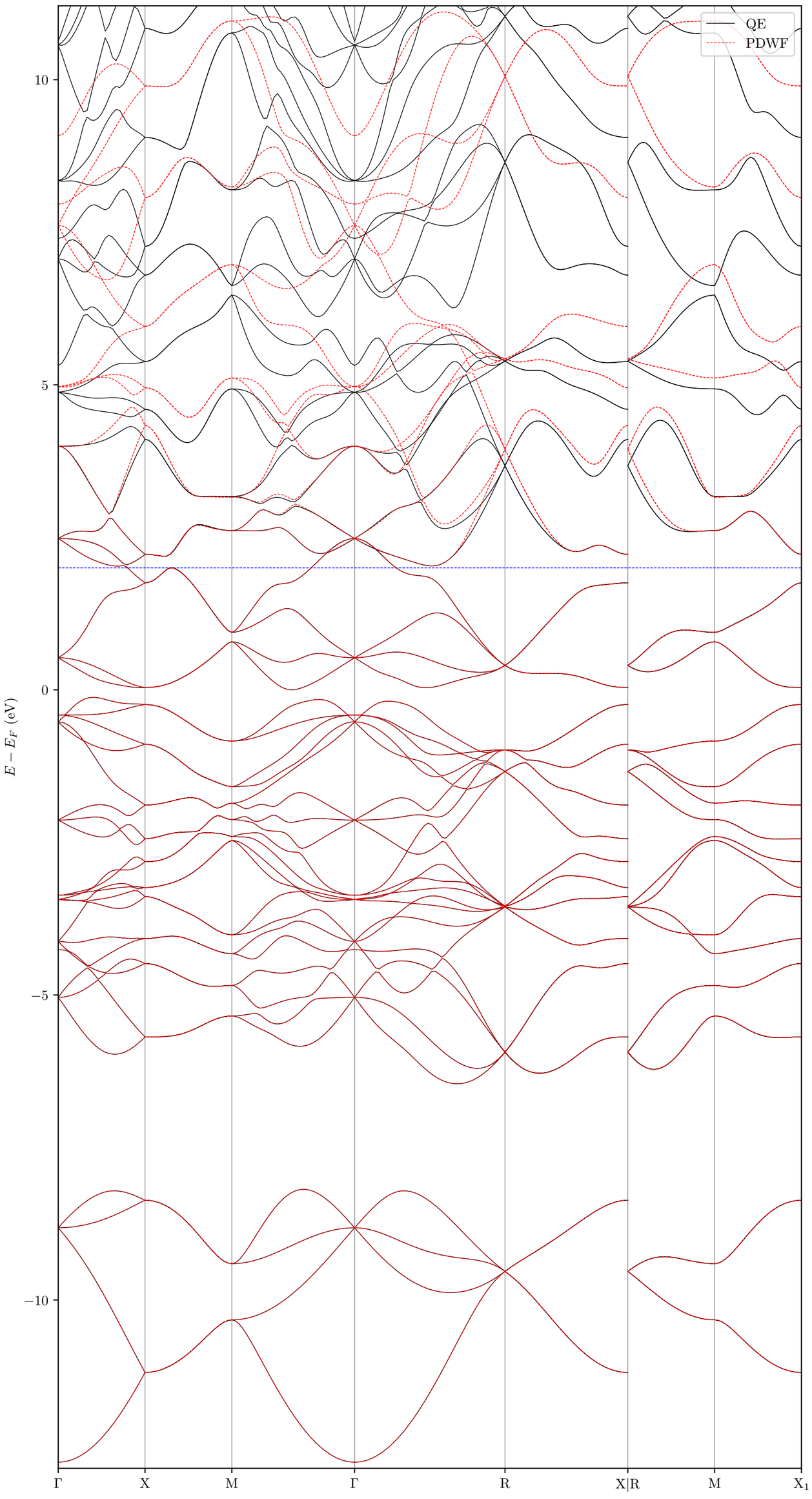

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.3 | 3.4 | 3.8 | 22.5 | 22.5 | 33.7 | 2.731 |

Hamiltonian decay



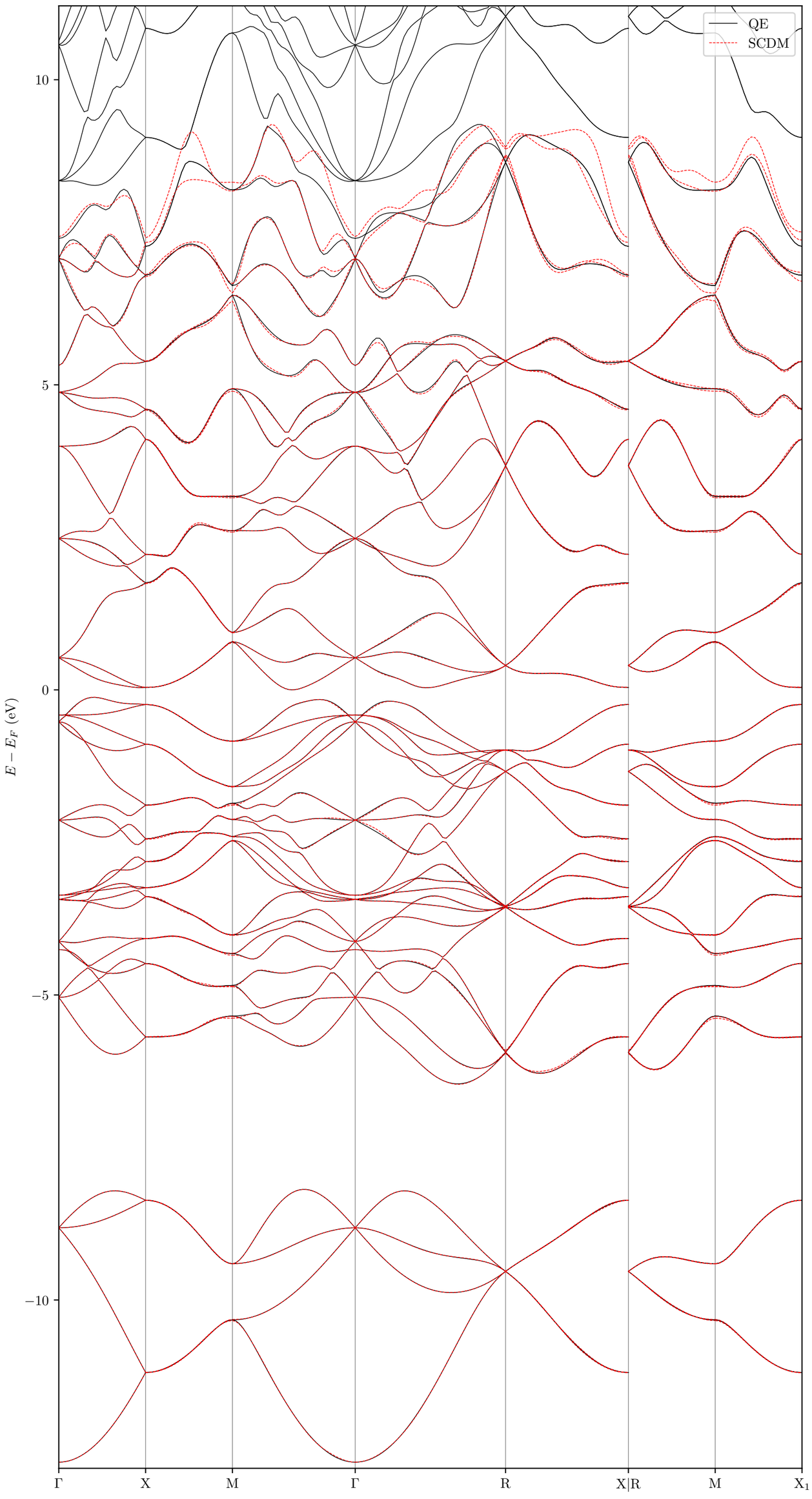
Ge4Ru4 exclude semicore
PW=50a71bf2-d203-46d7-a00f-8440b650f18f
W90=107769ea-a2c4-4d37-a819-d54b8ff3d6f5




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.4 | 1.5 | 27.9 | 8.4 | 8.4 | 235.8 | 2.278 |

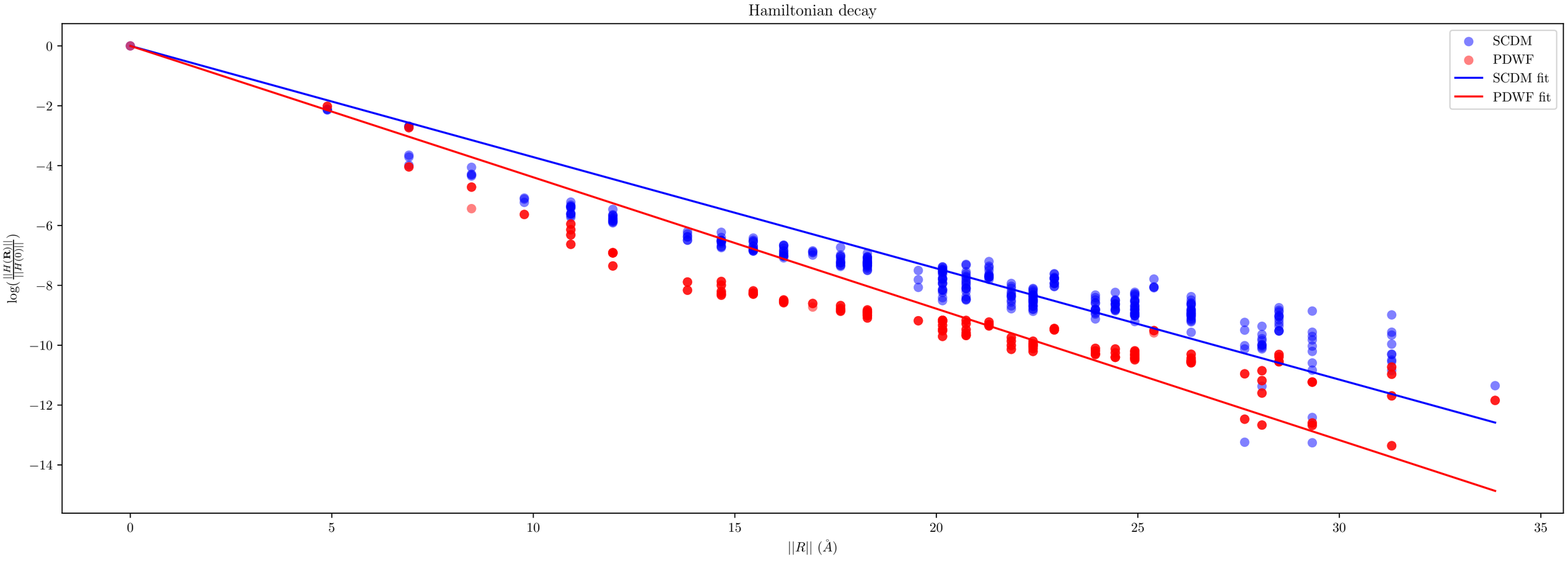
Ge4Ru4 exclude semicore
PW=50a71bf2-d203-46d7-a00f-8440b650f18f
W90=dc925161-ac64-4e6b-91de-0db98328c03b



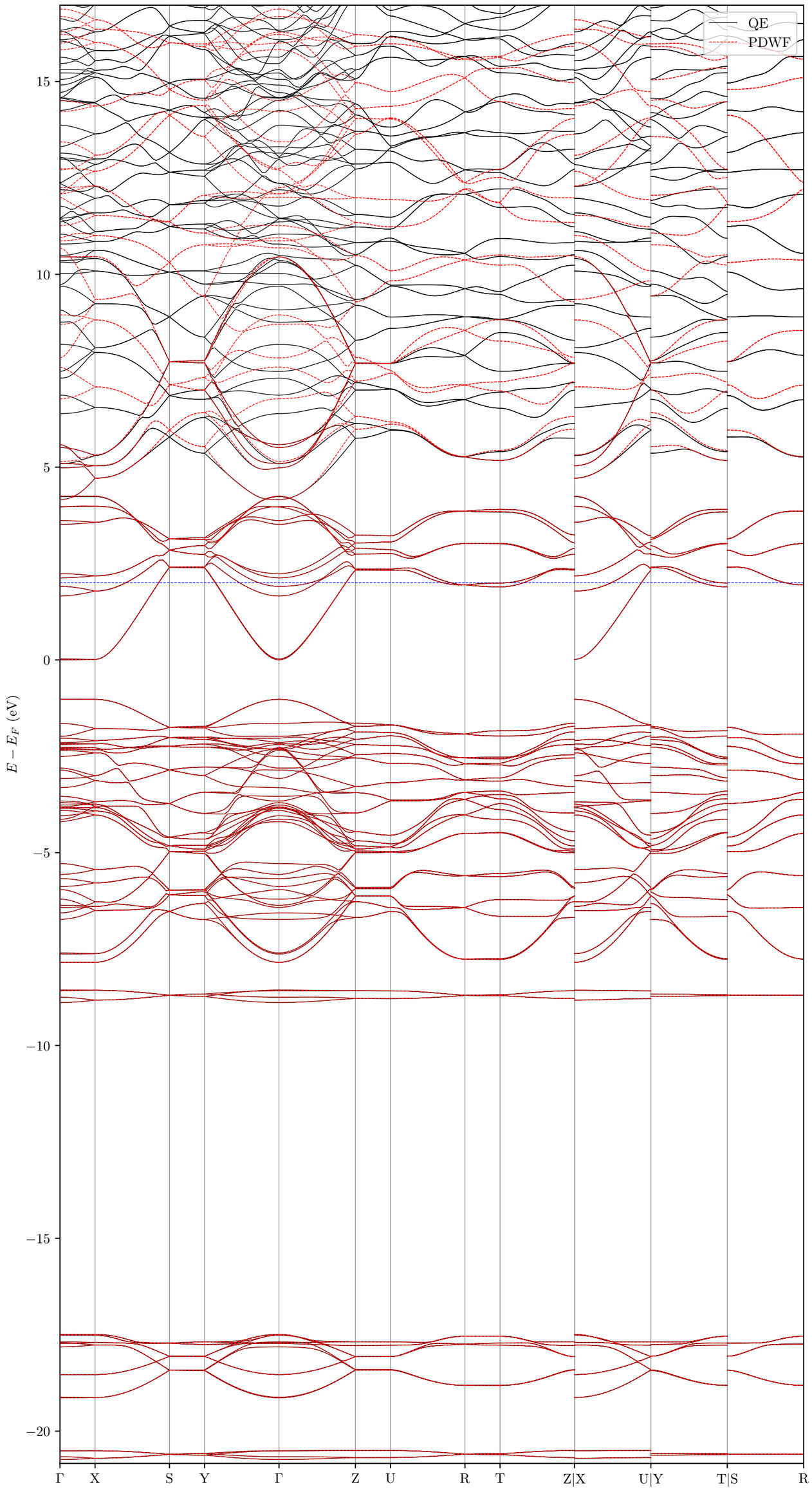

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.9 | 5.9 | 6.2 | 44.5 | 44.5 | 44.5 | 2.691 |

Hamiltonian decay



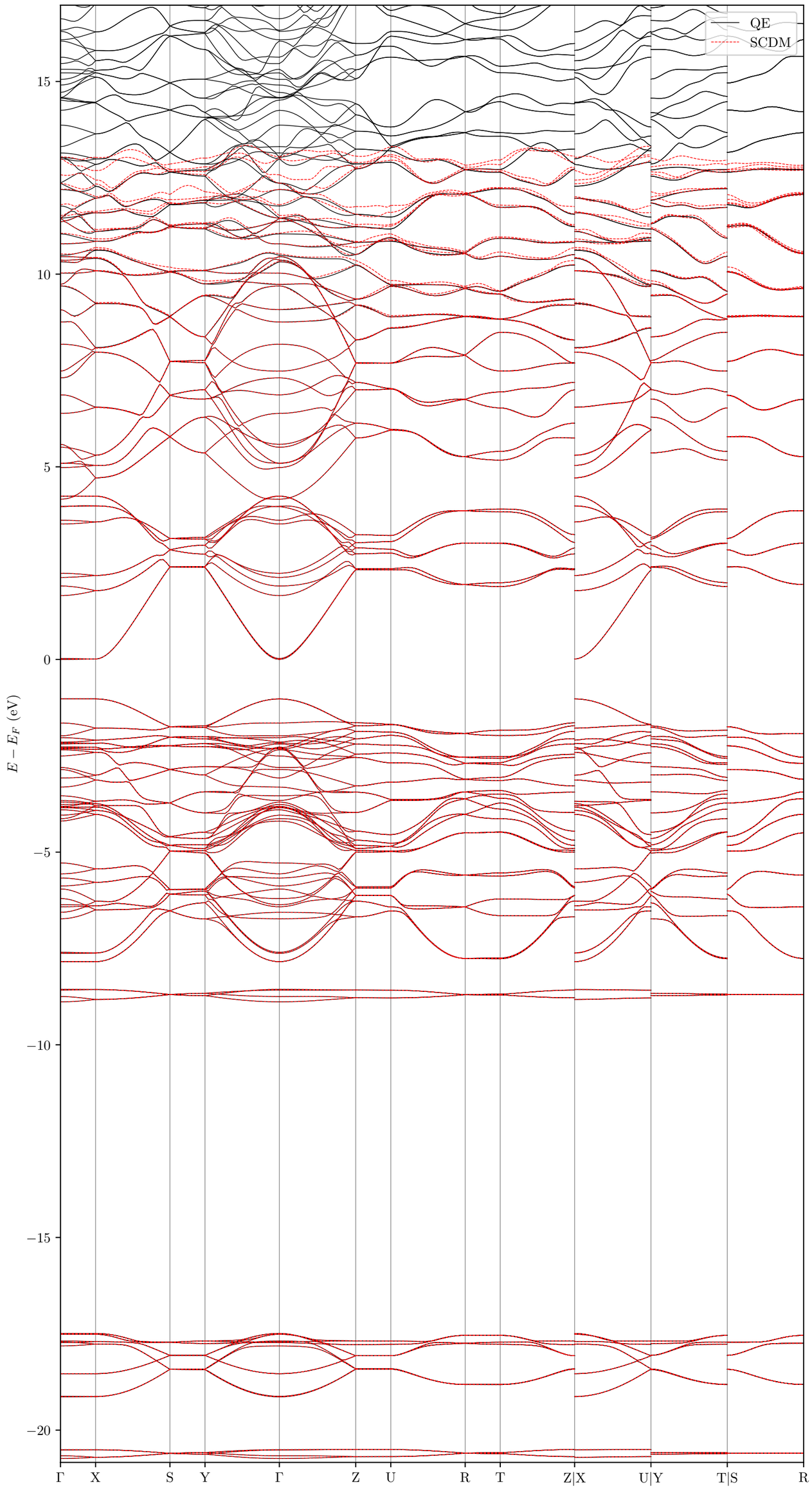
H8O16W4 exclude semicore
PW=c9f3fa41-9770-4367-9050-e4ba9921f1b0
W90=50a00ba1-e0ad-400d-a650-cd25f63248e7




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.2 | 0.3 | 2.8 | 2.8 | 2.9 | 2.556 |

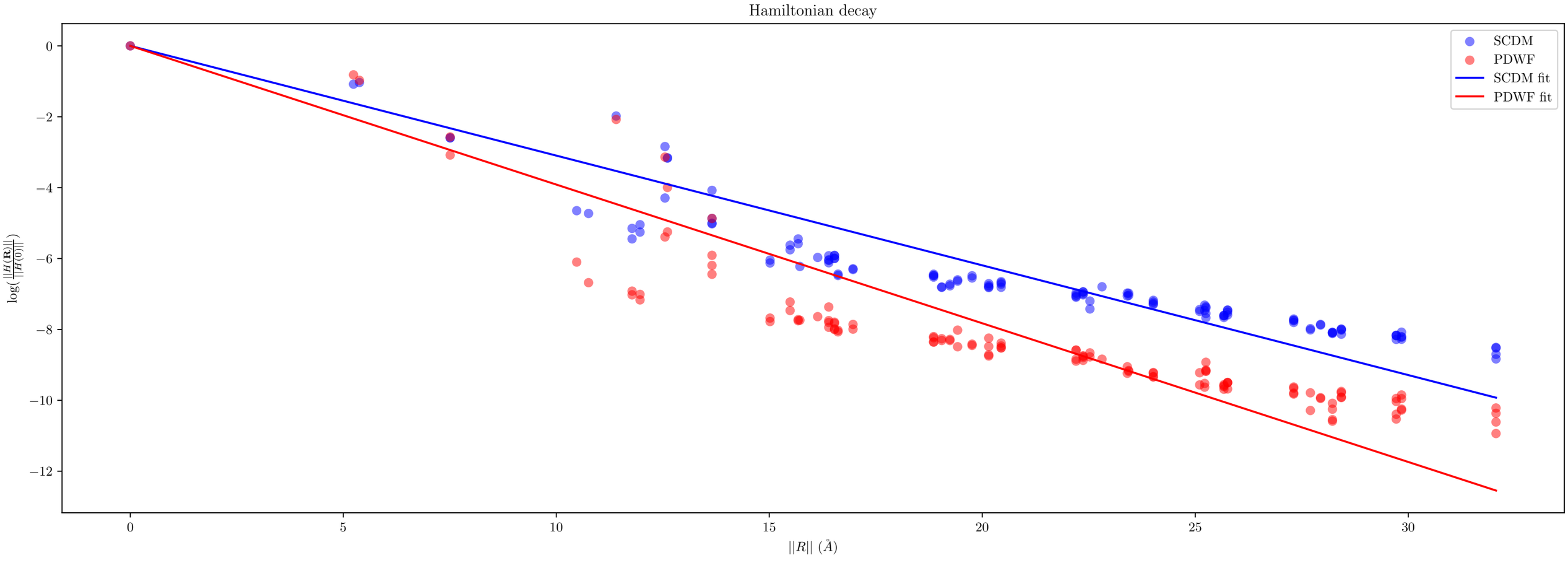
H8O16W4 exclude semicore
PW=c9f3fa41-9770-4367-9050-e4ba9921f1b0
W90=2757ecd8-beea-4d45-9116-2adecb32e1c3



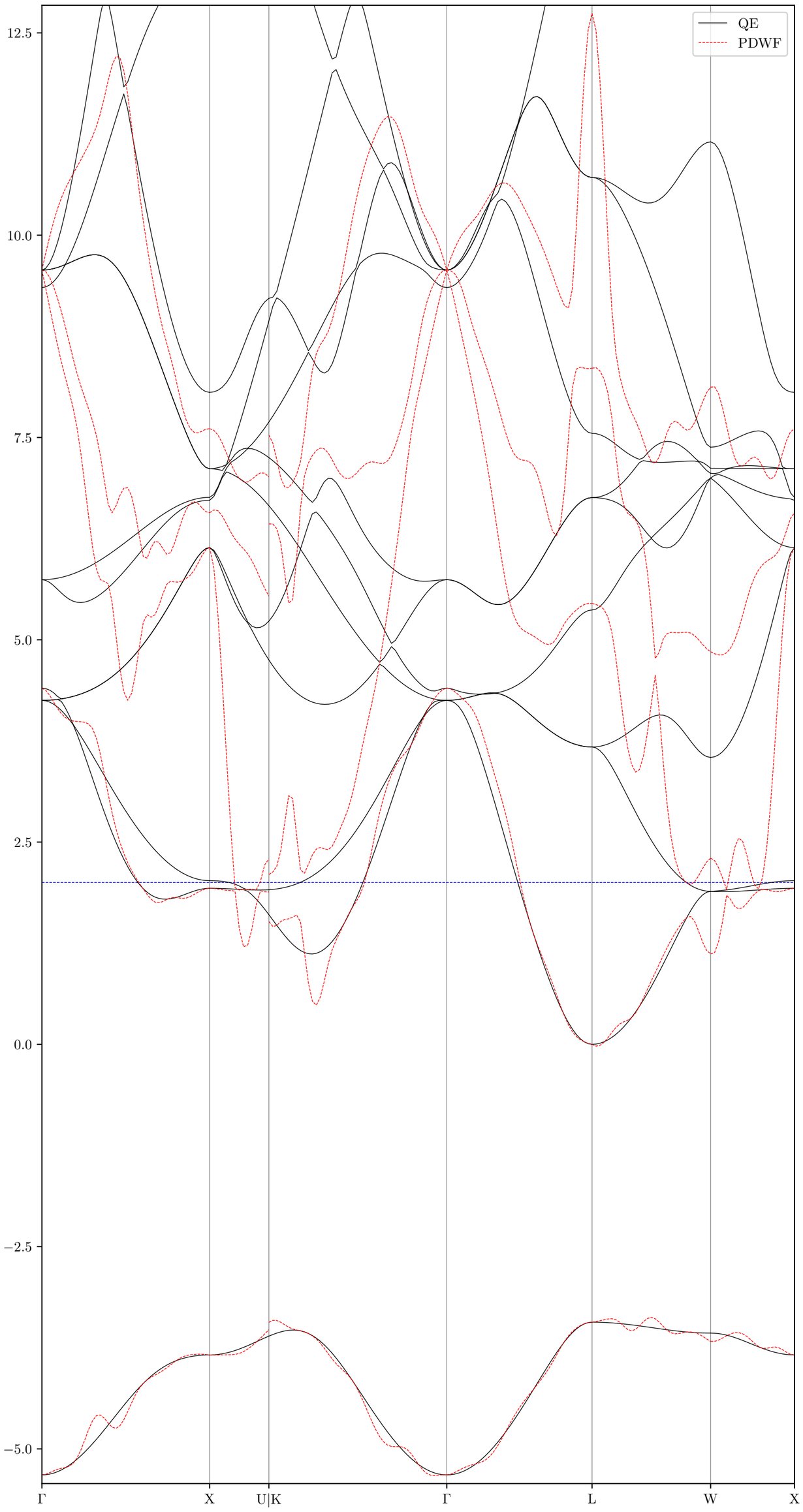

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.2 | 1.2 | 10.5 | 10.5 | 10.5 | 3.230 |

Hamiltonian decay



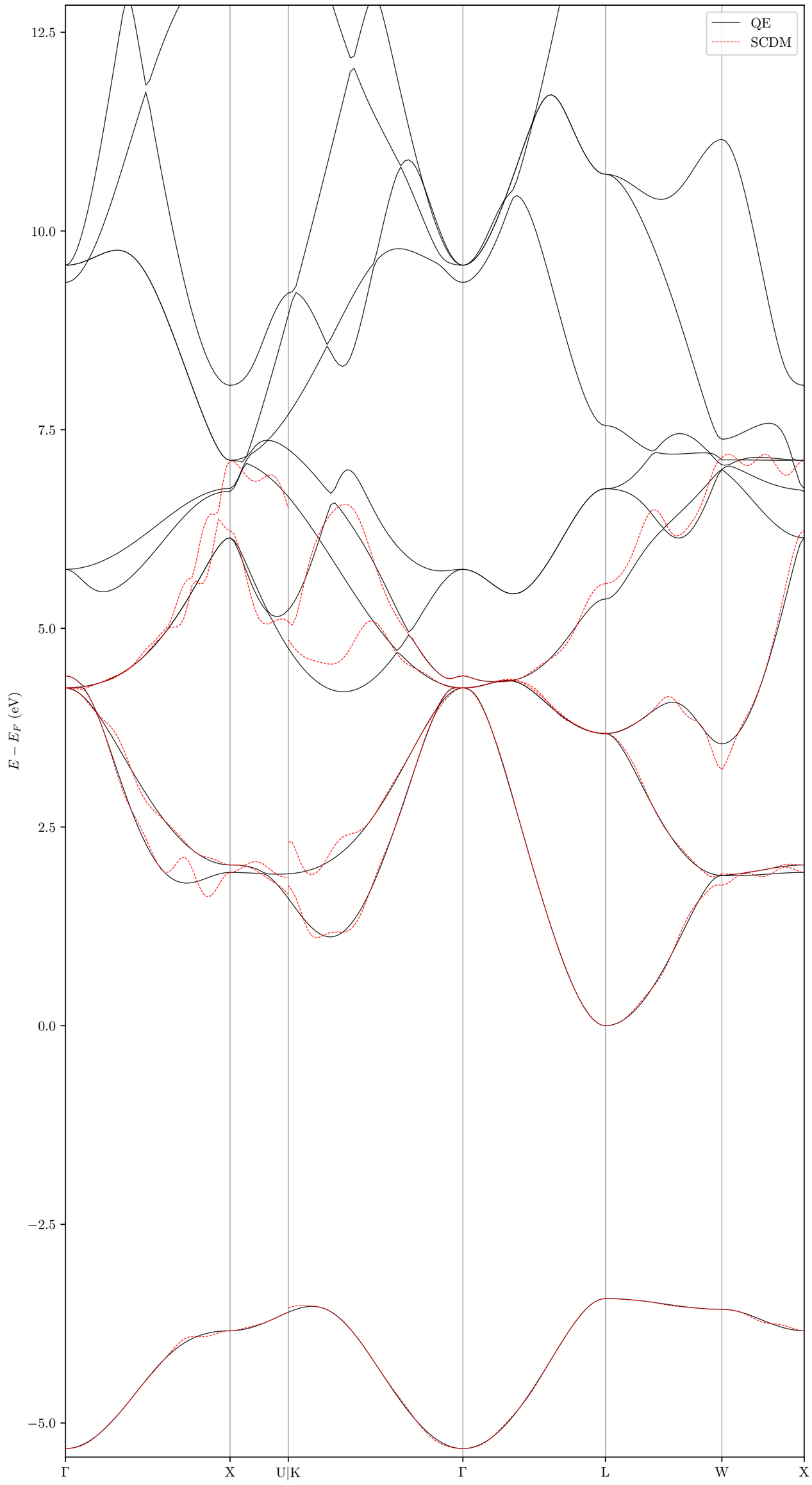
HK exclude semicore
PW=434eba76-3867-43f0-b94c-ad0a7c6e3a27
W90=0da14412-410e-474d-9f81-82e03efd2798




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 72.2 | 72.2 | 130.0 | 292.3 | 292.3 | 640.5 | 3.482 |

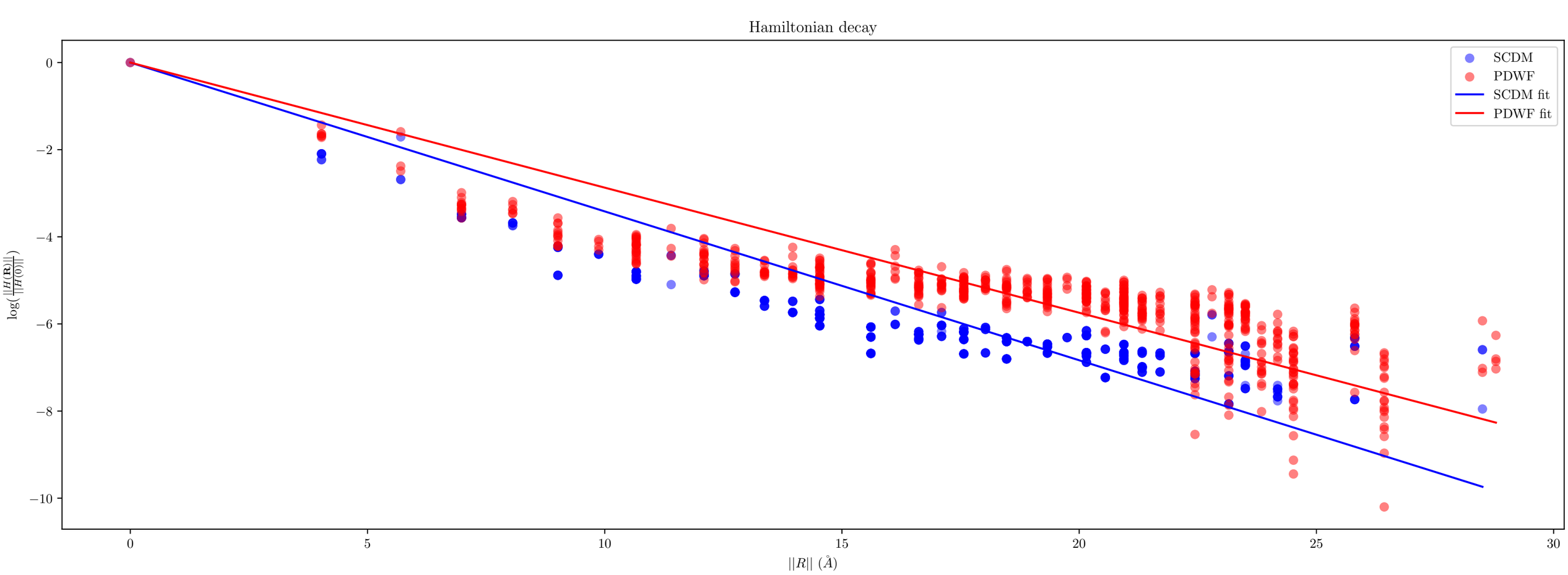
HK exclude semicore
PW=434eba76-3867-43f0-b94c-ad0a7c6e3a27
W90=d5081427-b385-4015-b63c-57cfcf833089

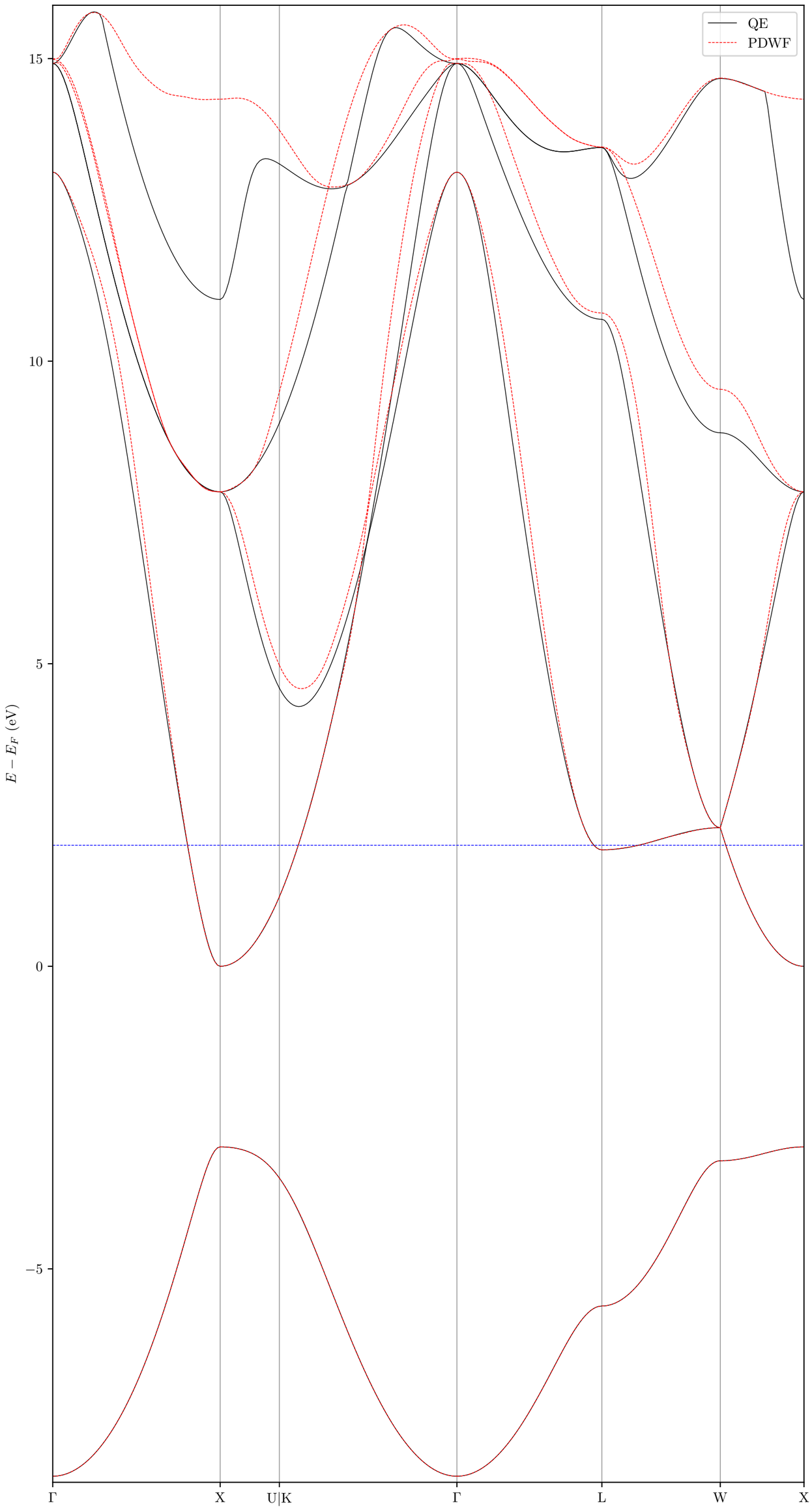



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 13.9 | 13.9 | 31.5 | 51.9 | 51.9 | 102.9 | 2.927 |

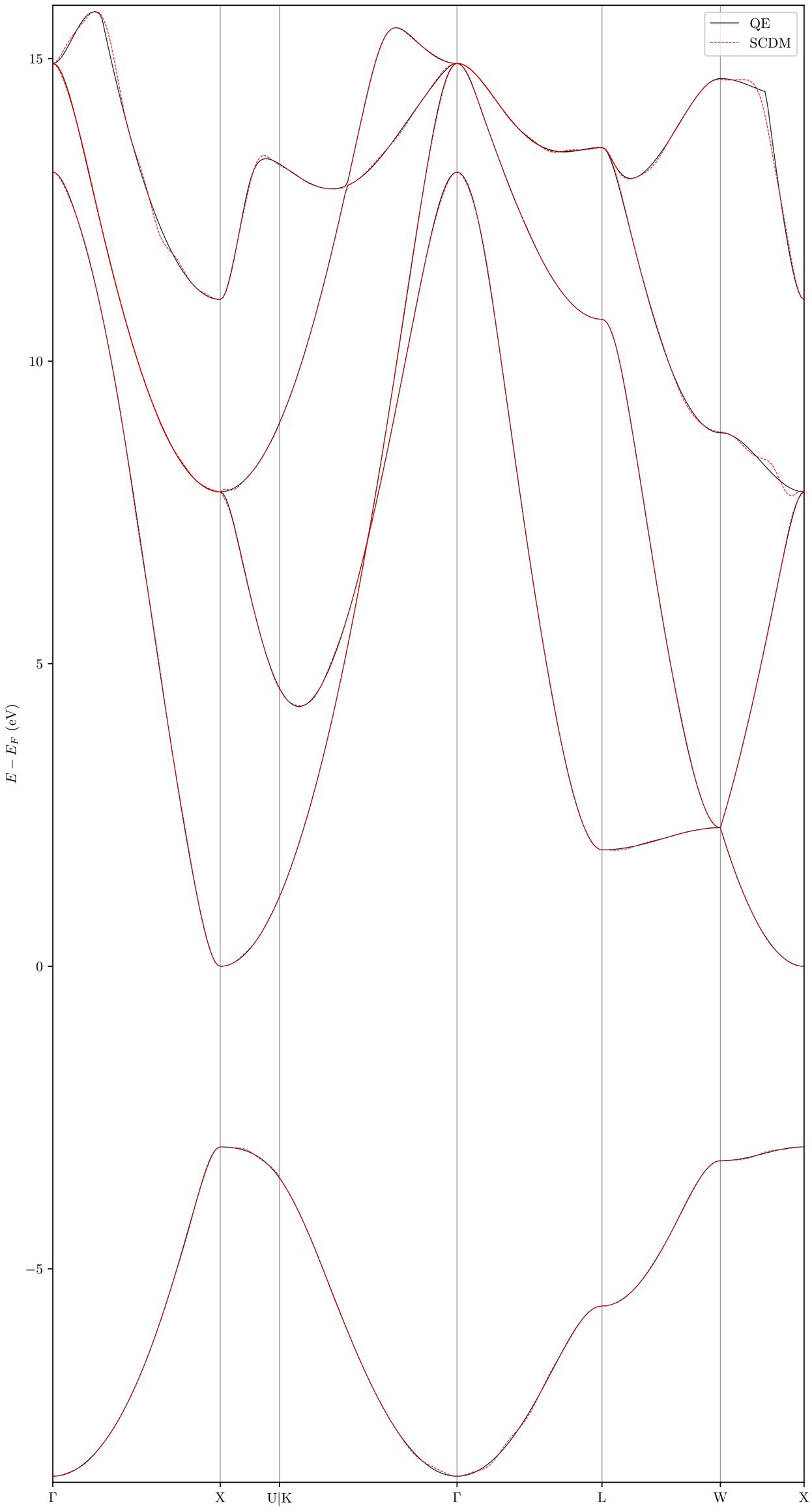
Hamiltonian decay





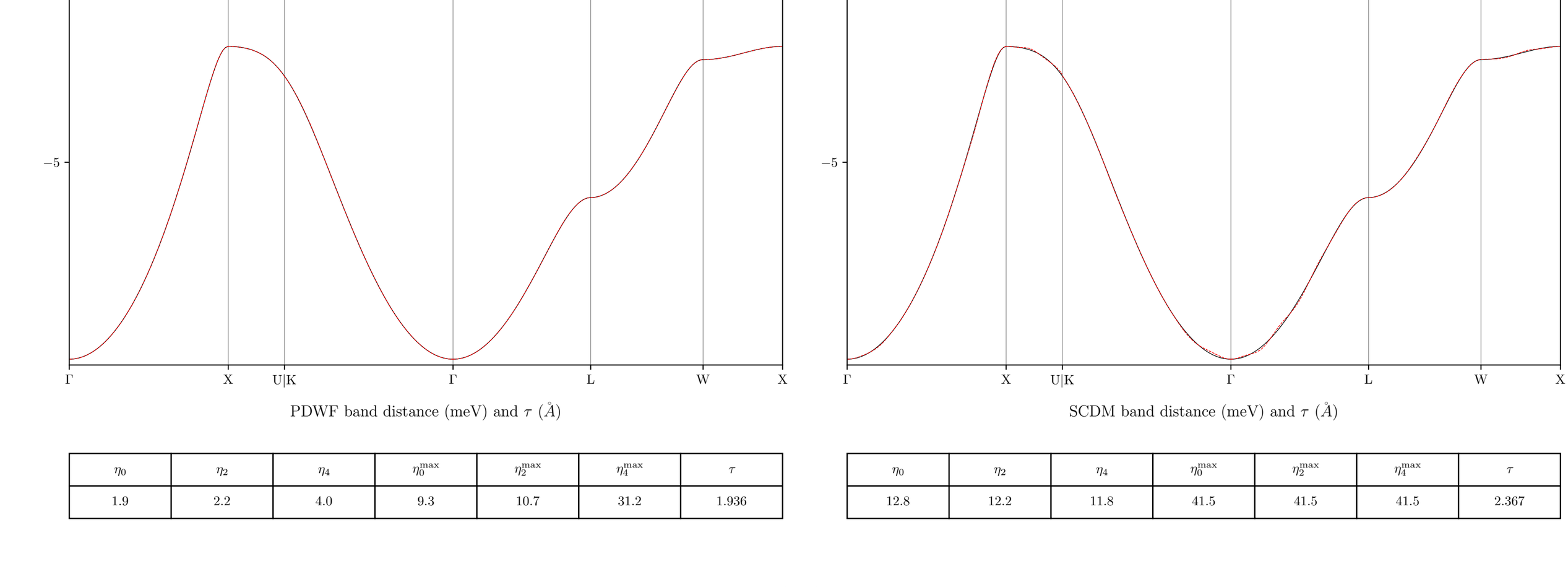

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.9 | 2.2 | 4.0 | 9.3 | 10.7 | 31.2 | 1.936 |

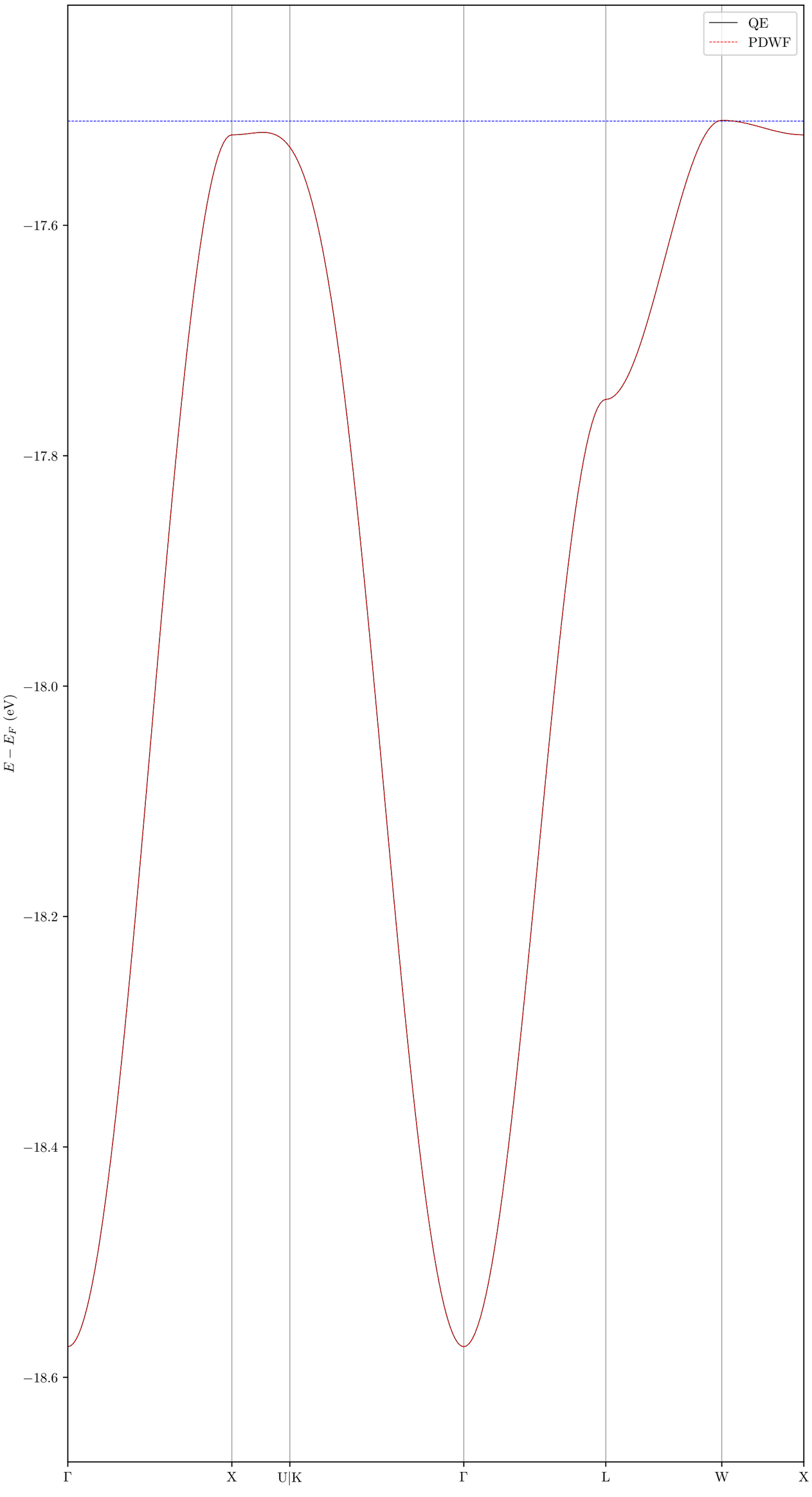



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 12.8 | 12.2 | 11.8 | 41.5 | 41.5 | 41.5 | 2.367 |



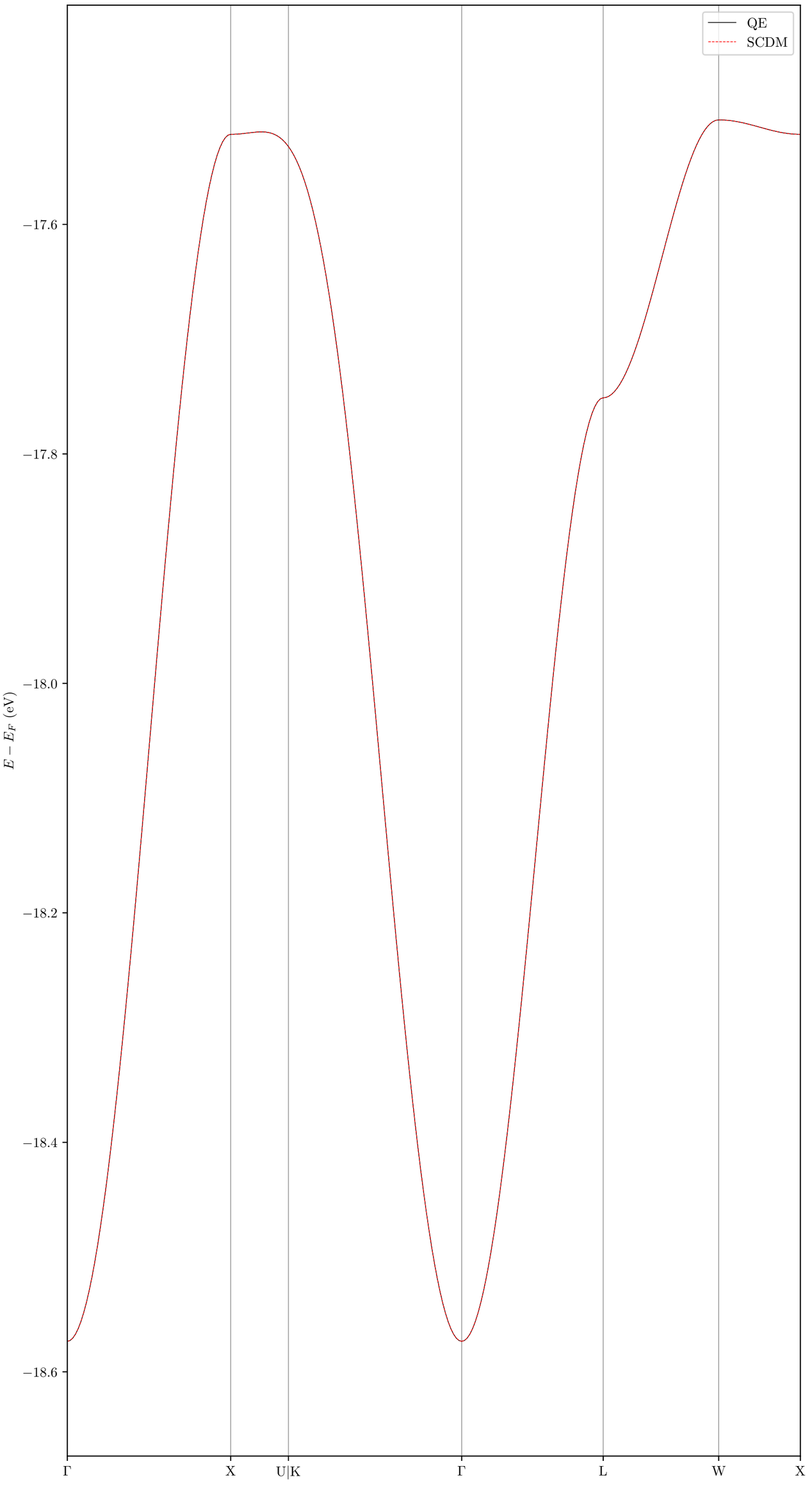
He exclude semicore
PW=c7ea0a4c-7444-408b-8ba4-3525033c5612
W90=0b3e1266-69f1-42aa-90f5-ae6c816c8c80




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.880 |

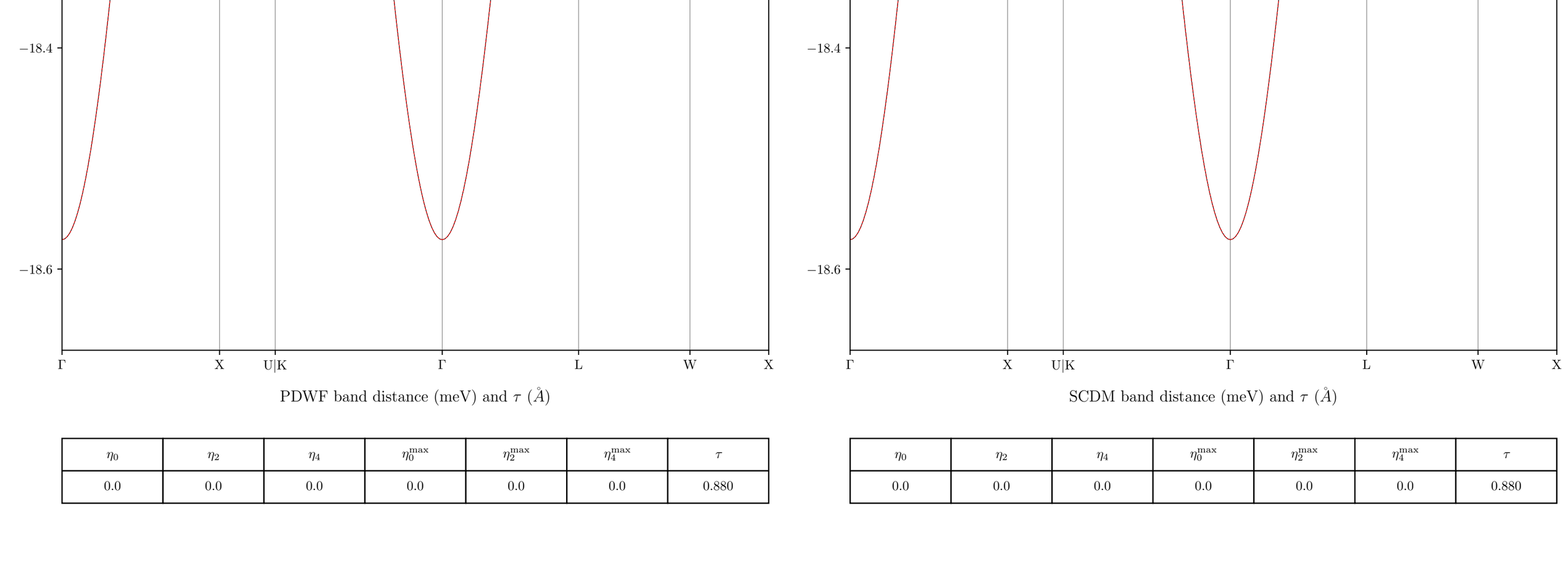
He exclude semicore
PW=c7ea0a4c-7444-408b-8ba4-3525033c5612
W90=b8e10025-ad8c-4dda-947a-7a13a0bf3a30



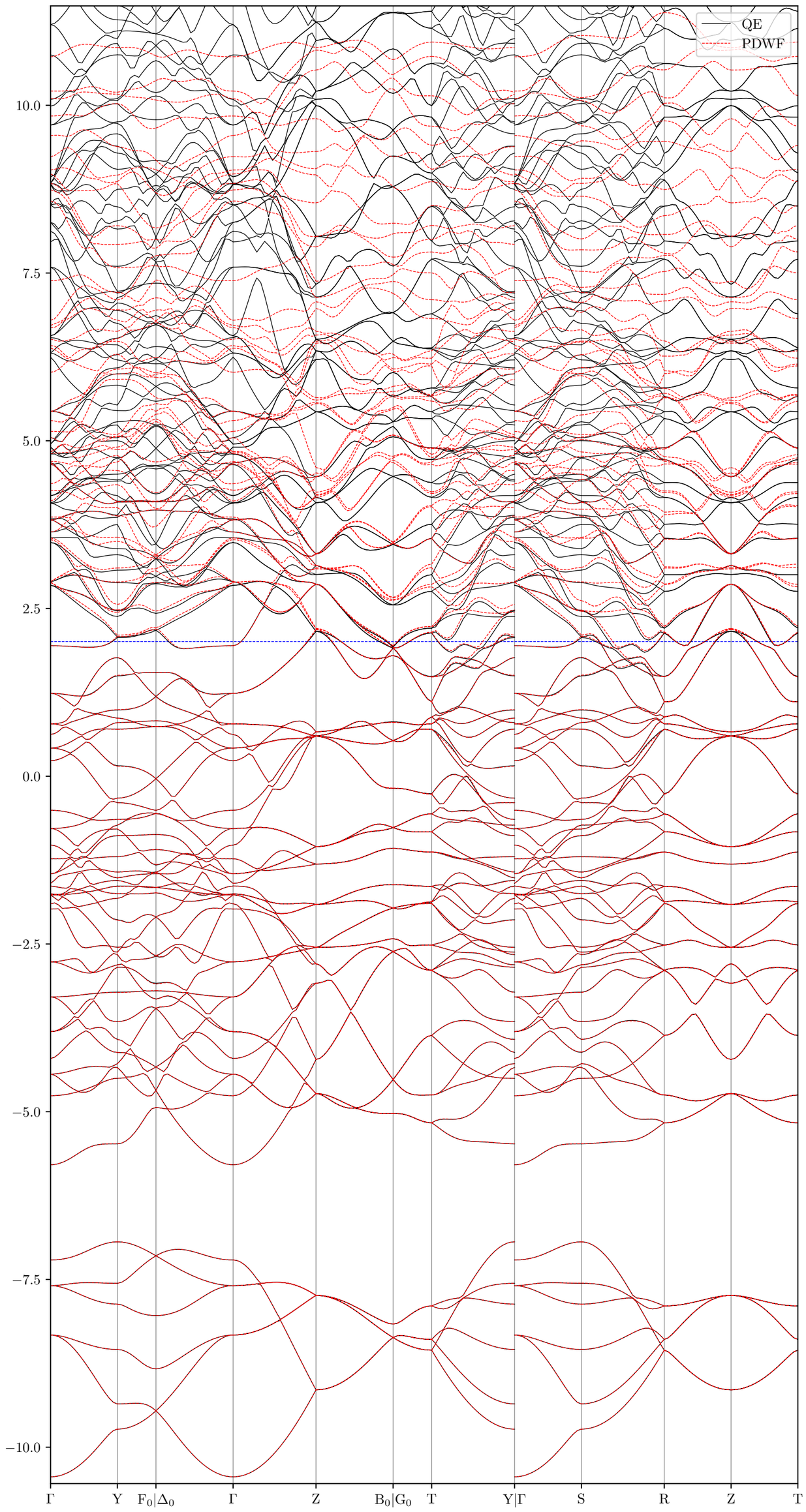

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.880 |

Hamiltonian decay



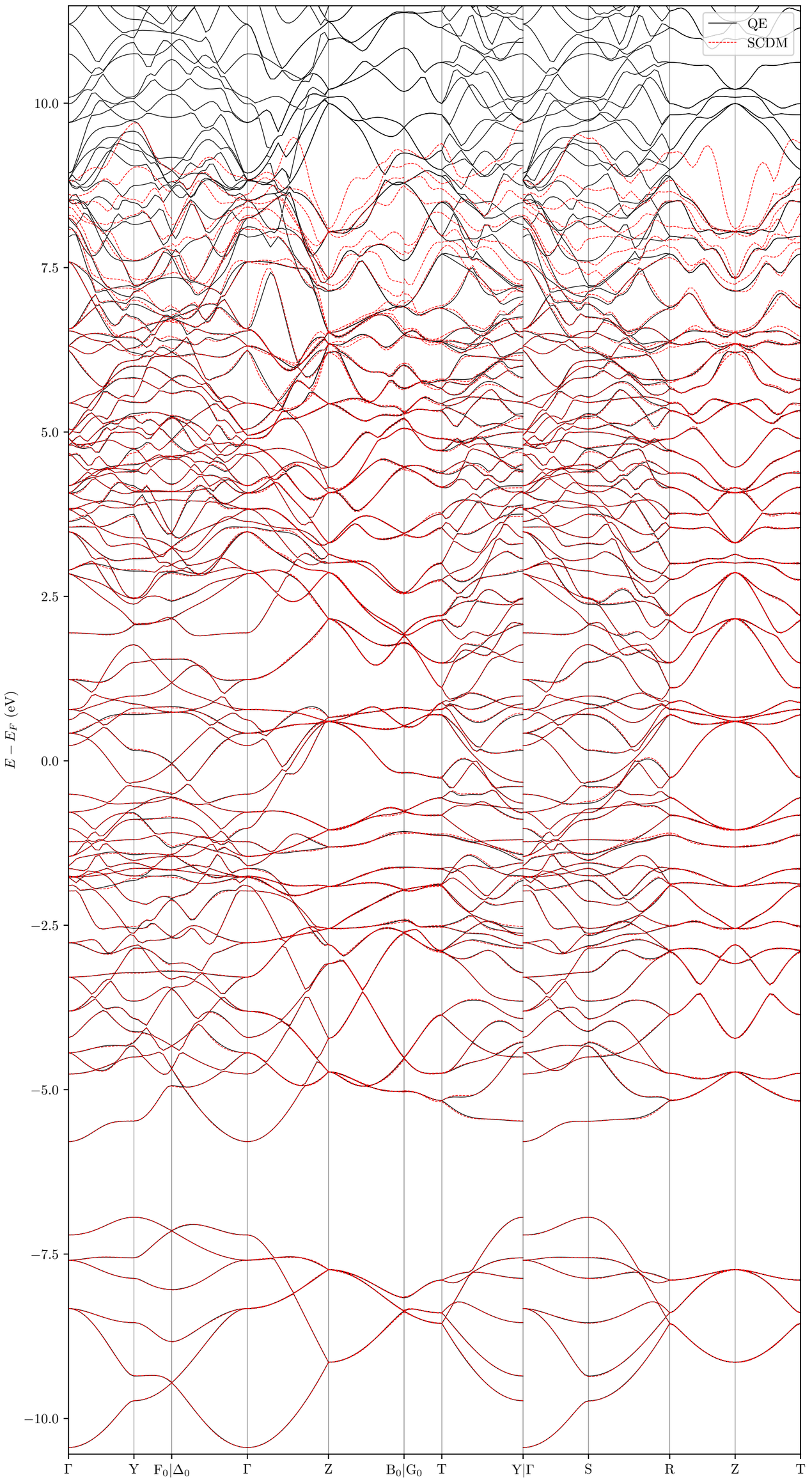
Hf10Si6 exclude semicore
PW=d5ec18e6-9241-45a4-b086-d2a19a2a0445
W90=b19d276e-0a34-4787-9592-570ddcbb3502




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.8 | 3.9 | 51.9 | 13.5 | 52.2 | 415.7 | 2.791 |

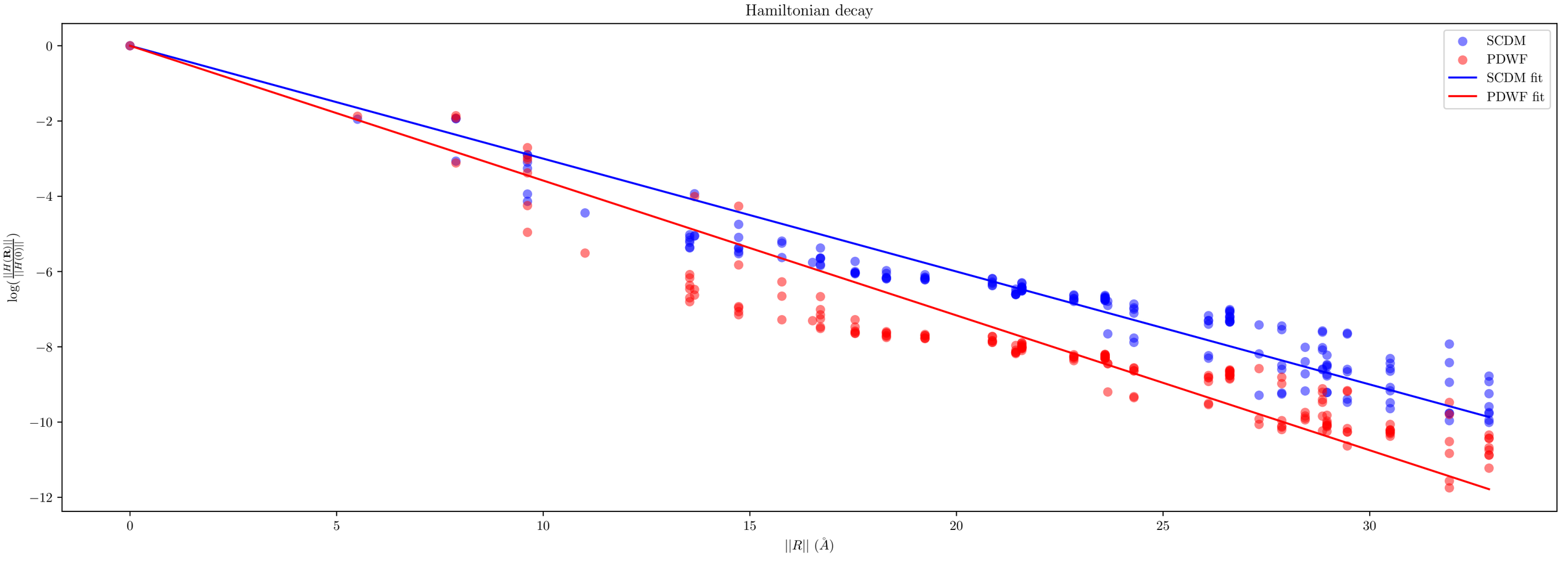
Hf10Si6 exclude semicore
PW=d5ec18e6-9241-45a4-b086-d2a19a2a0445
W90=47fc958b-9224-4fa0-80db-5eae77094183

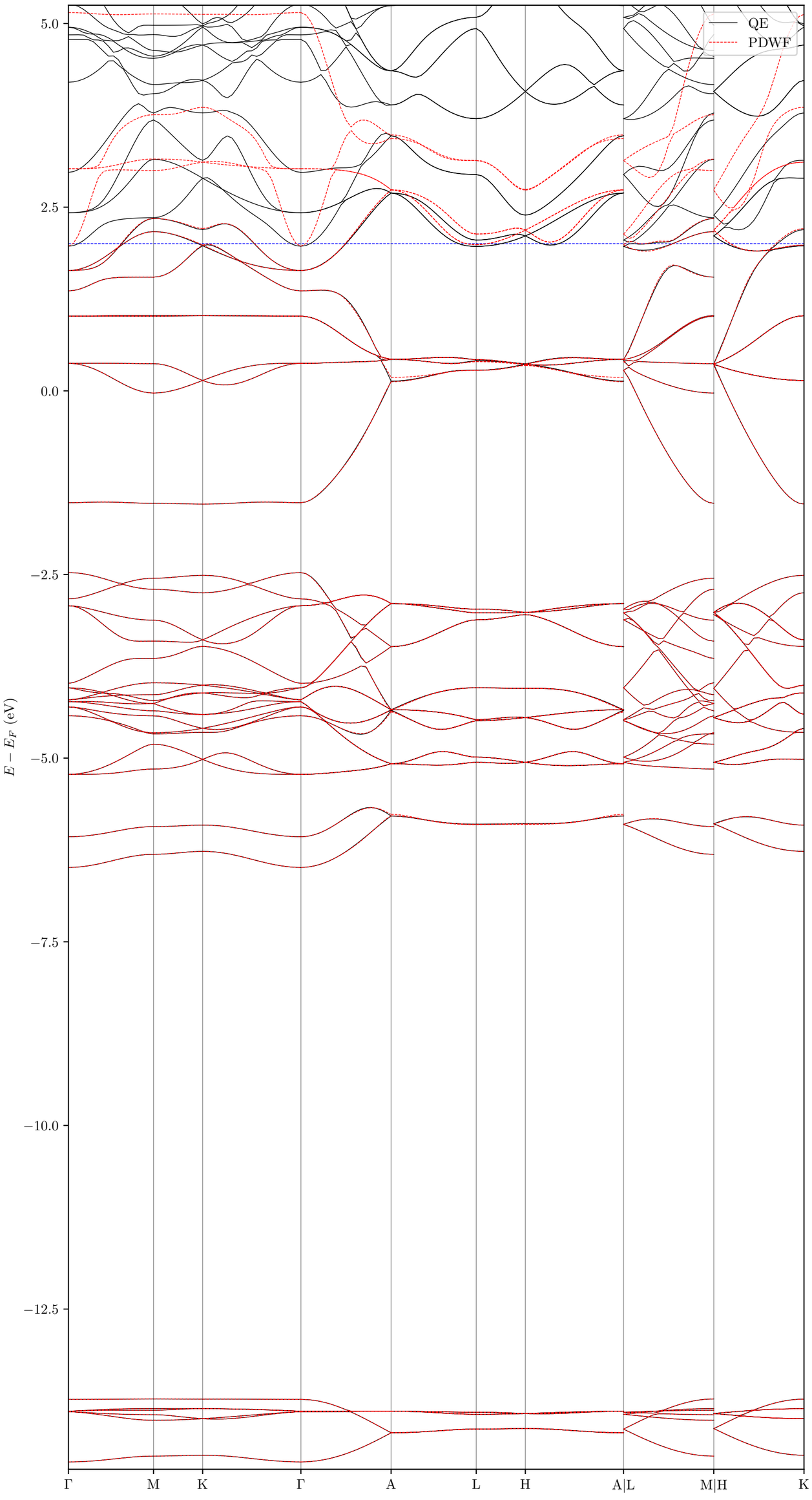



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.3 | 7.2 | 7.5 | 45.1 | 45.1 | 45.1 | 3.334 |

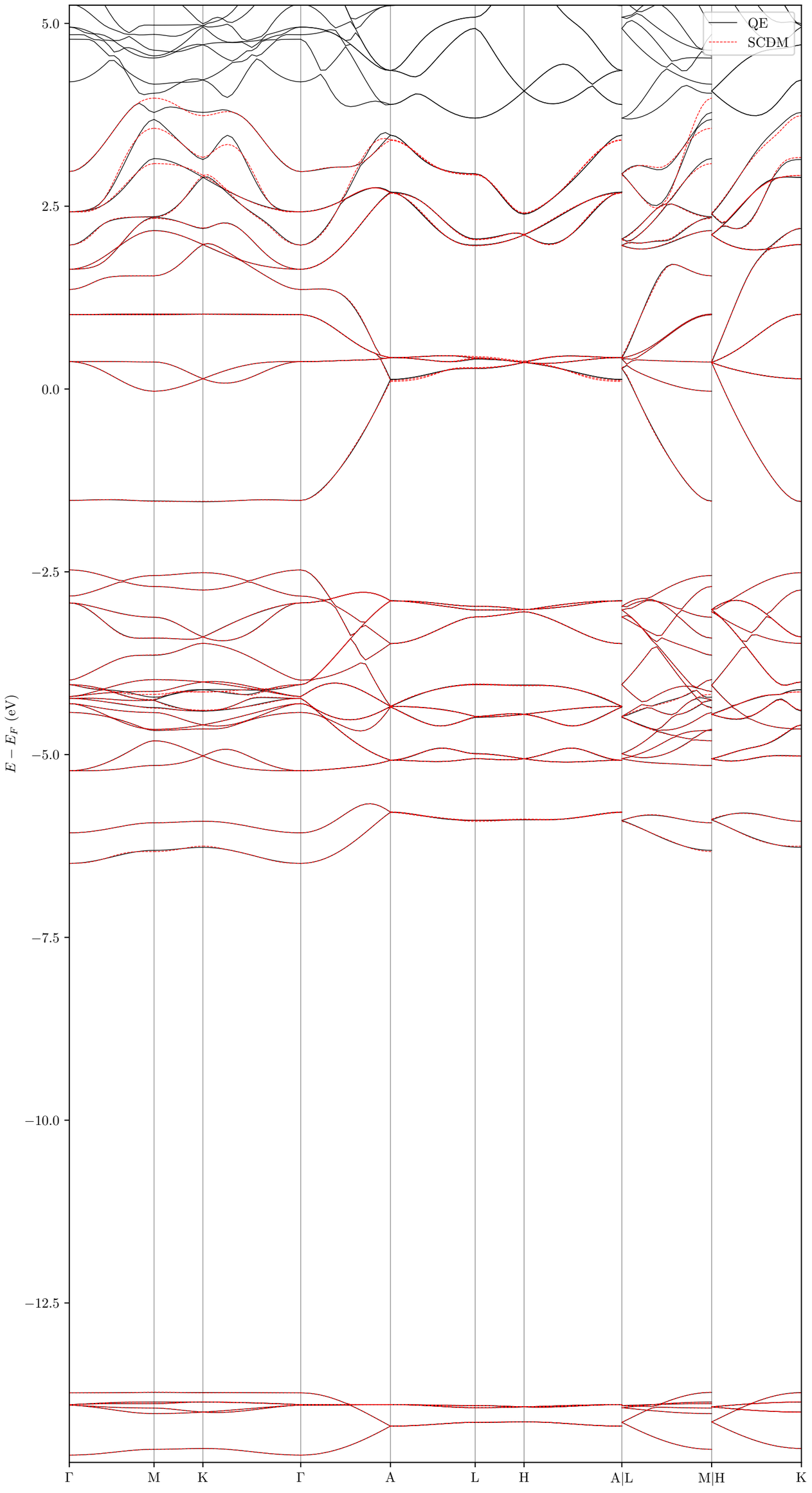
Hamiltonian decay





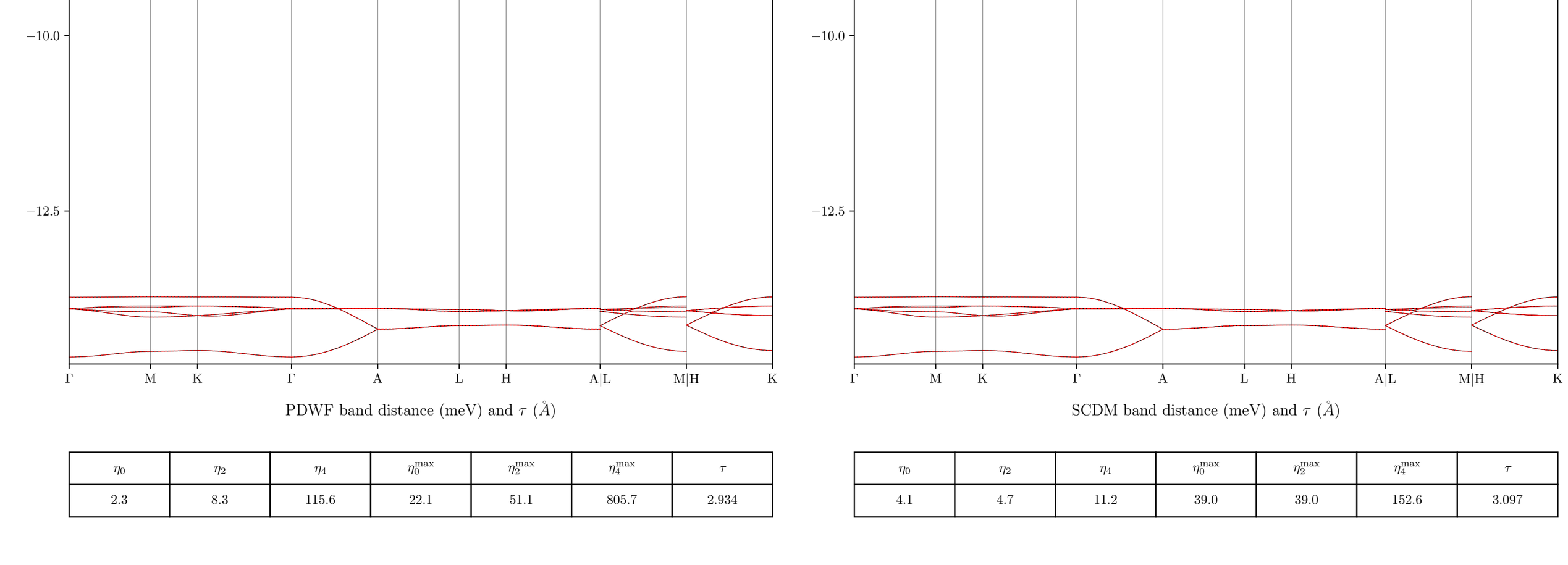

PDWF band distance (meV) and $\tau$ ($\AA$)

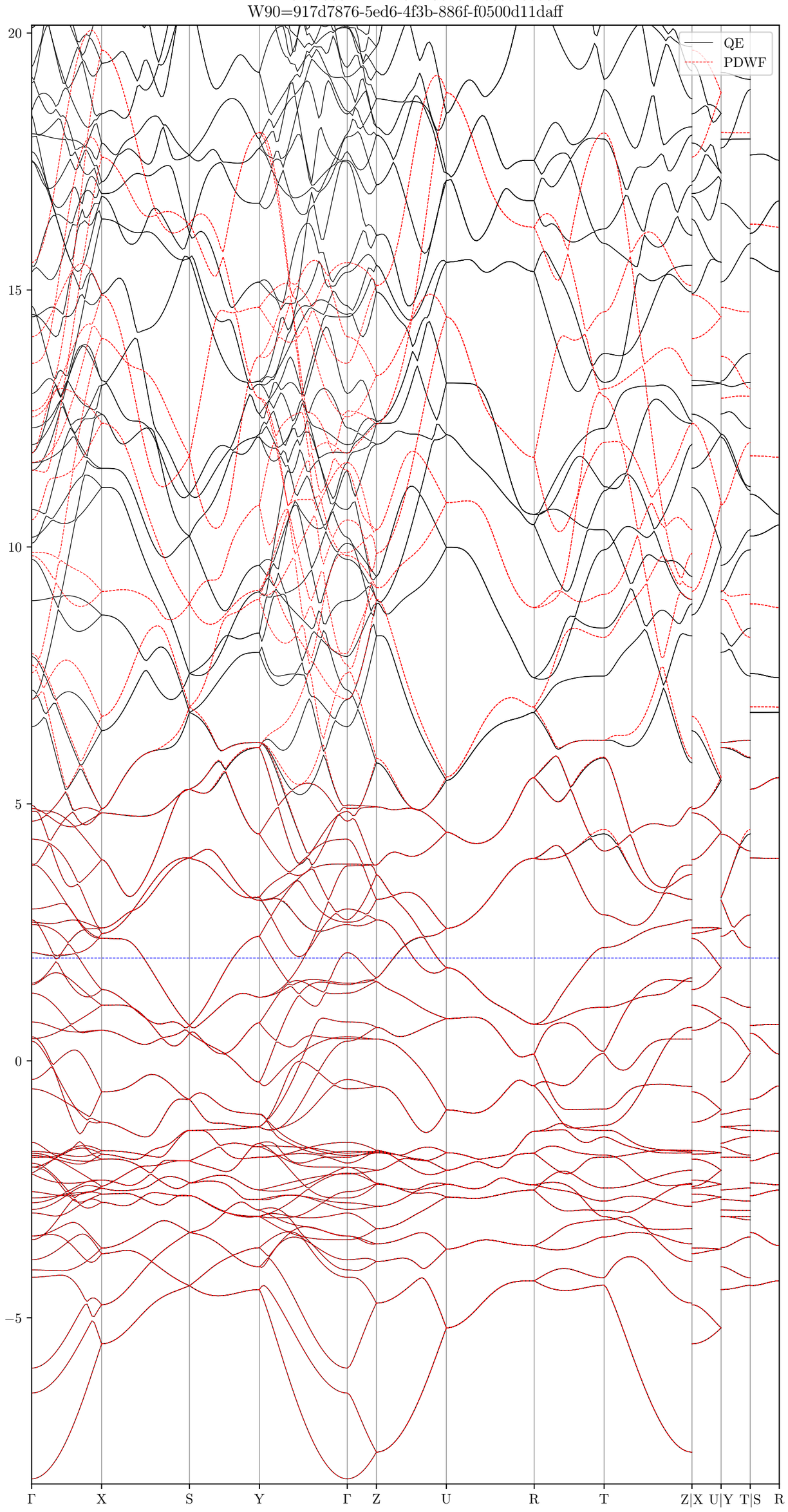
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.3 | 8.3 | 115.6 | 22.1 | 51.1 | 805.7 | 2.934 |




SCDM band distance (meV) and $\tau$ ($\AA$)

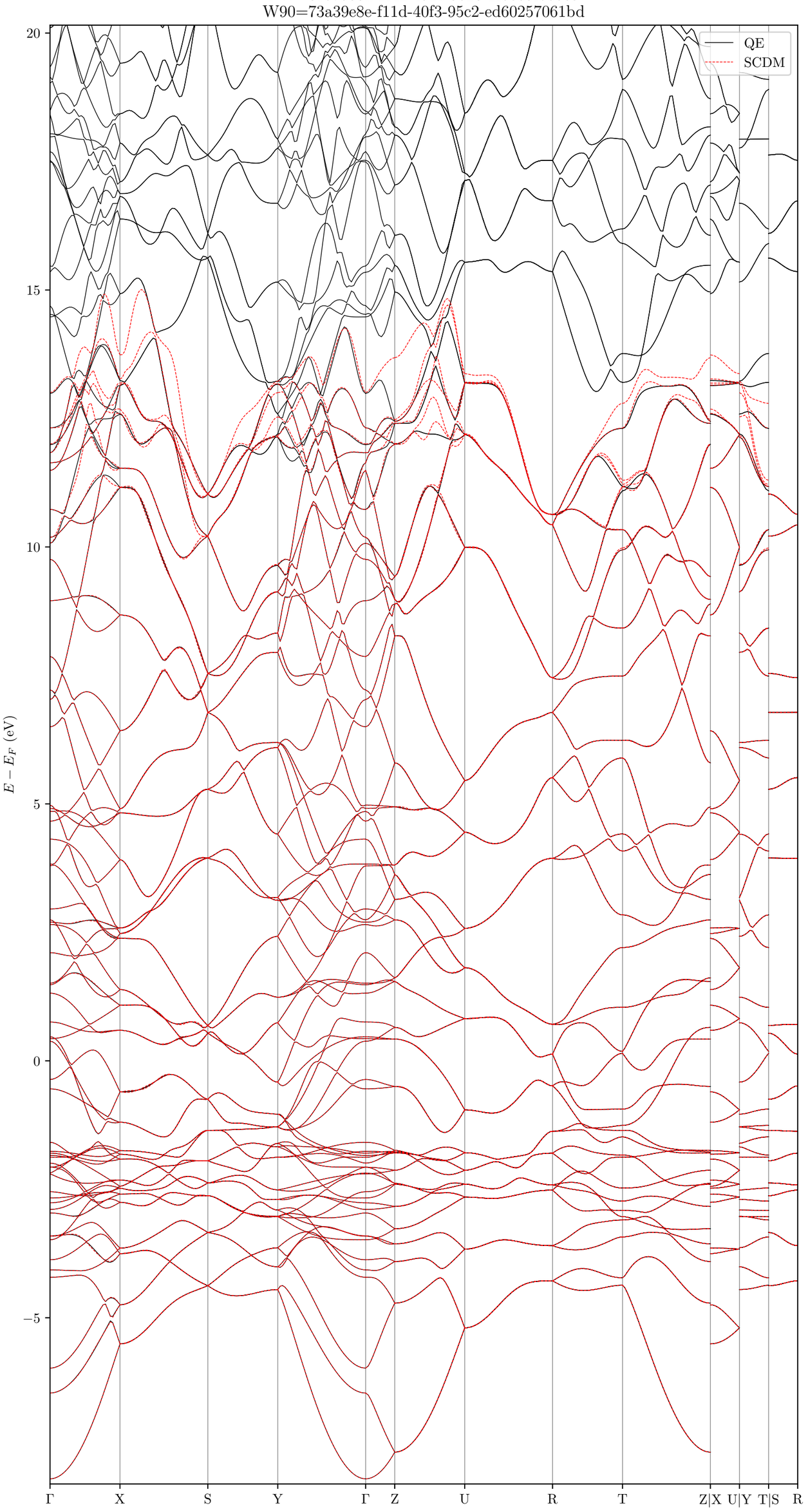
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.1 | 4.7 | 11.2 | 39.0 | 39.0 | 152.6 | 3.097 |





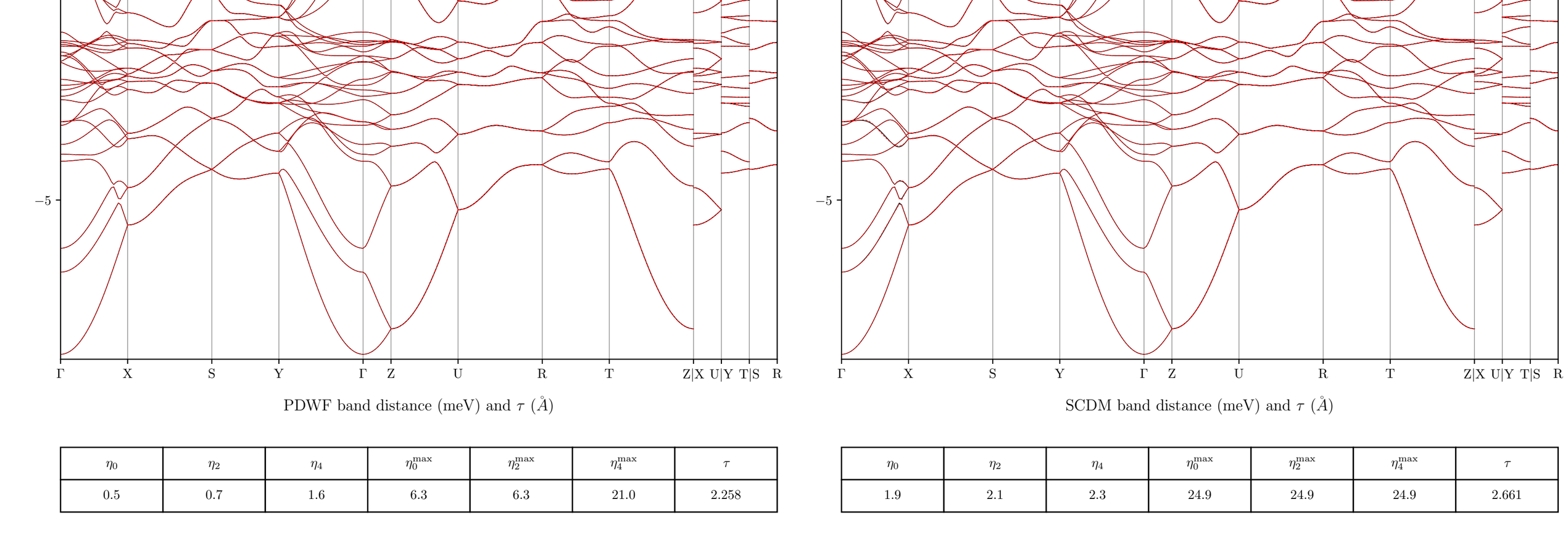

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

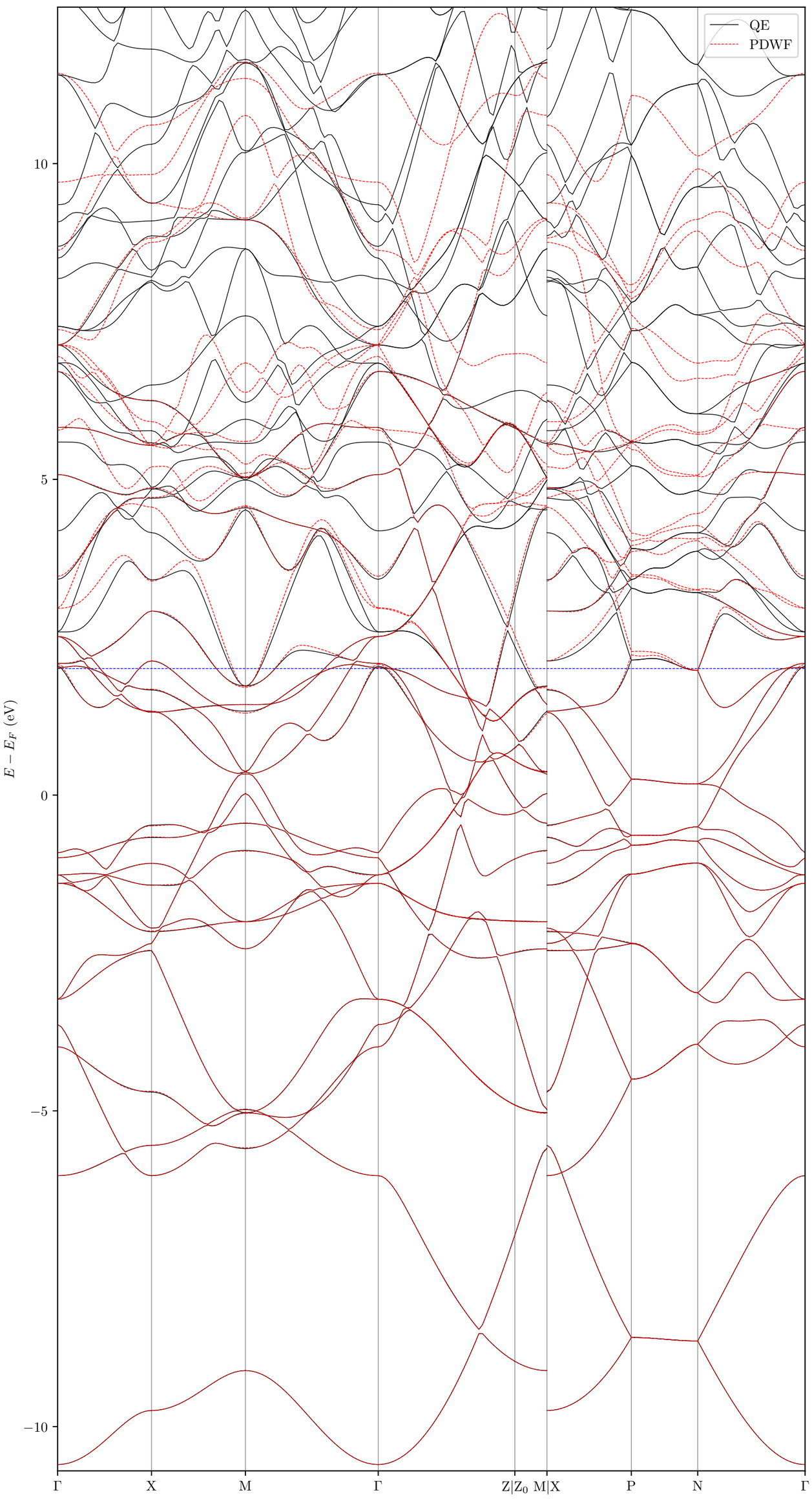
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.7 | 1.6 | 6.3 | 6.3 | 21.0 | 2.258 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

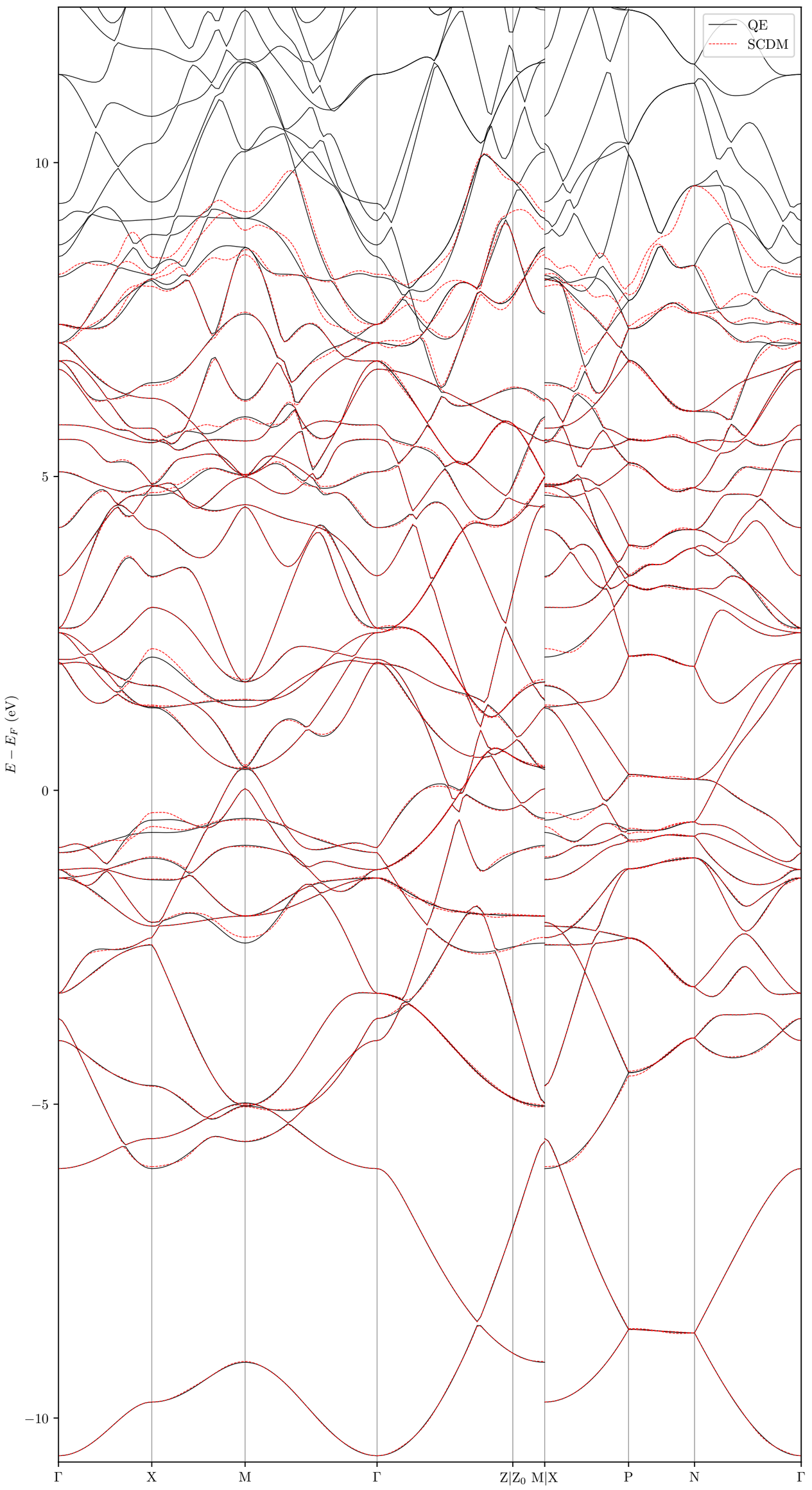
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.9 | 2.1 | 2.3 | 24.9 | 24.9 | 24.9 | 2.661 |





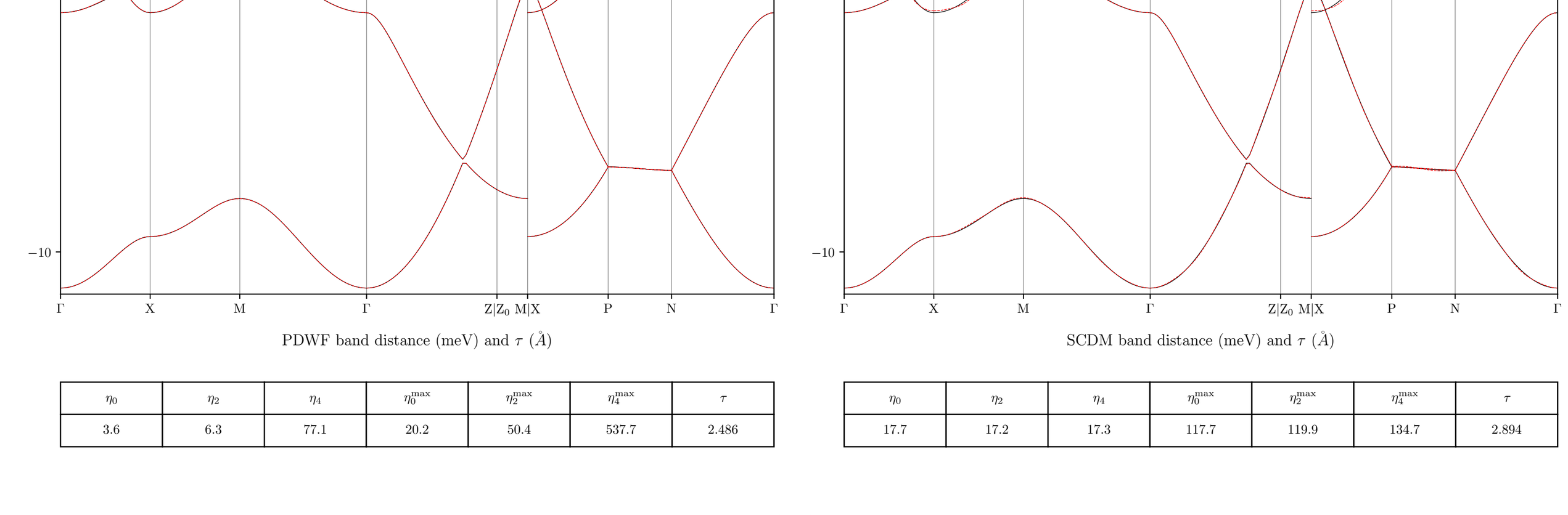

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.6 | 6.3 | 77.1 | 20.2 | 50.4 | 537.7 | 2.486 |

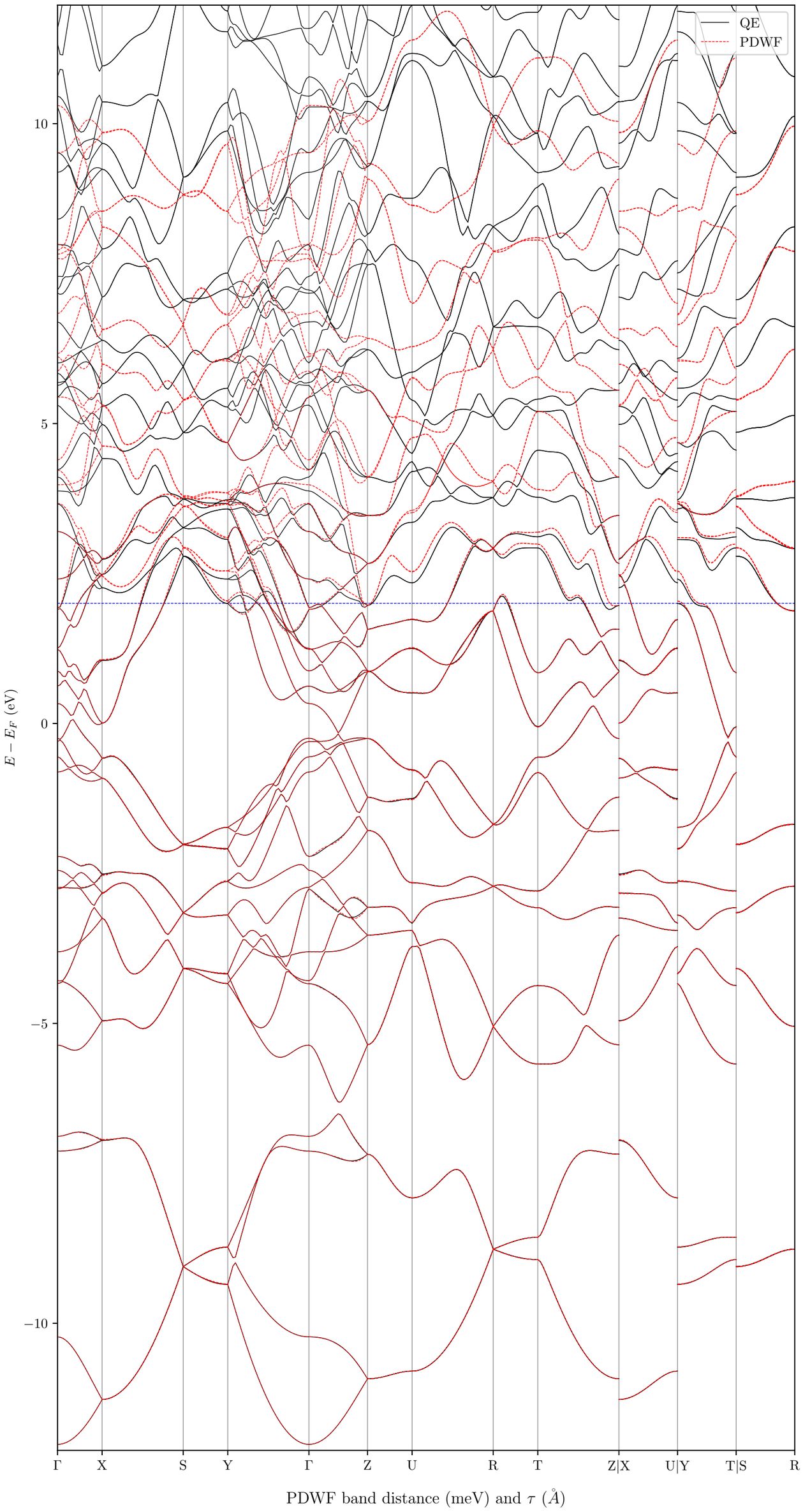



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 17.7 | 17.2 | 17.3 | 117.7 | 119.9 | 134.7 | 2.894 |



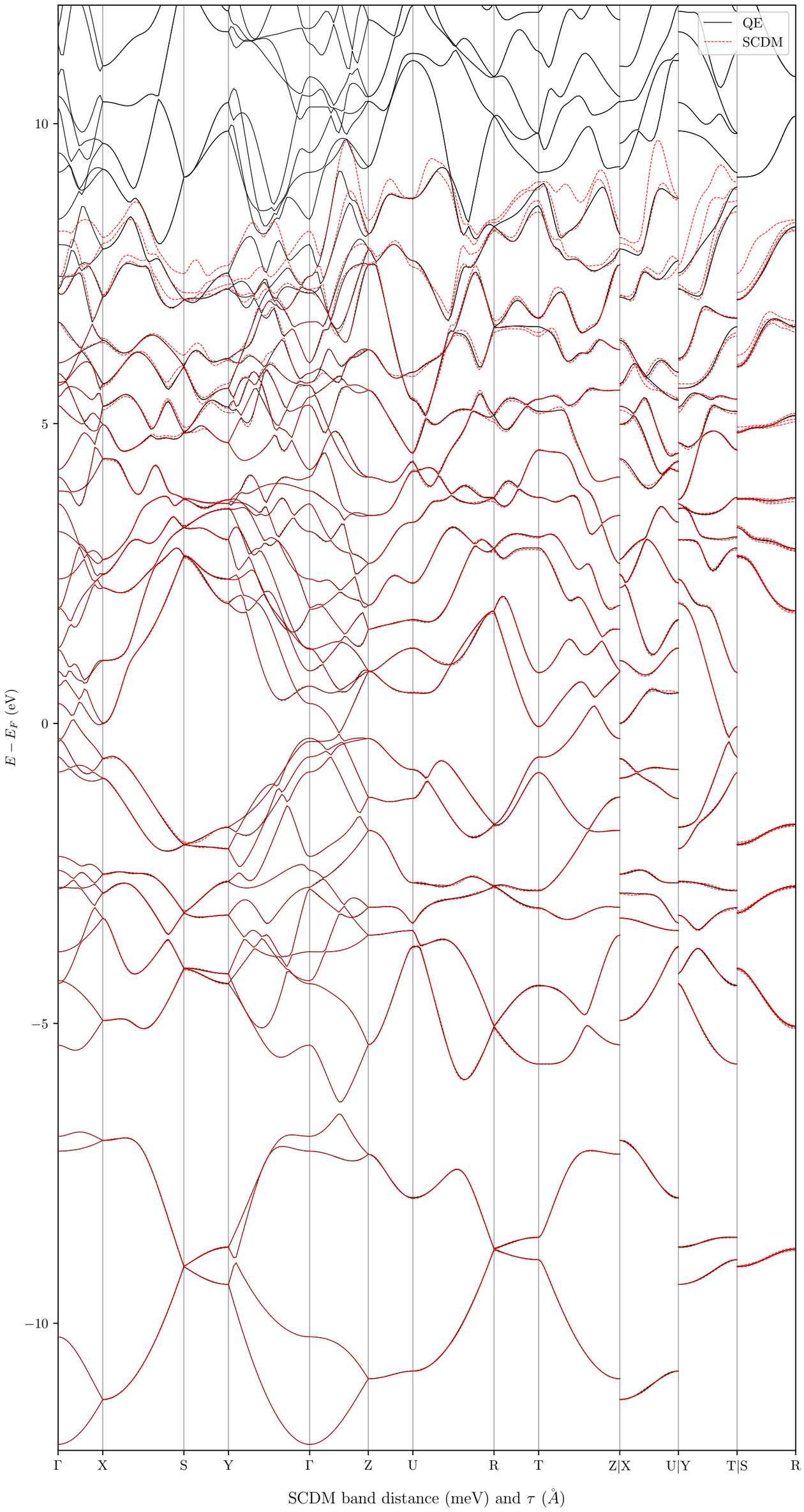
Hf4Si4 exclude semicore
PW=8e16896b-ae76-474c-8b3f-cd6019b59fc2
W90=a51b785e-8966-4013-a677-1f0e51170cb6




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.2 | 8.4 | 76.6 | 29.1 | 75.1 | 514.6 | 2.521 |

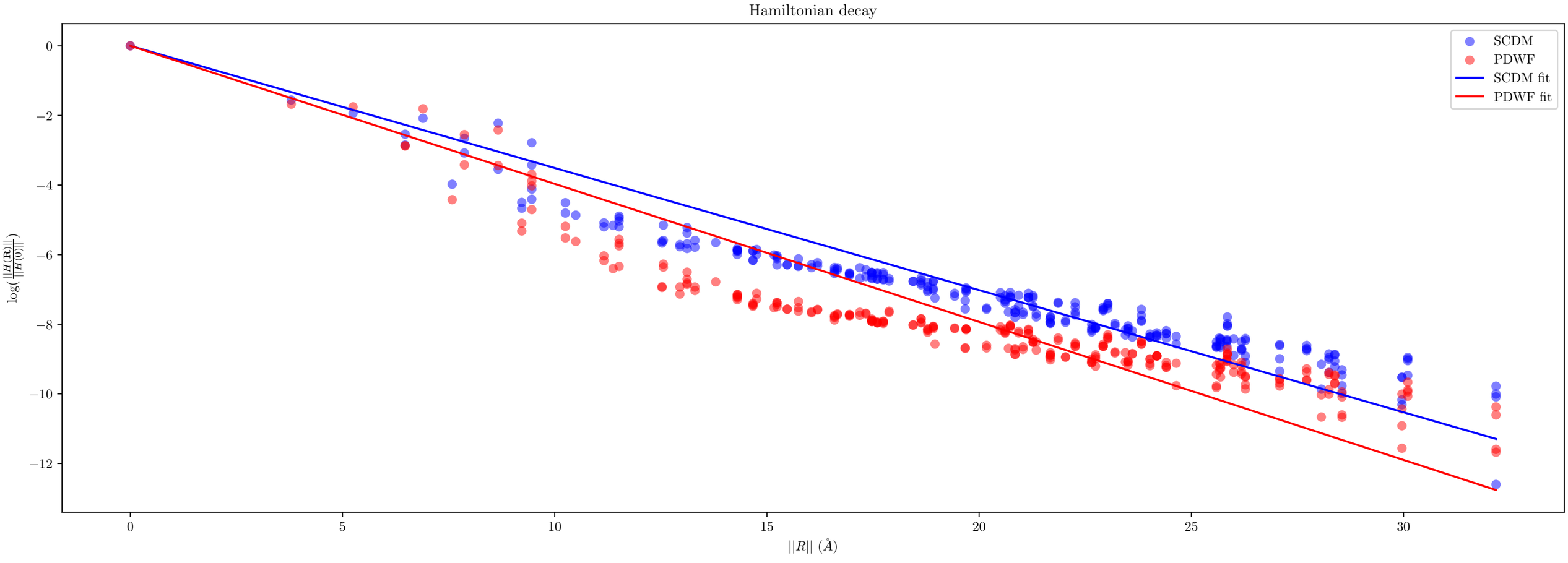
Hf4Si4 exclude semicore
PW=8e16896b-ae76-474c-8b3f-cd6019b59fc2
W90=1541541e-f995-4ac9-b448-039de0768315



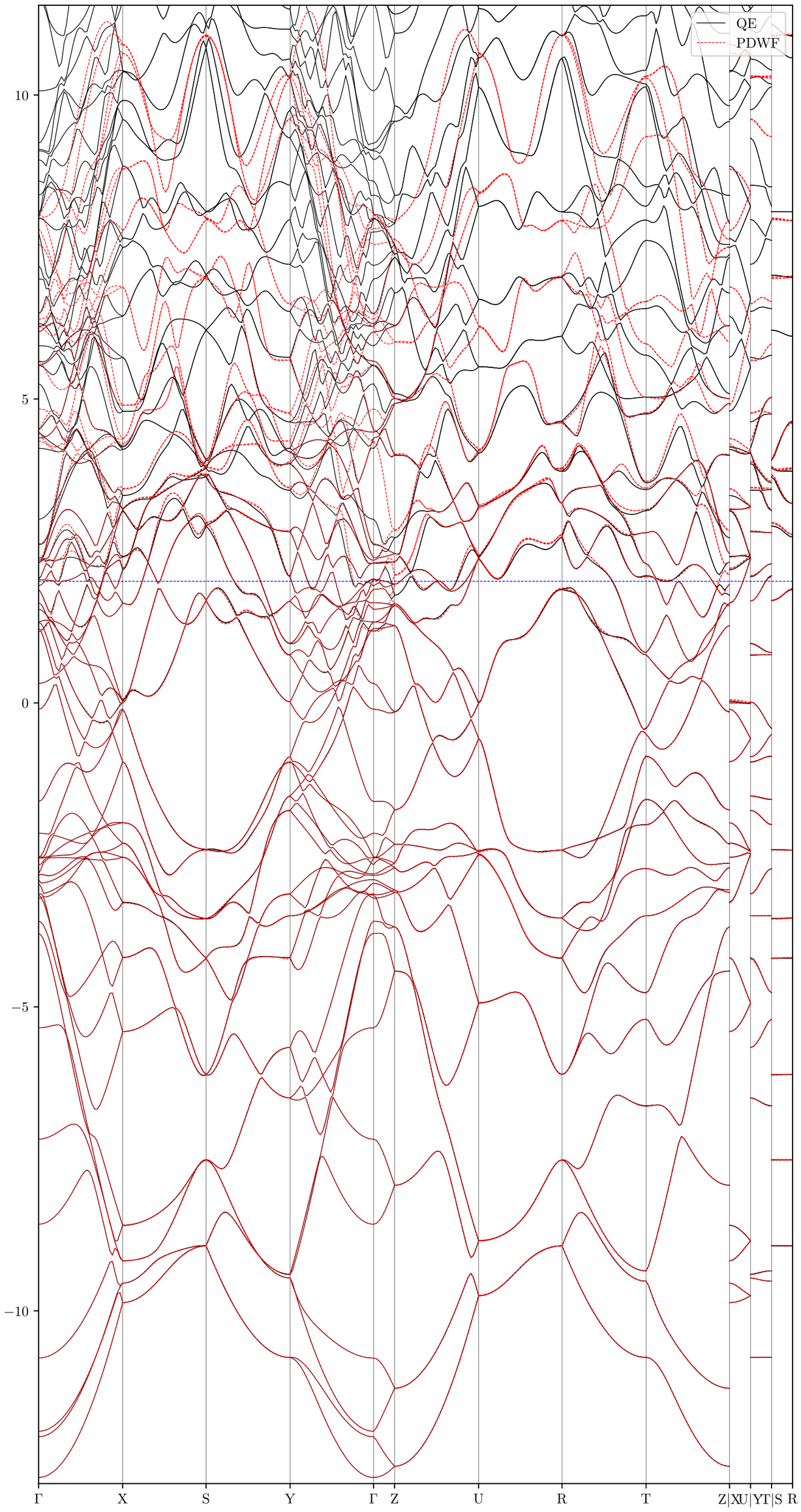

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.5 | 8.8 | 10.0 | 43.2 | 43.2 | 62.2 | 2.849 |

Hamiltonian decay



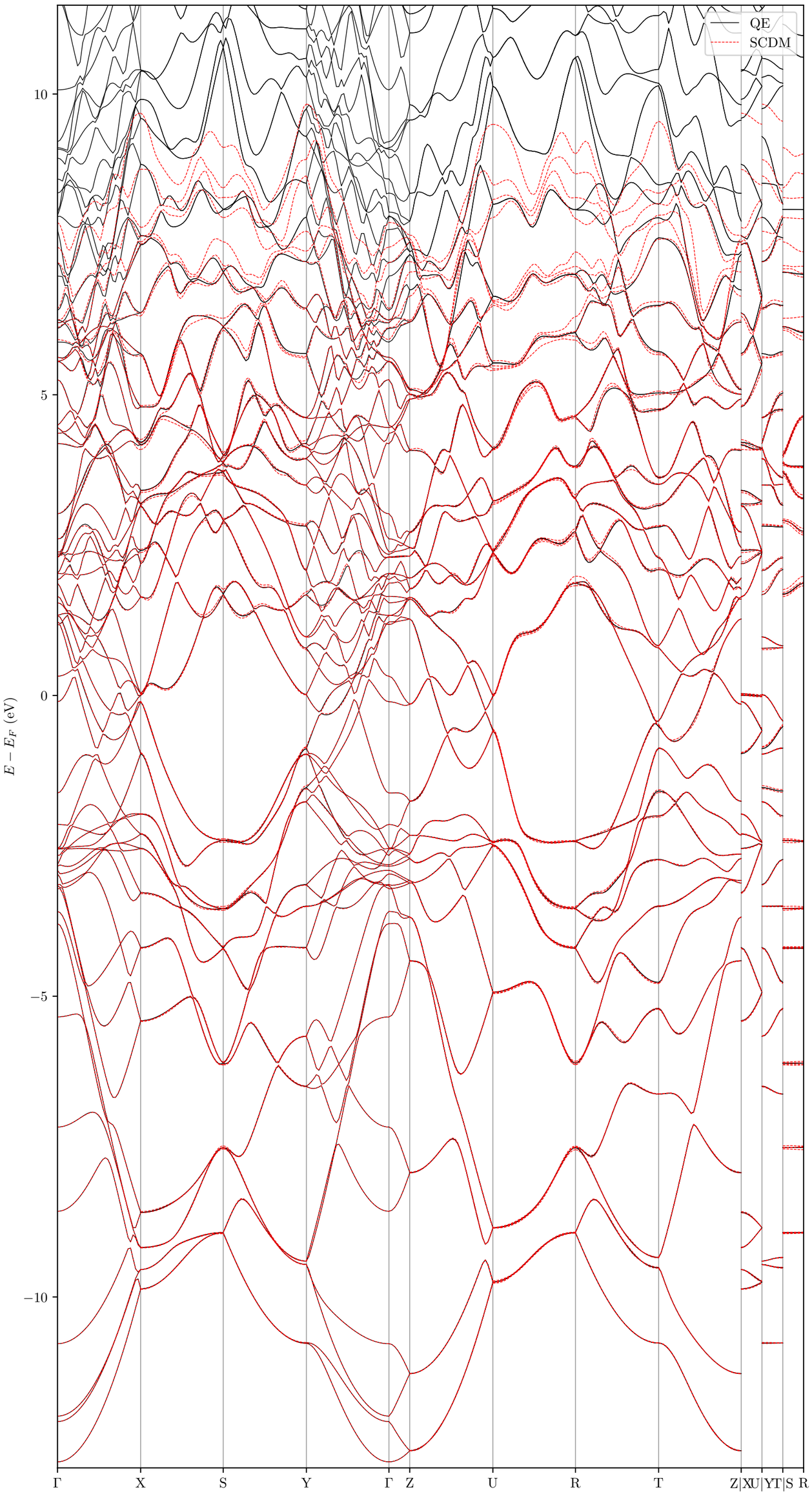
Hf4Si8 exclude semicore
PW=7c563ad4-6e17-4eed-ac8d-c829a000ea10
W90=753ce7b2-3ad8-4baf-8897-eac700d98c57




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.6 | 10.4 | 47.3 | 23.3 | 136.8 | 1095.8 | 3.200 |

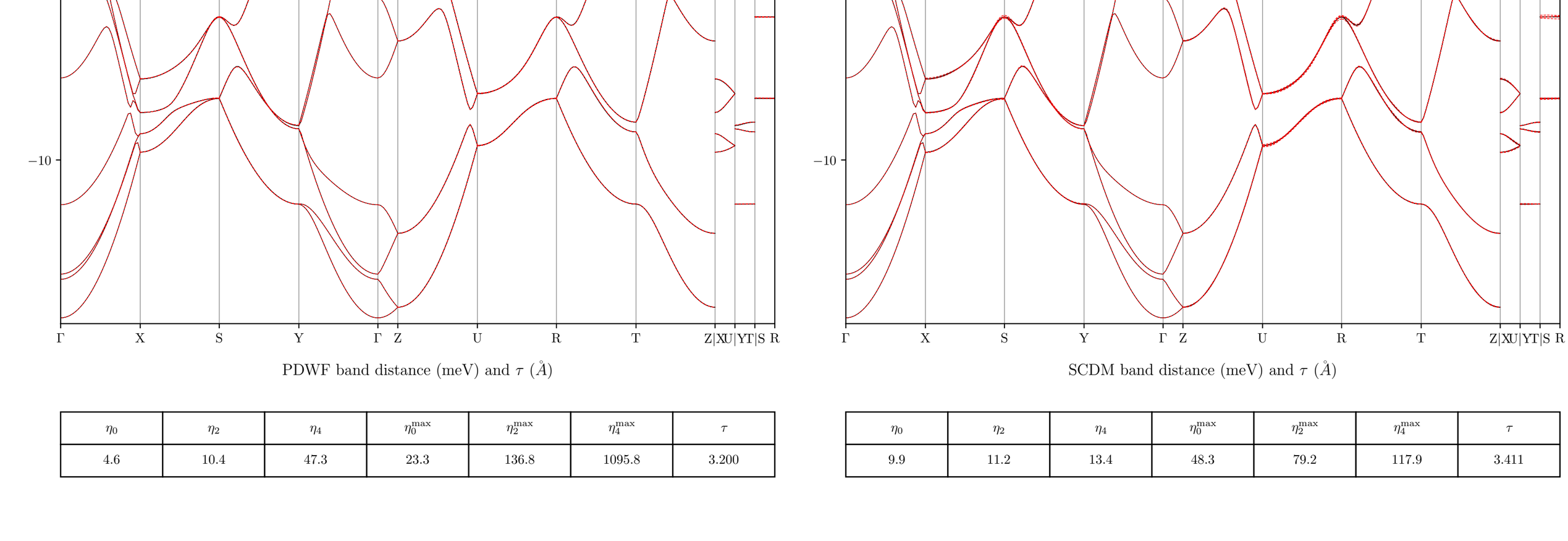
Hf4Si8 exclude semicore
PW=7c563ad4-6e17-4eed-ac8d-c829a000ea10
W90=cd6a6f5b-0125-43f9-a241-2896117b22b9



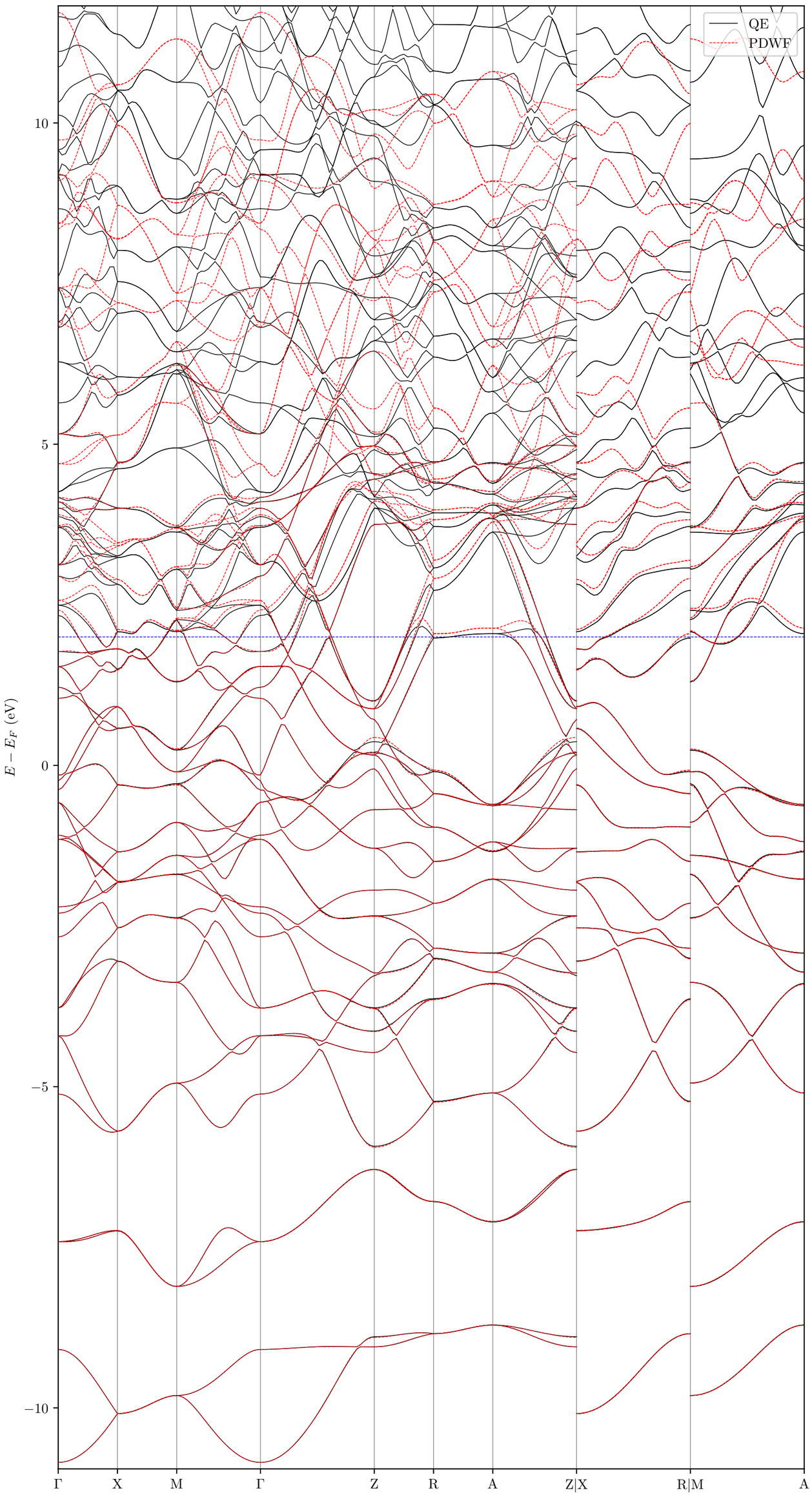

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 9.9 | 11.2 | 13.4 | 48.3 | 79.2 | 117.9 | 3.411 |

Hamiltonian decay



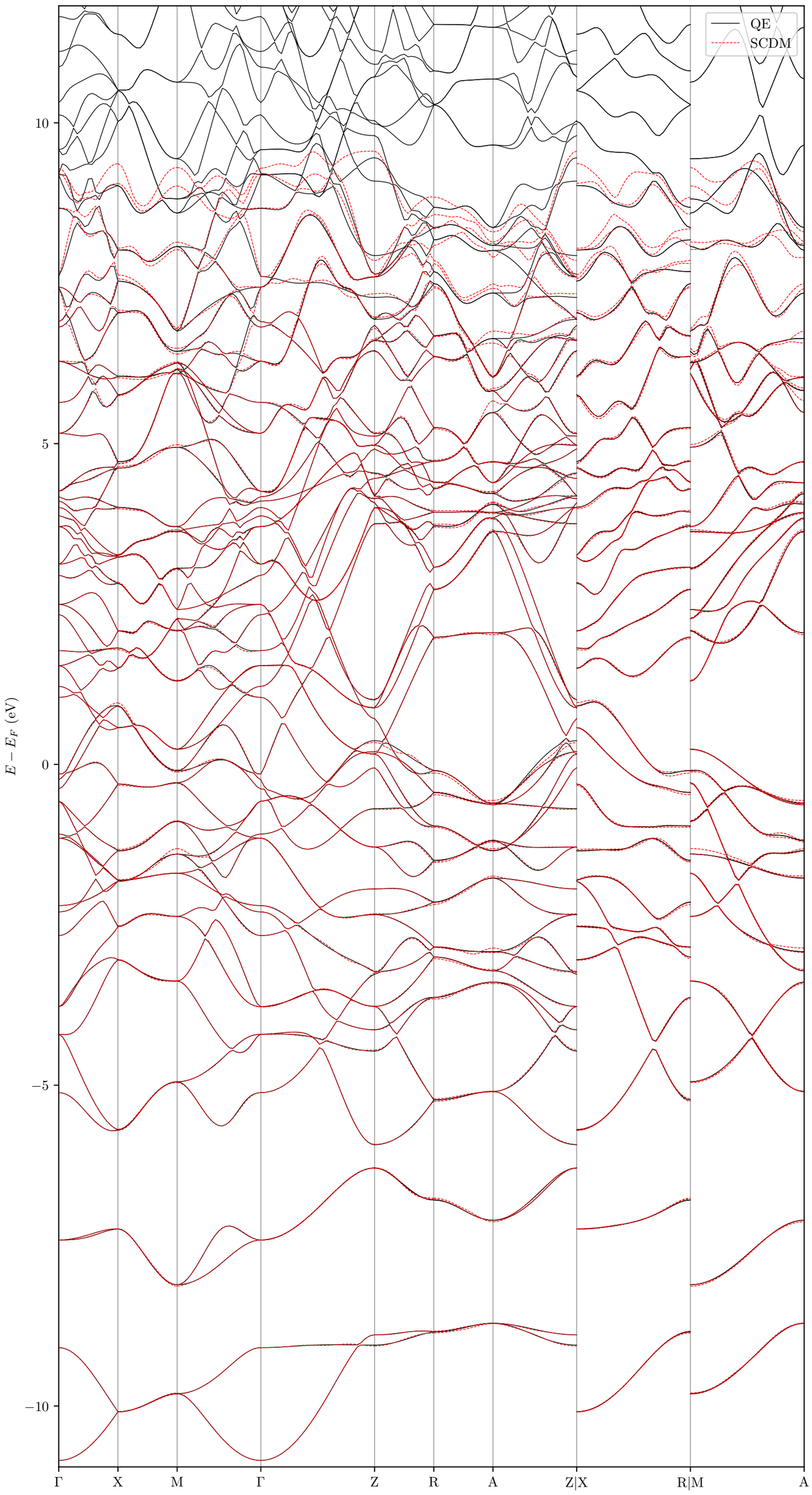
Hf6Si4 exclude semicore
PW=001cf403-f6e0-46d1-9606-29f7533613ff
W90=08ea1dfa-c326-4d87-b0a1-48eac2f5f170




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.5 | 9.3 | 52.8 | 26.8 | 66.1 | 425.5 | 2.749 |

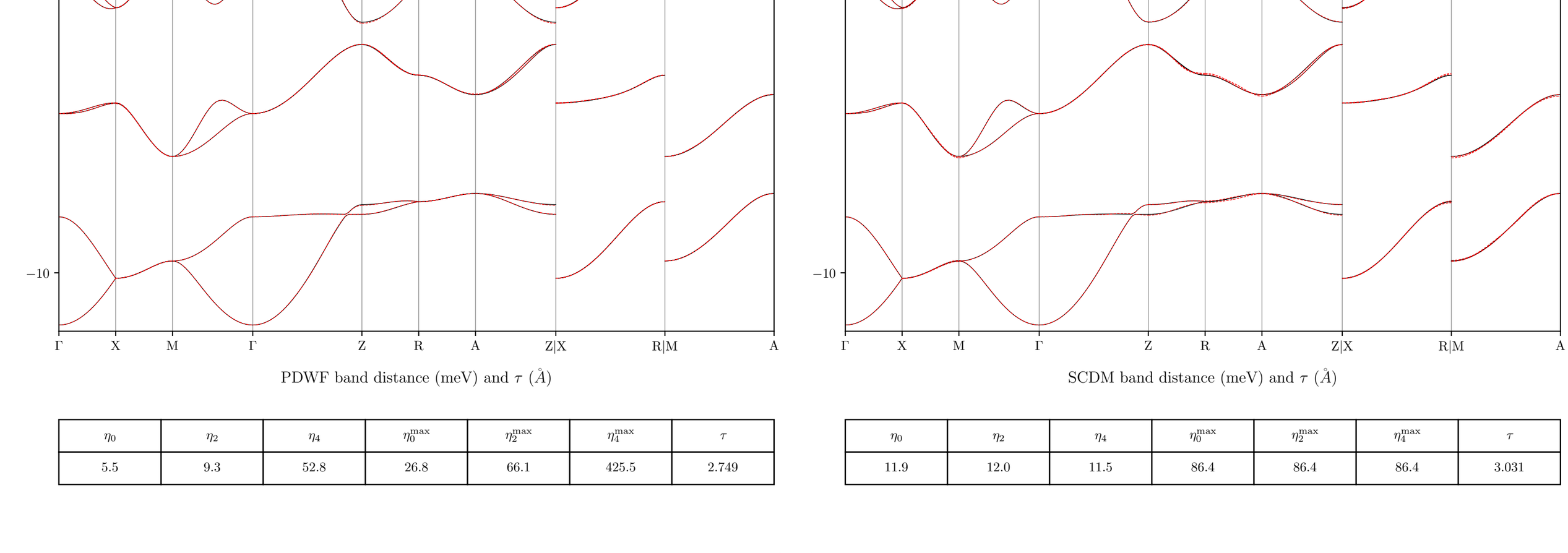
Hf6Si4 exclude semicore
PW=001cf403-f6e0-46d1-9606-29f7533613ff
W90=b6f3565c-3e94-4a78-a618-8085fc433046

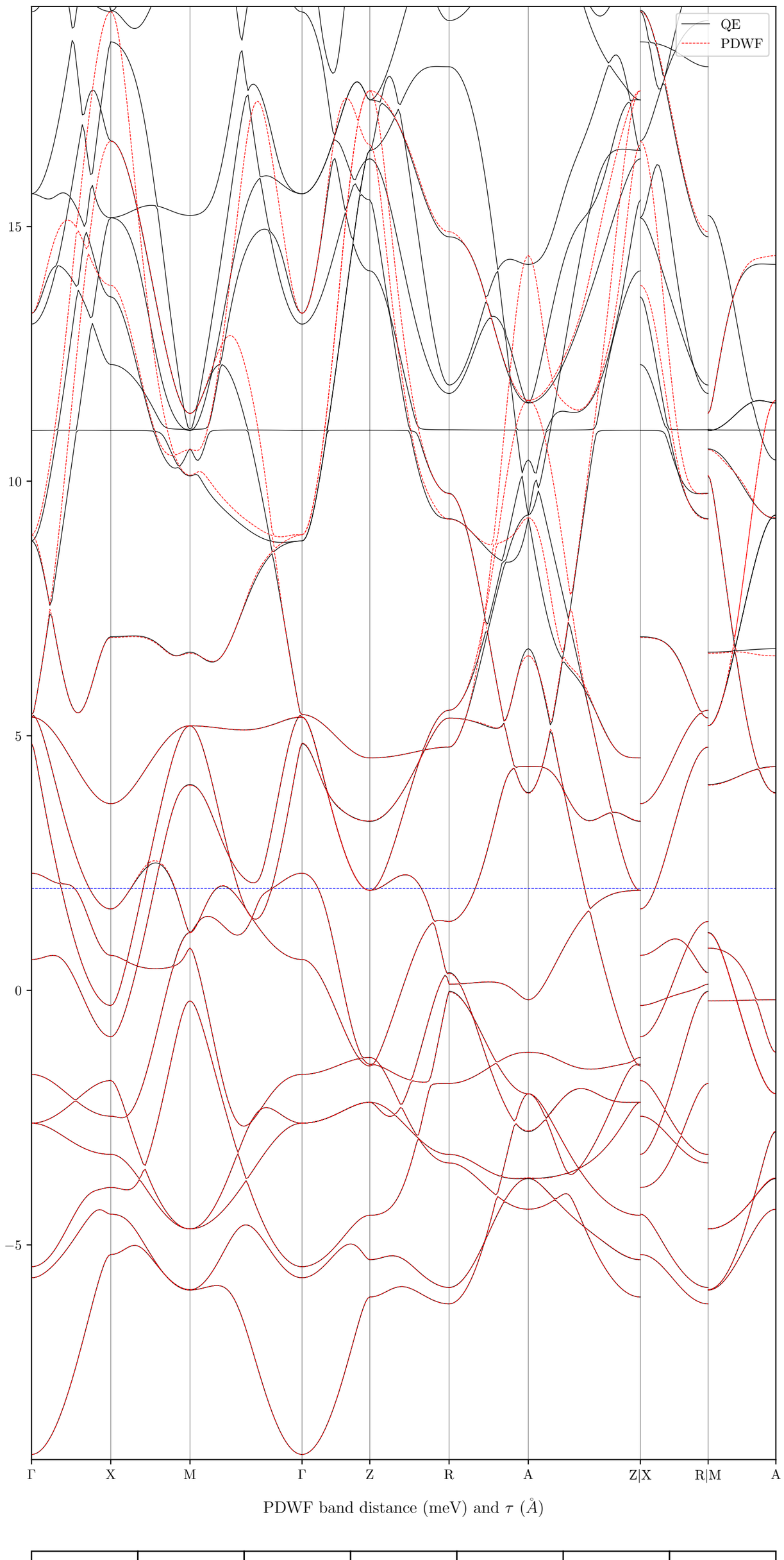



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 11.9 | 12.0 | 11.5 | 86.4 | 86.4 | 86.4 | 3.031 |

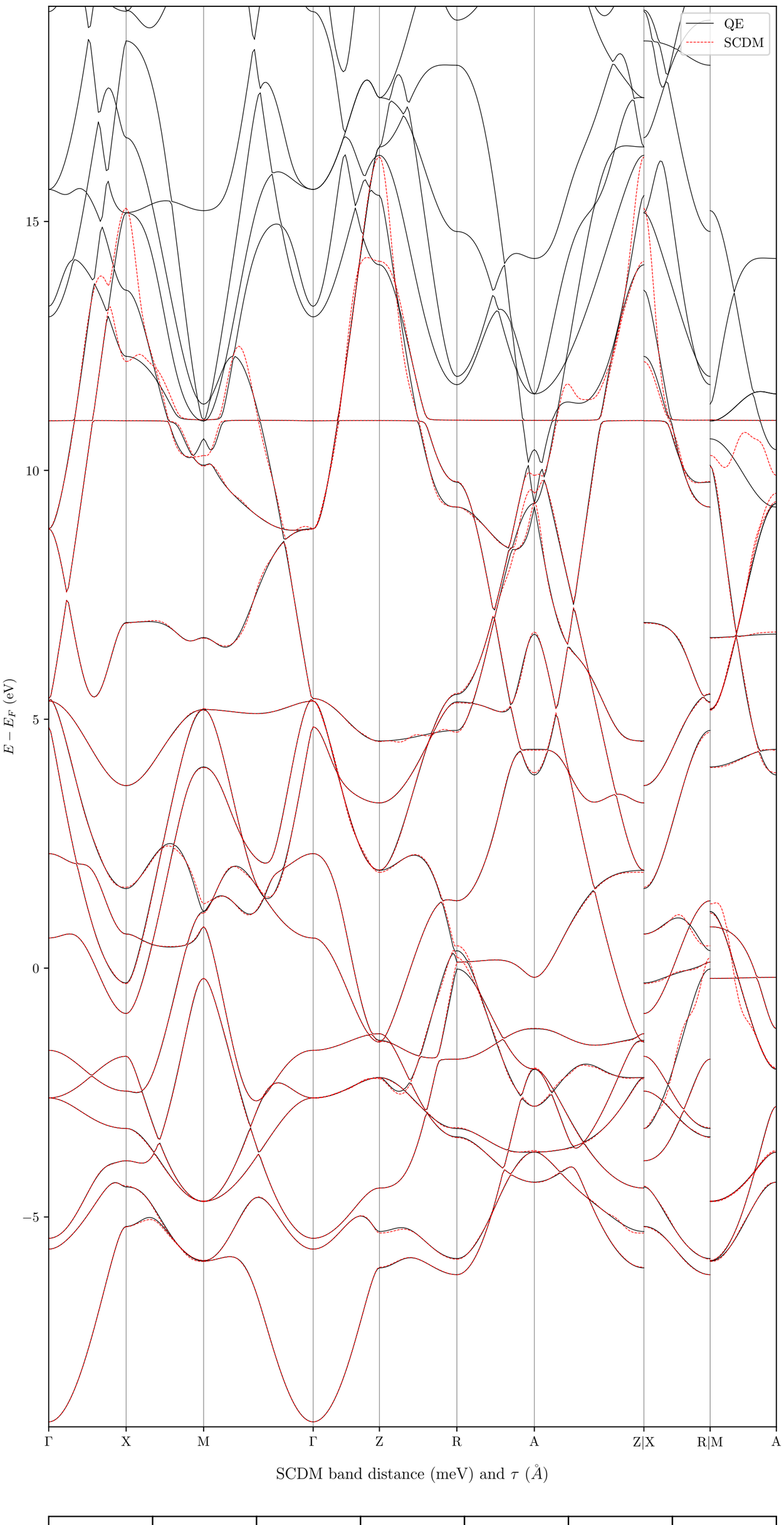
Hamiltonian decay





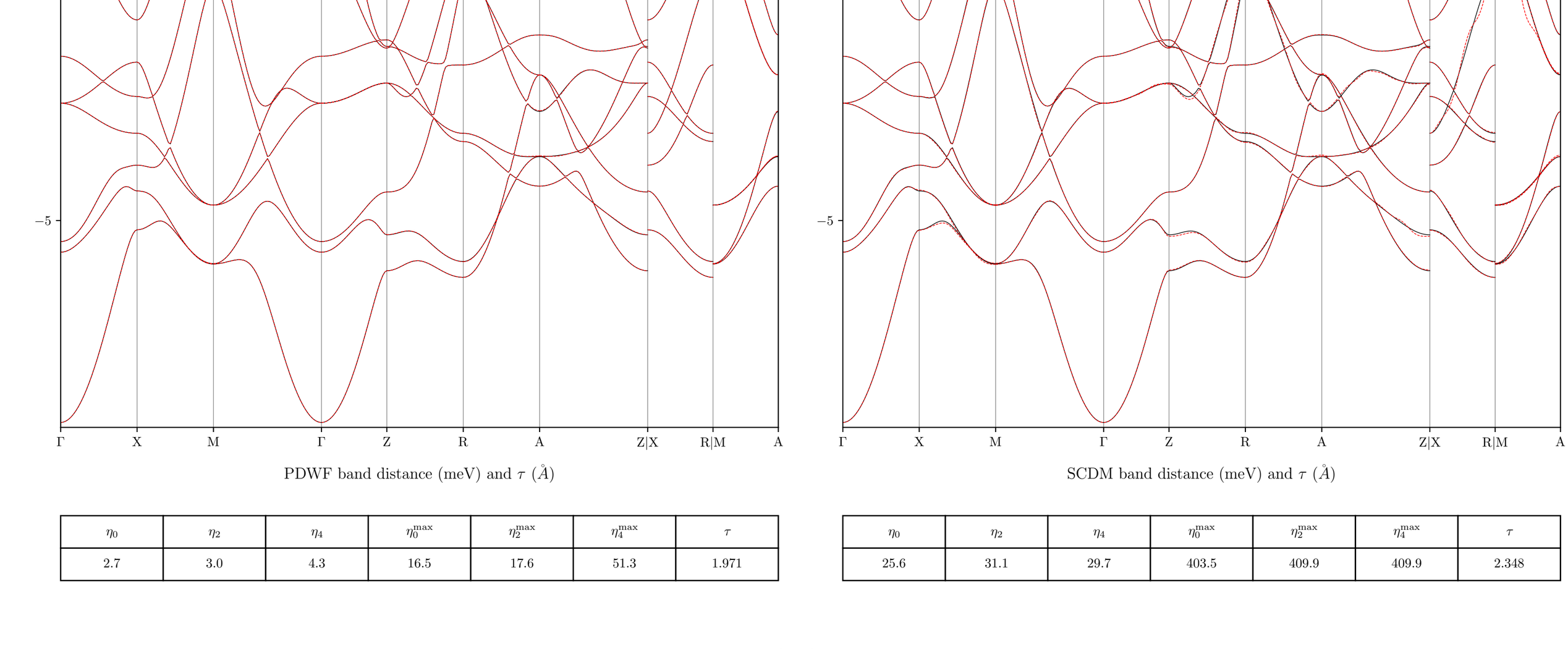

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

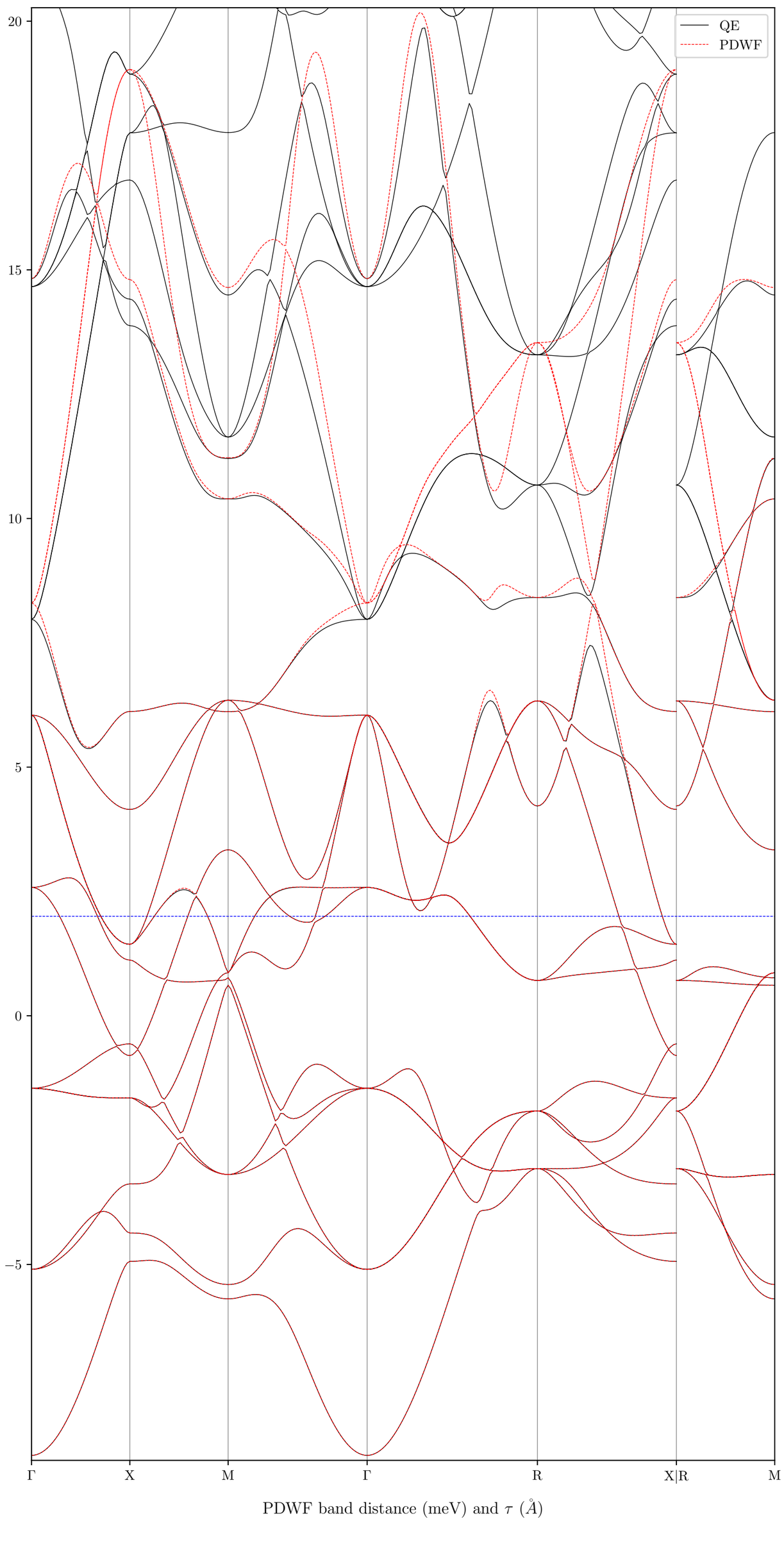
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.7 | 3.0 | 4.3 | 16.5 | 17.6 | 51.3 | 1.971 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

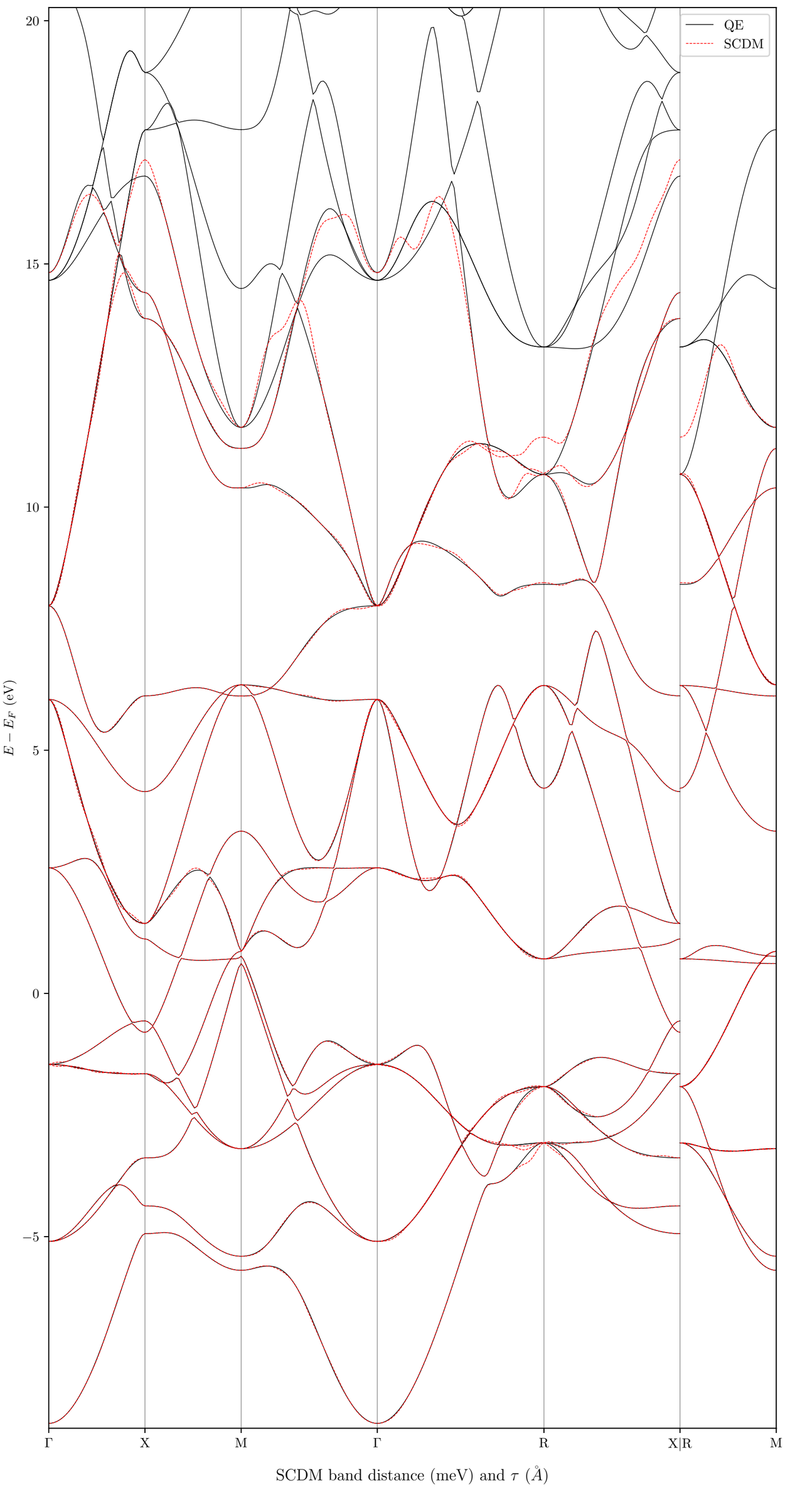
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 25.6 | 31.1 | 29.7 | 403.5 | 409.9 | 409.9 | 2.348 |





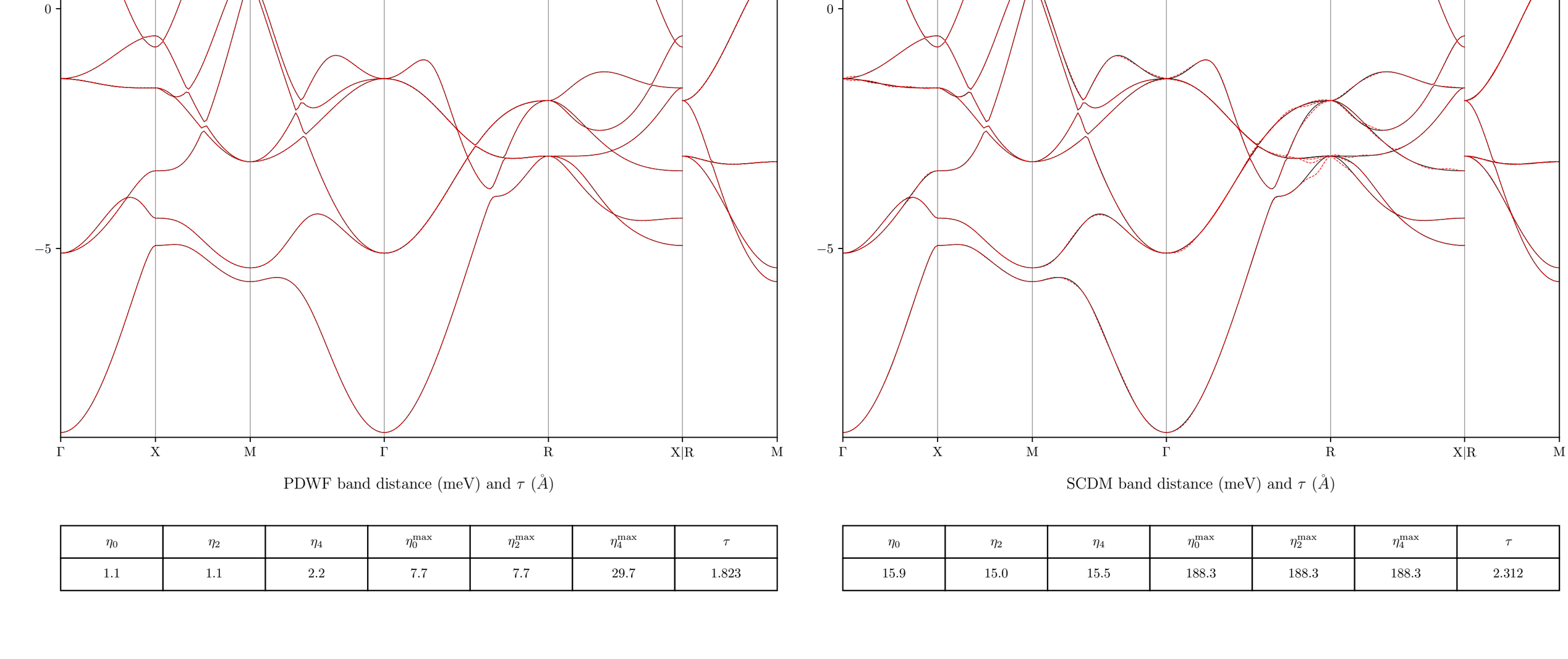

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.1 | 2.2 | 7.7 | 7.7 | 29.7 | 1.823 |

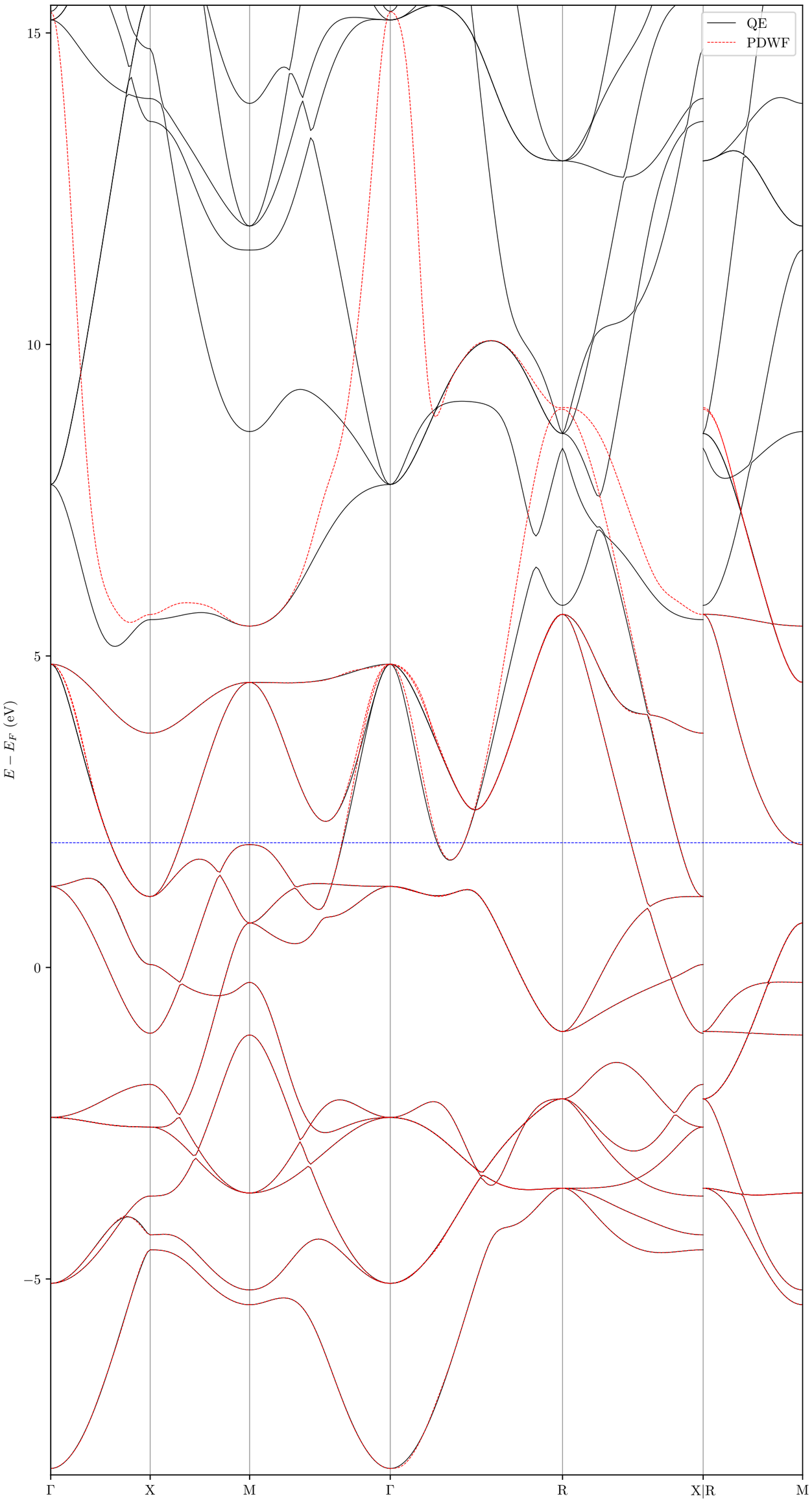



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 15.9 | 15.0 | 15.5 | 188.3 | 188.3 | 188.3 | 2.312 |



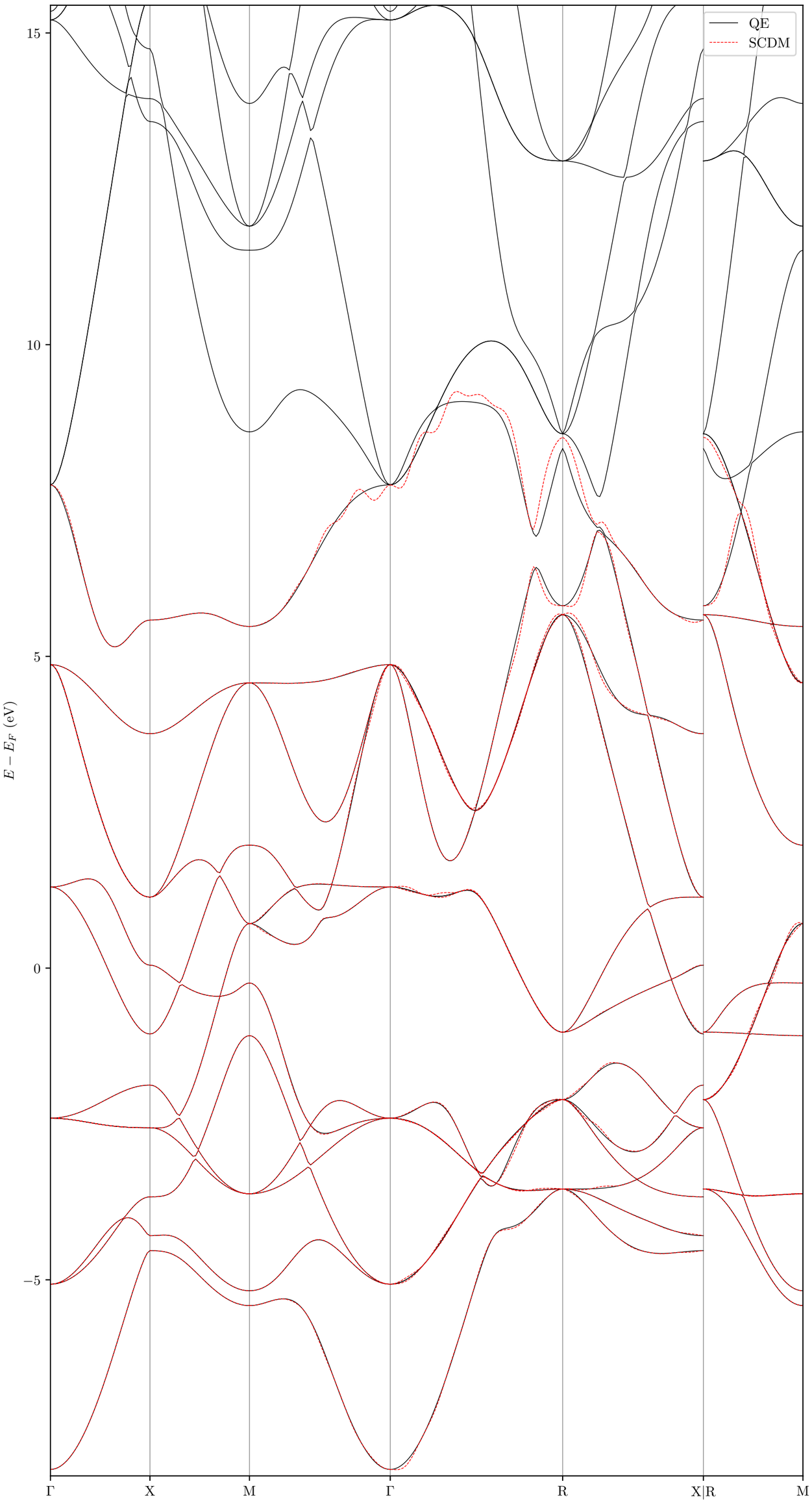
HfRh exclude semicore
PW=59c9b04b-5b4f-4e4d-b6de-9948c0c891eb
W90=de962245-a500-4968-a57f-dfe70976deeb




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.6 | 3.9 | 22.7 | 35.9 | 35.9 | 227.0 | 2.083 |

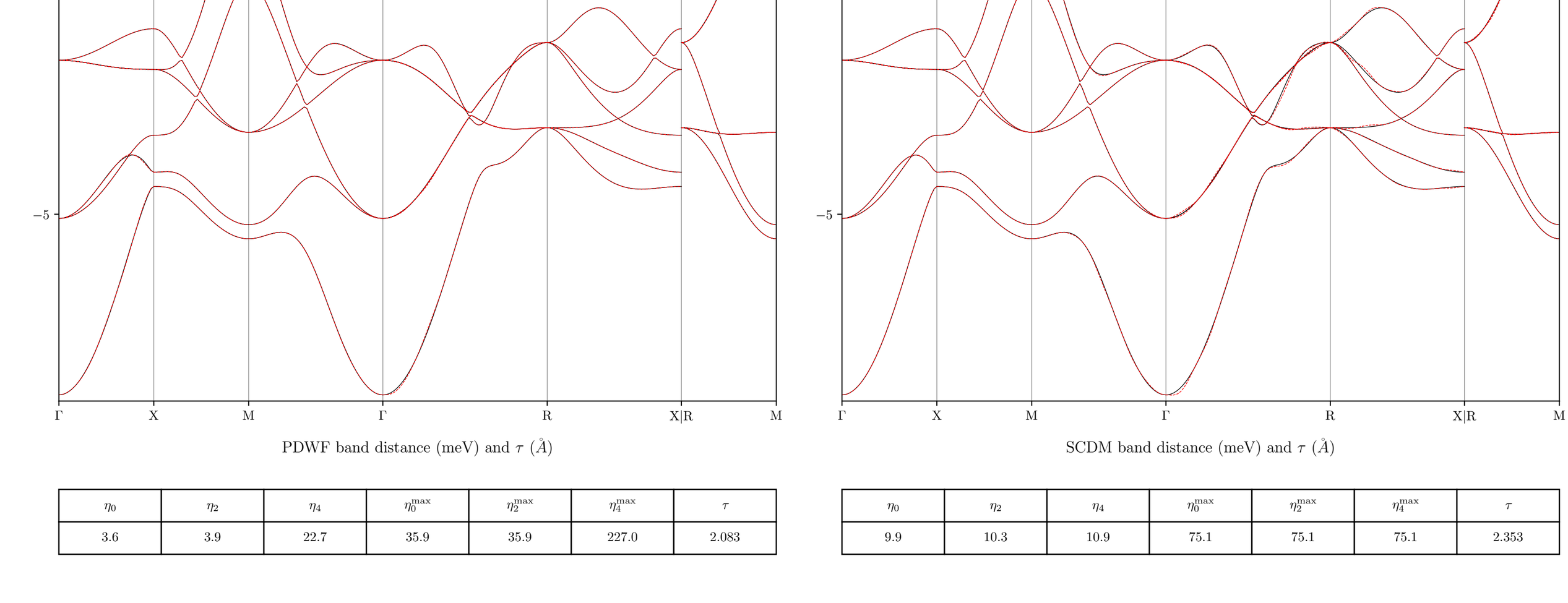
HfRh exclude semicore
PW=59c9b04b-5b4f-4e4d-b6de-9948c0c891eb
W90=a3fa9425-7f0d-47fe-b587-e3afa742a405



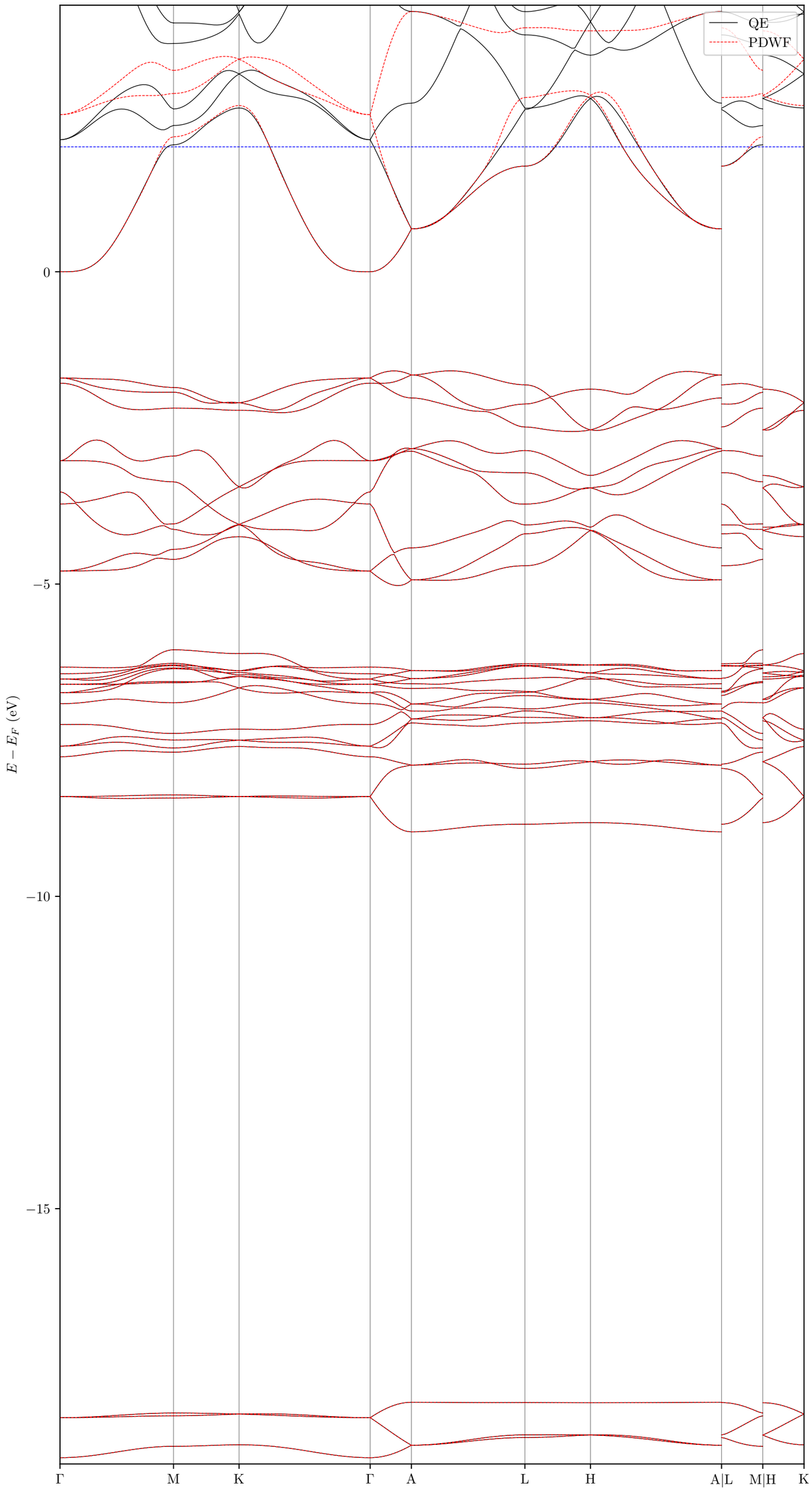

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 9.9 | 10.3 | 10.9 | 75.1 | 75.1 | 75.1 | 2.353 |

Hamiltonian decay



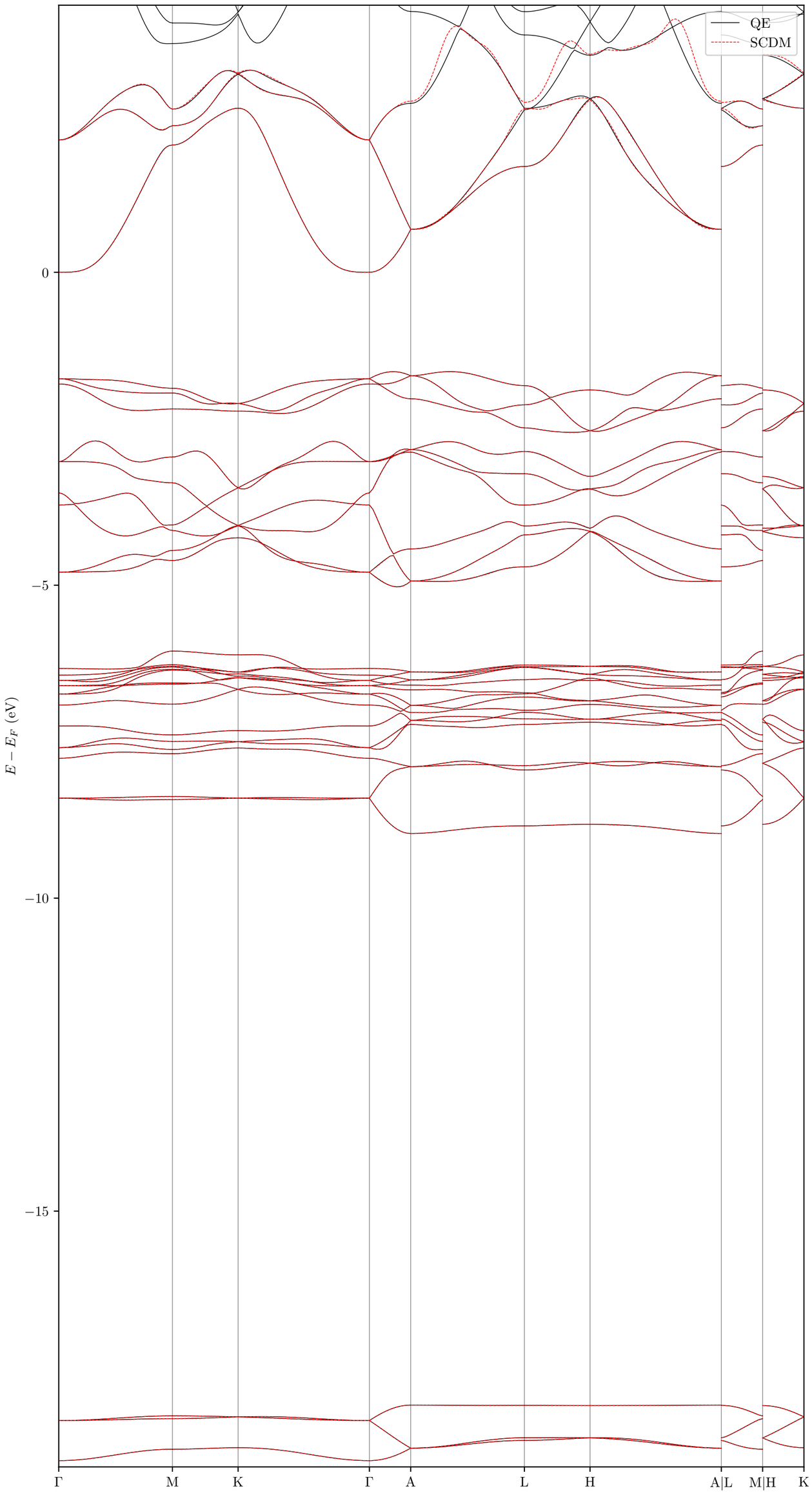
Hg3O3 exclude semicore
PW=07d5814a-0991-48a7-b248-ee70497434ce
W90=e4ec8362-80b8-49d1-ab91-0e17cbcd4f3c




PDWF band distance (meV) and $\tau$ ($\AA$)

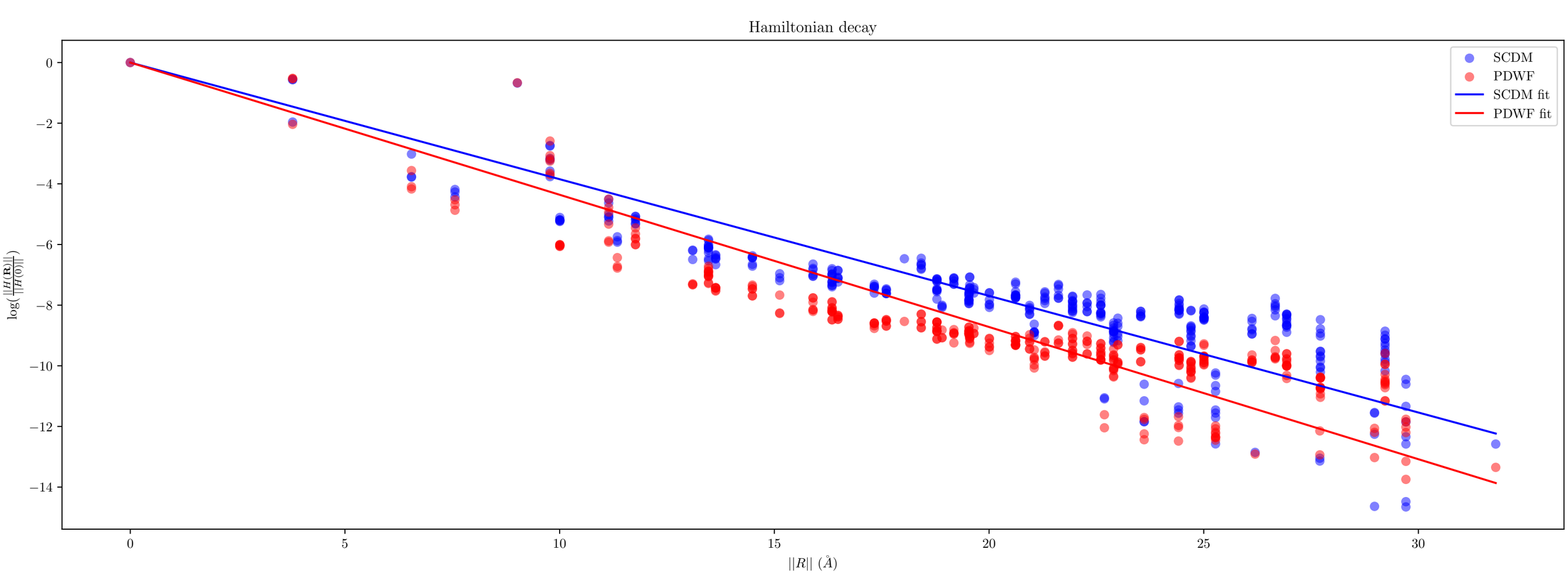
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.6 | 56.6 | 2.3 | 12.4 | 556.3 | 2.293 |

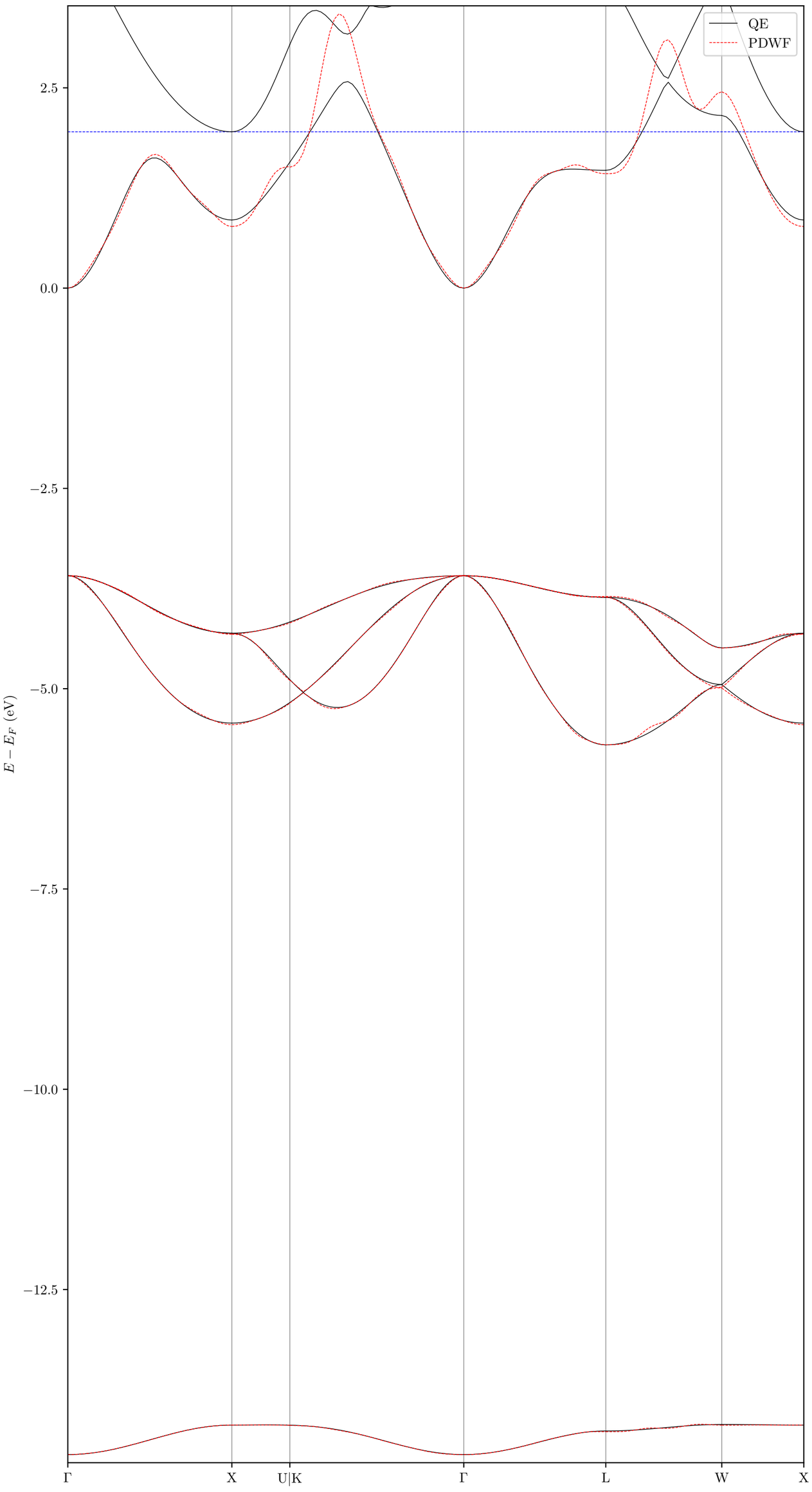
Hg3O3 exclude semicore
PW=07d5814a-0991-48a7-b248-ee70497434ce
W90=b9e24e49-ea40-4fef-af6a-19715af44655




SCDM band distance (meV) and $\tau$ ($\AA$)

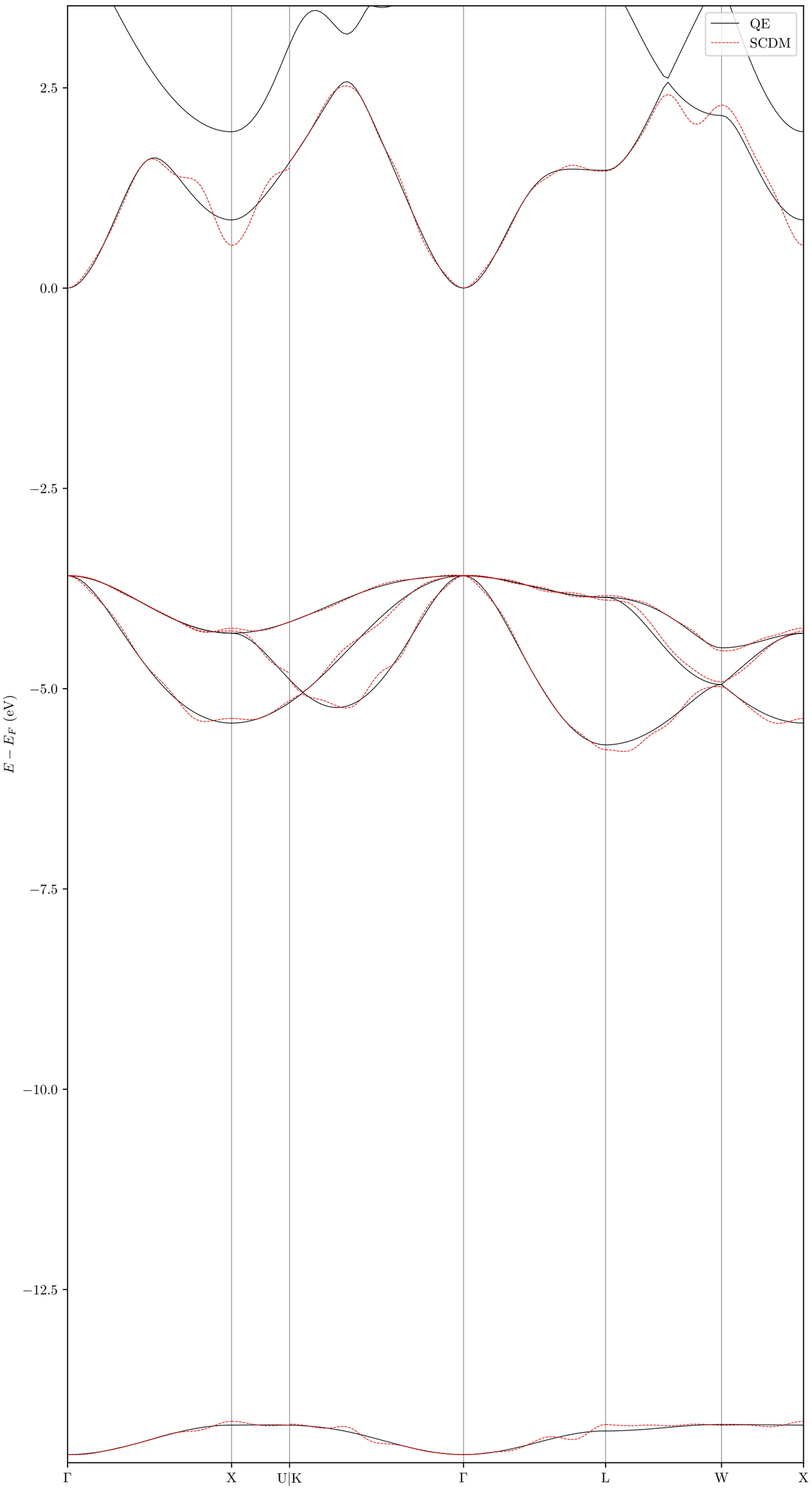
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.9 | 1.1 | 7.2 | 7.3 | 16.3 | 125.3 | 2.599 |





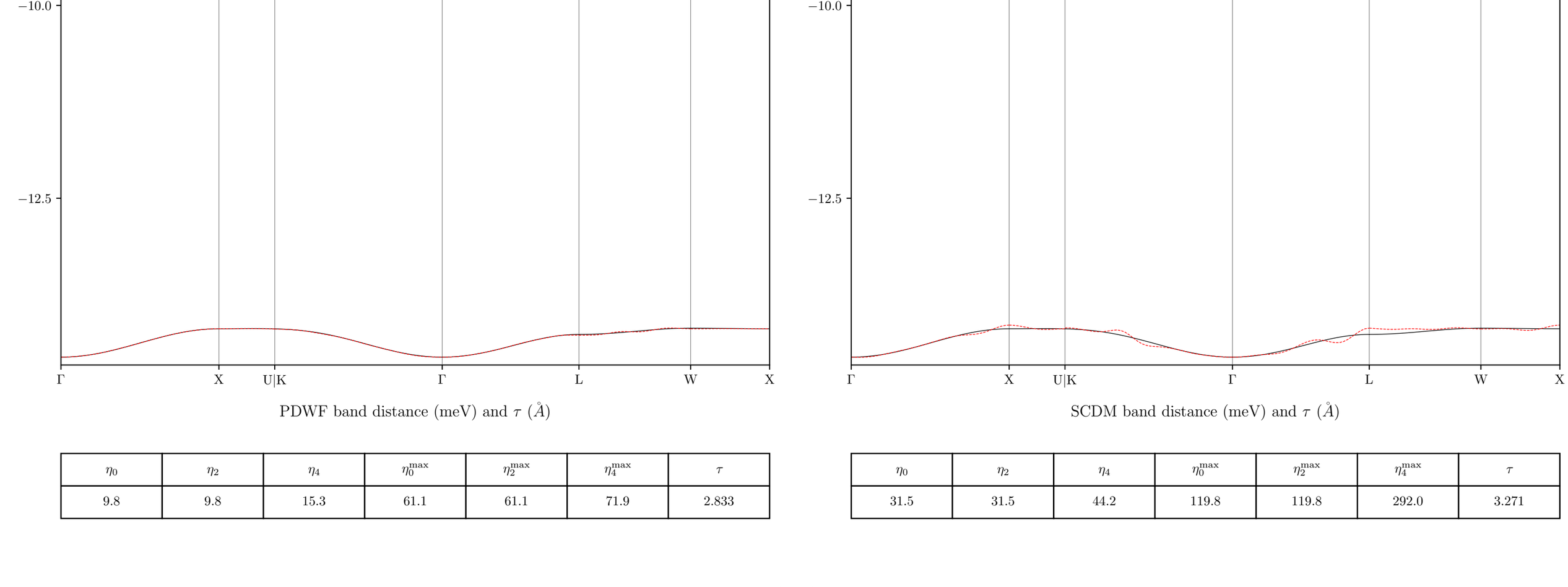

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 9.8 | 9.8 | 15.3 | 61.1 | 61.1 | 71.9 | 2.833 |

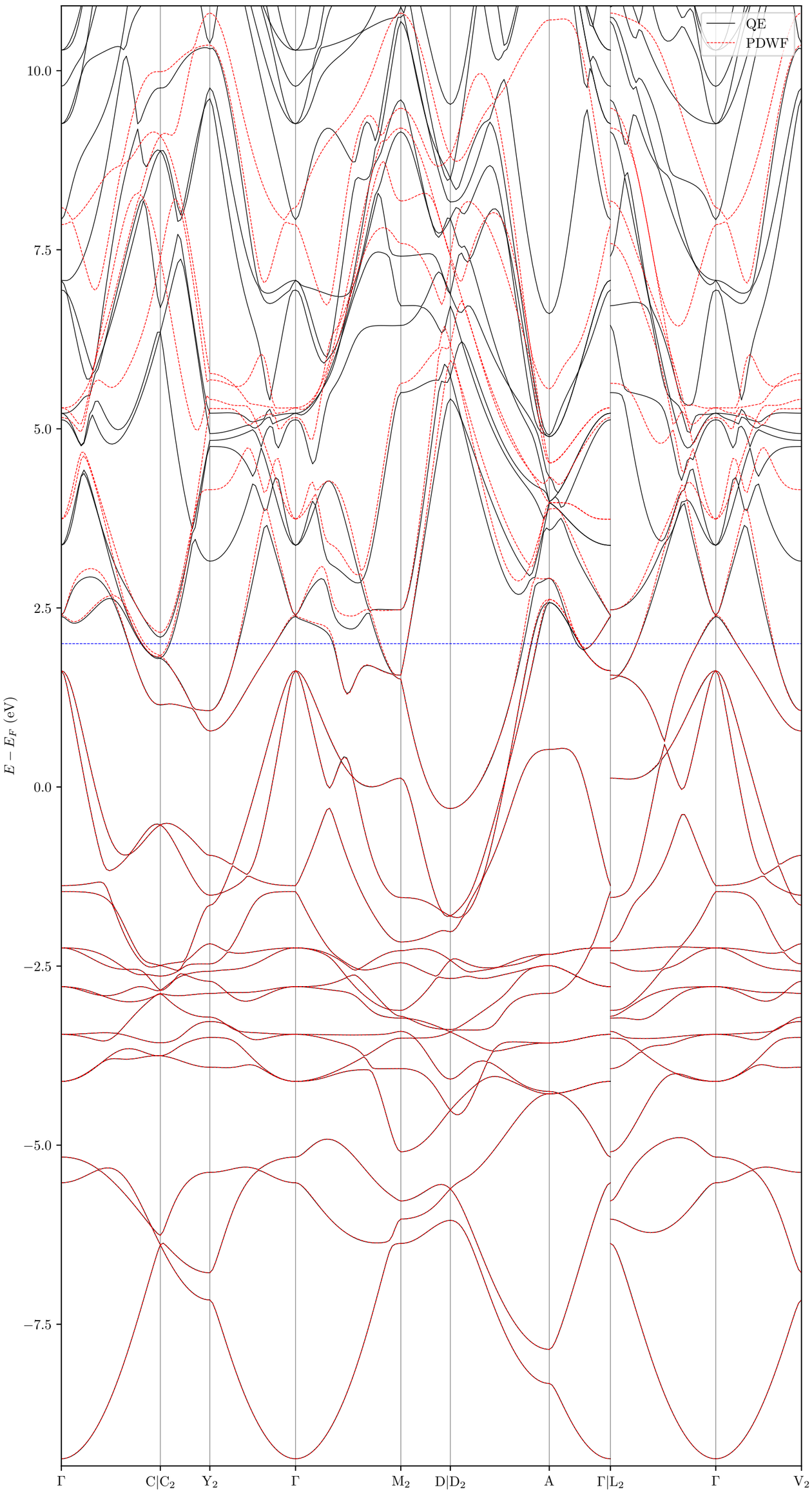



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 31.5 | 31.5 | 44.2 | 119.8 | 119.8 | 292.0 | 3.271 |



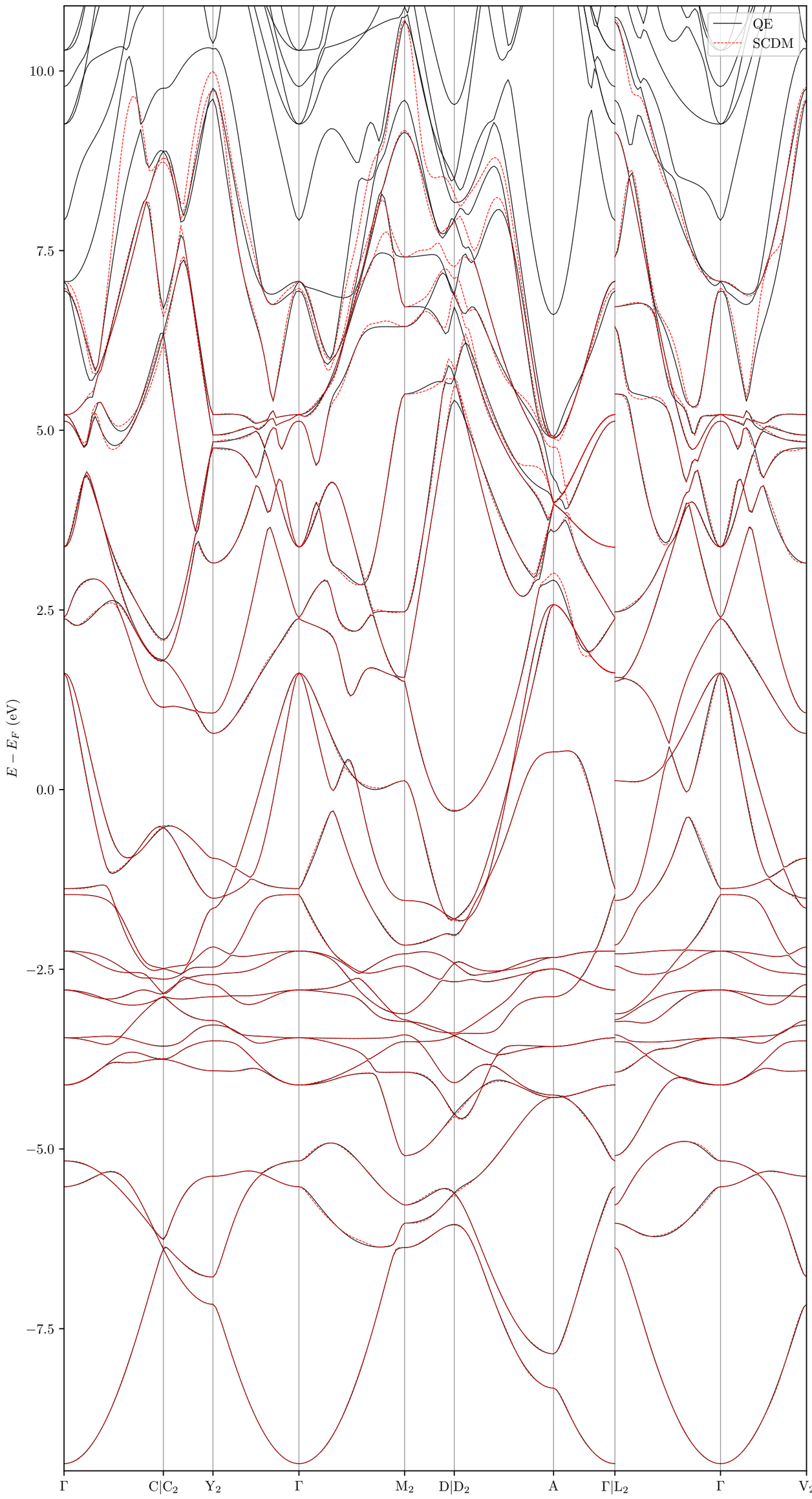
In3Pd2 exclude semicore
PW=7725590b-9952-4a8c-9671-cdab879a633c
W90=ba5b8bec-f0dd-4b5d-9717-cd073eb75dfd




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.6 | 5.4 | 72.8 | 10.7 | 82.4 | 454.0 | 2.286 |

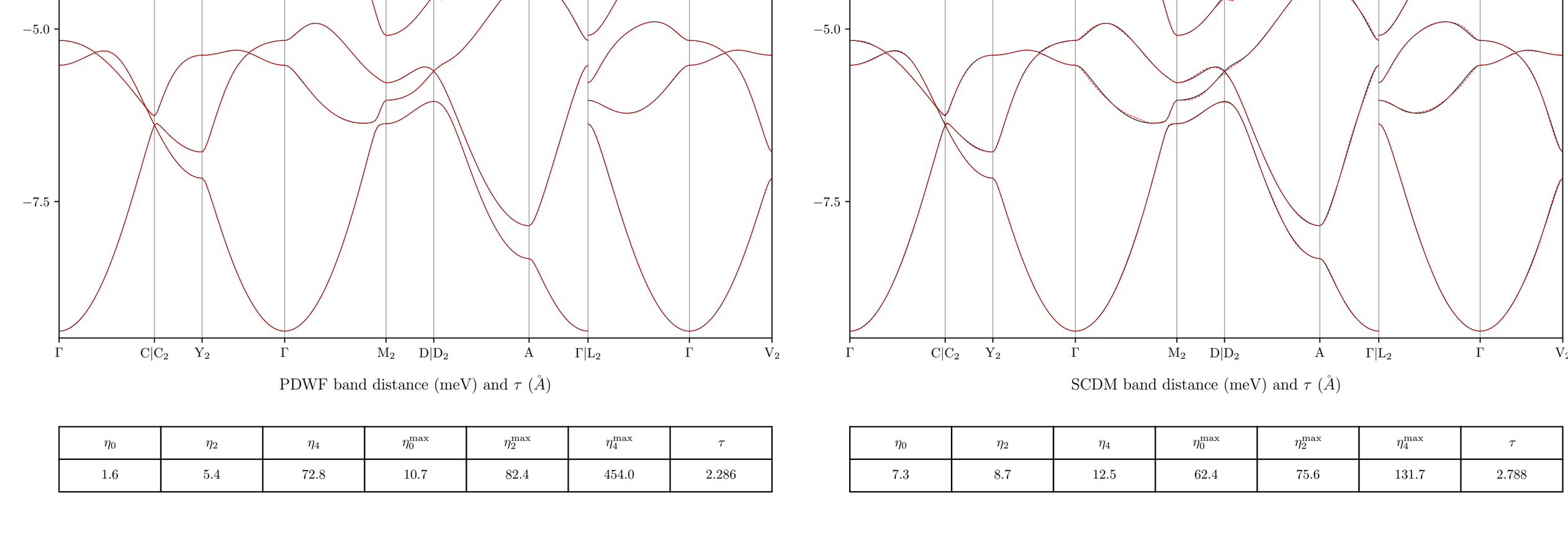
In3Pd2 exclude semicore
PW=7725590b-9952-4a8c-9671-cdab879a633c
W90=9cf90882-4405-4357-aecd-11d381923f6b

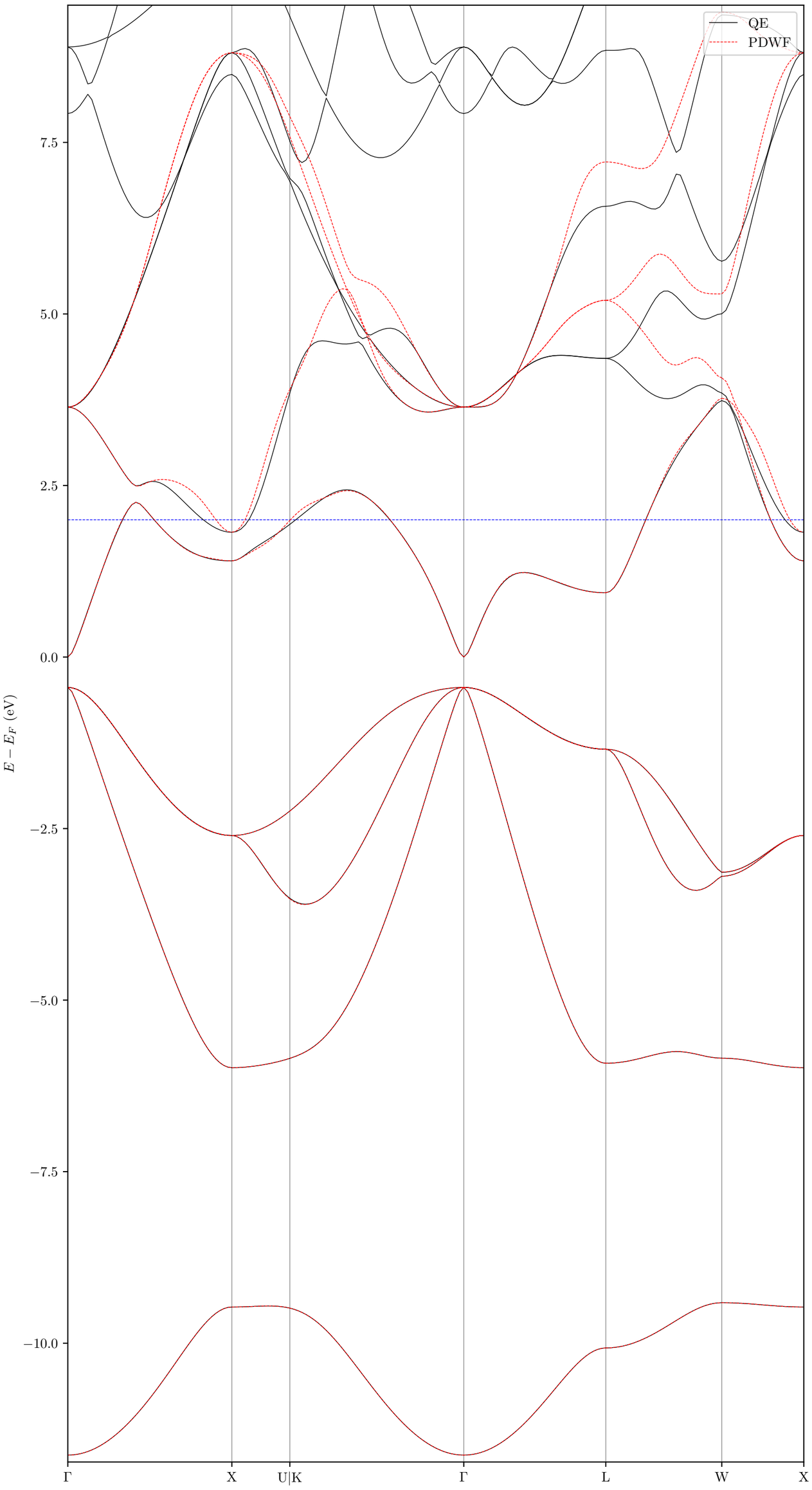



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.3 | 8.7 | 12.5 | 62.4 | 75.6 | 131.7 | 2.788 |

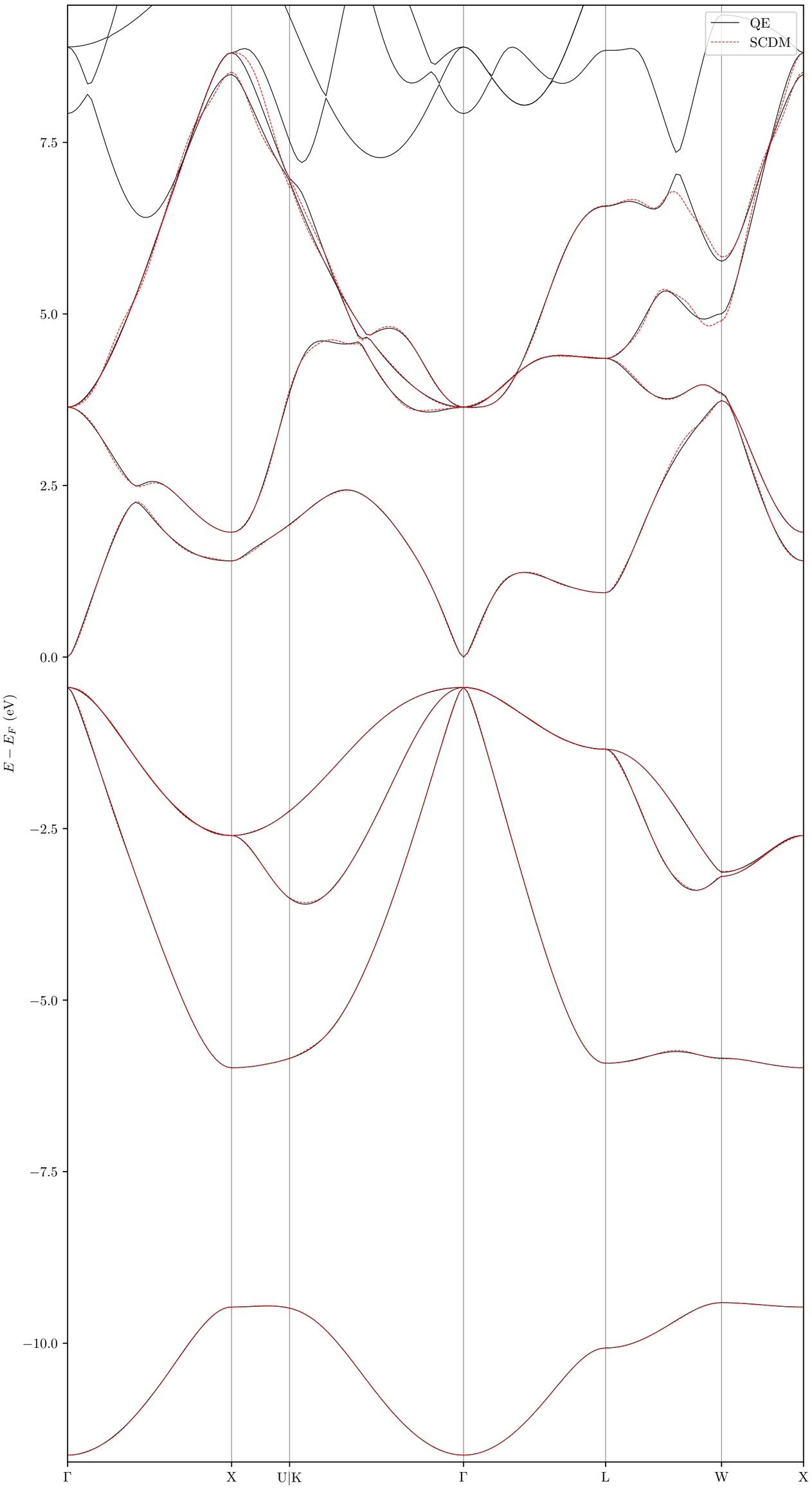
Hamiltonian decay





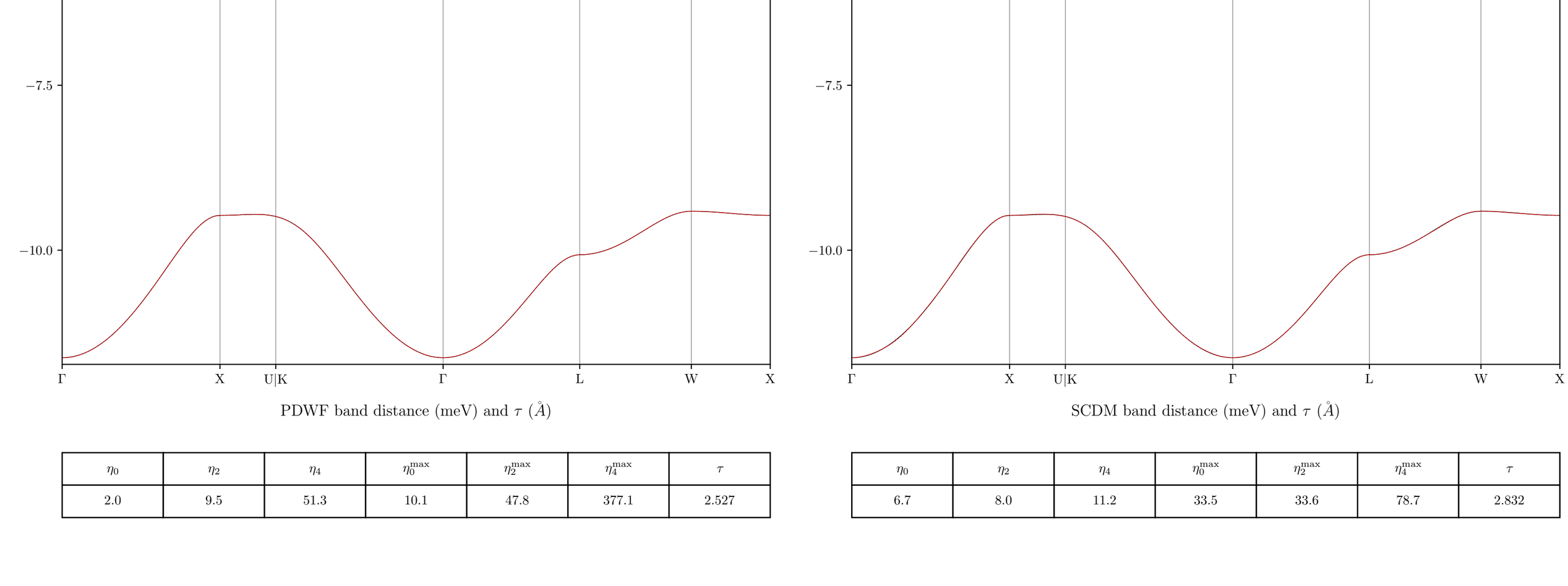

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

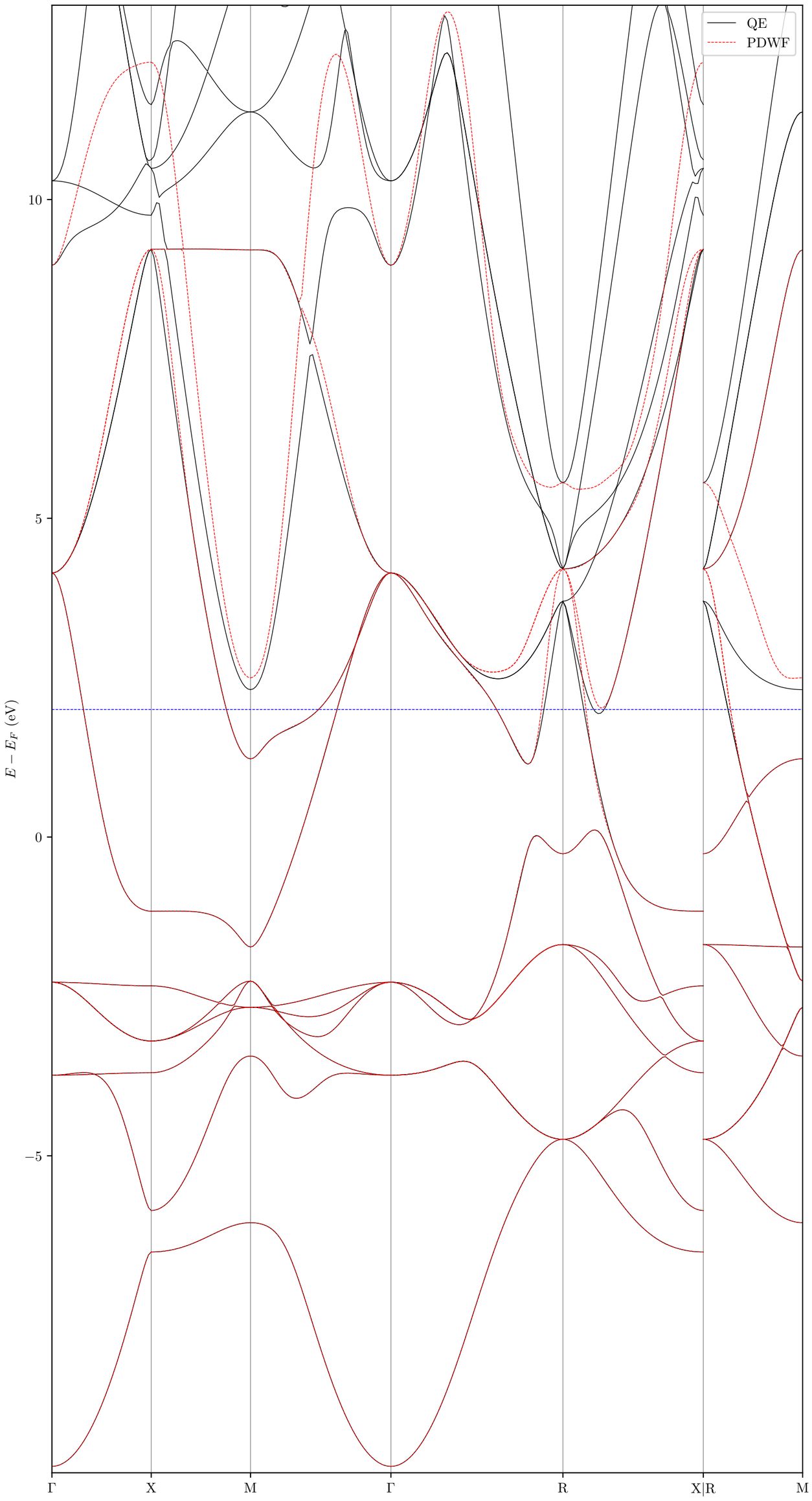
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.0 | 9.5 | 51.3 | 10.1 | 47.8 | 377.1 | 2.527 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

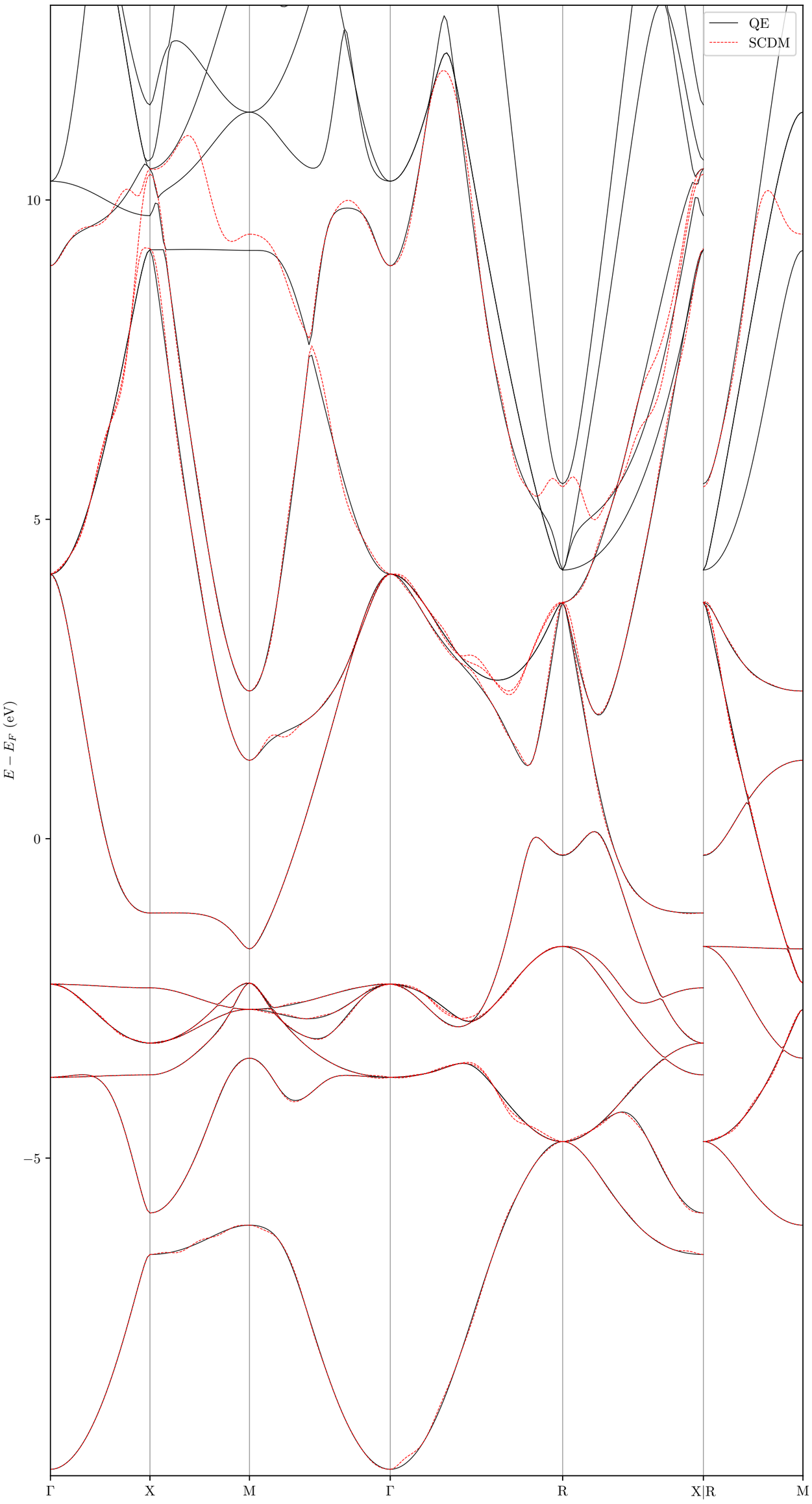
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.7 | 8.0 | 11.2 | 33.5 | 33.6 | 78.7 | 2.832 |





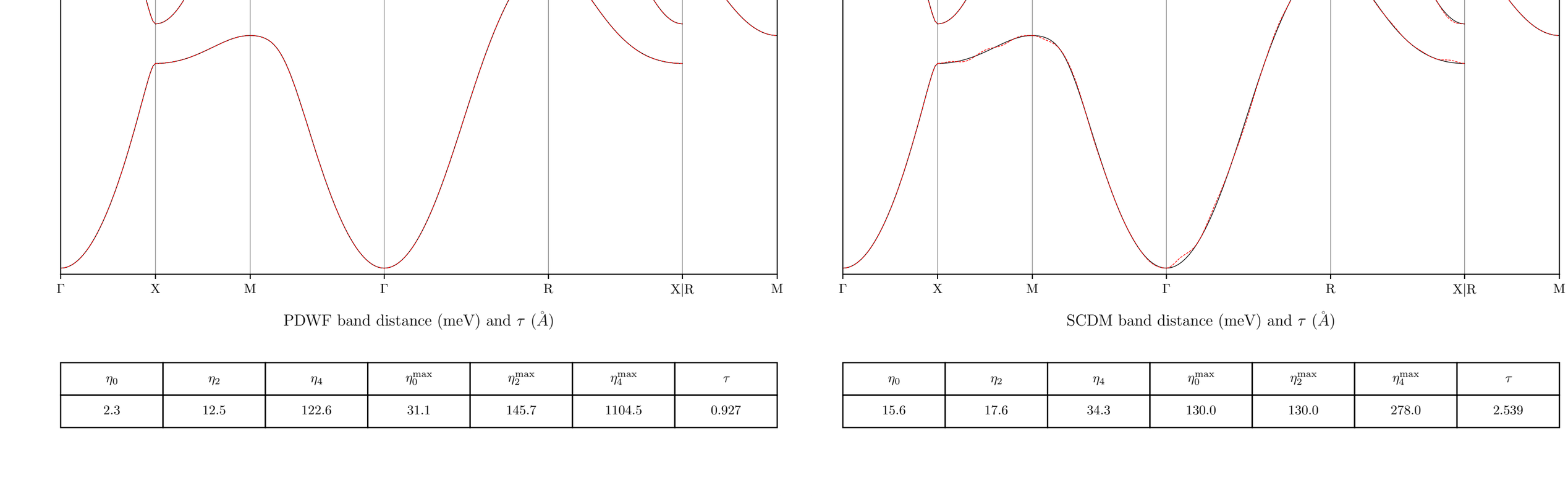

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.3 | 12.5 | 122.6 | 31.1 | 145.7 | 1104.5 | 0.927 |

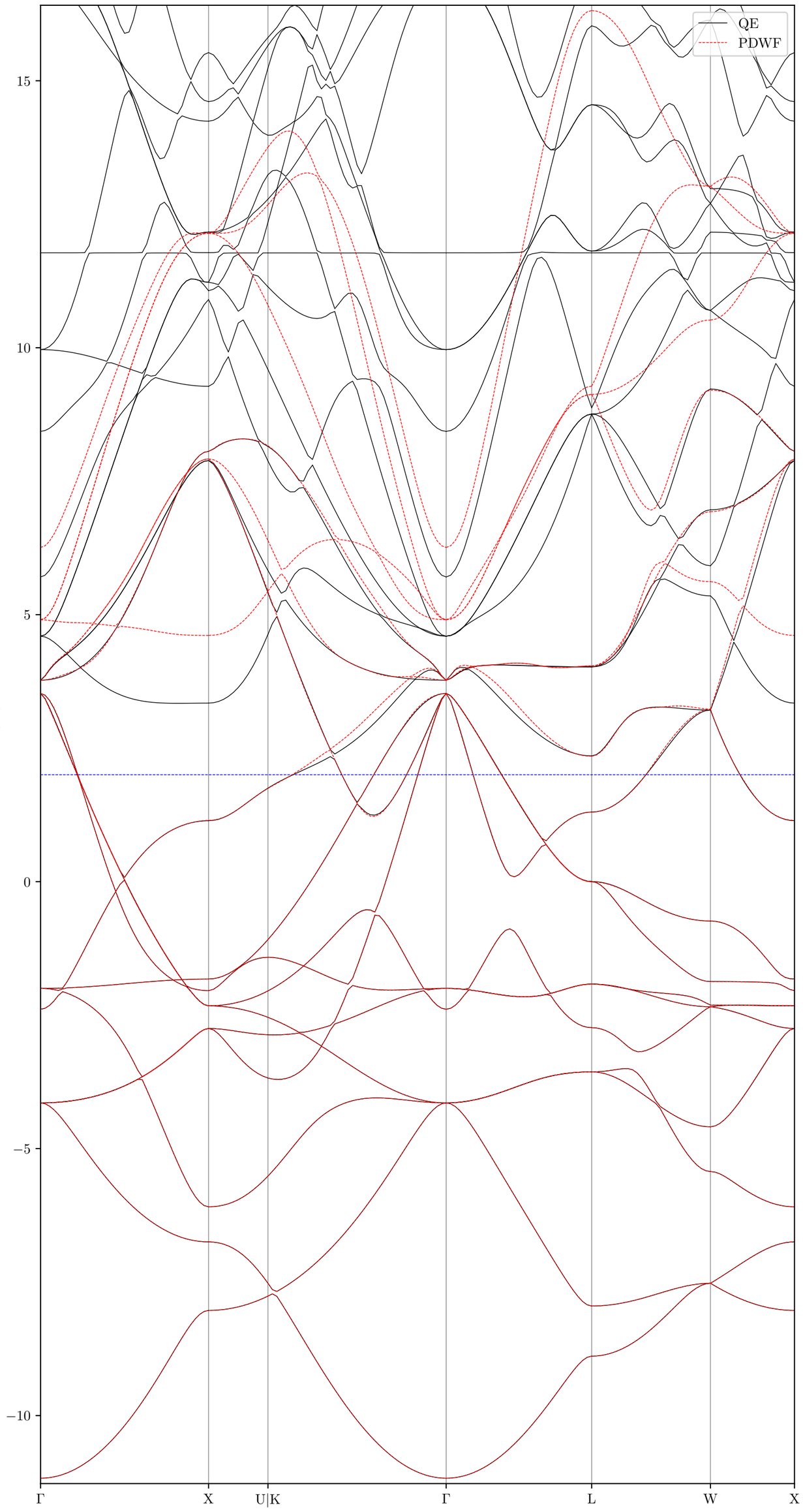



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 15.6 | 17.6 | 34.3 | 130.0 | 130.0 | 278.0 | 2.539 |



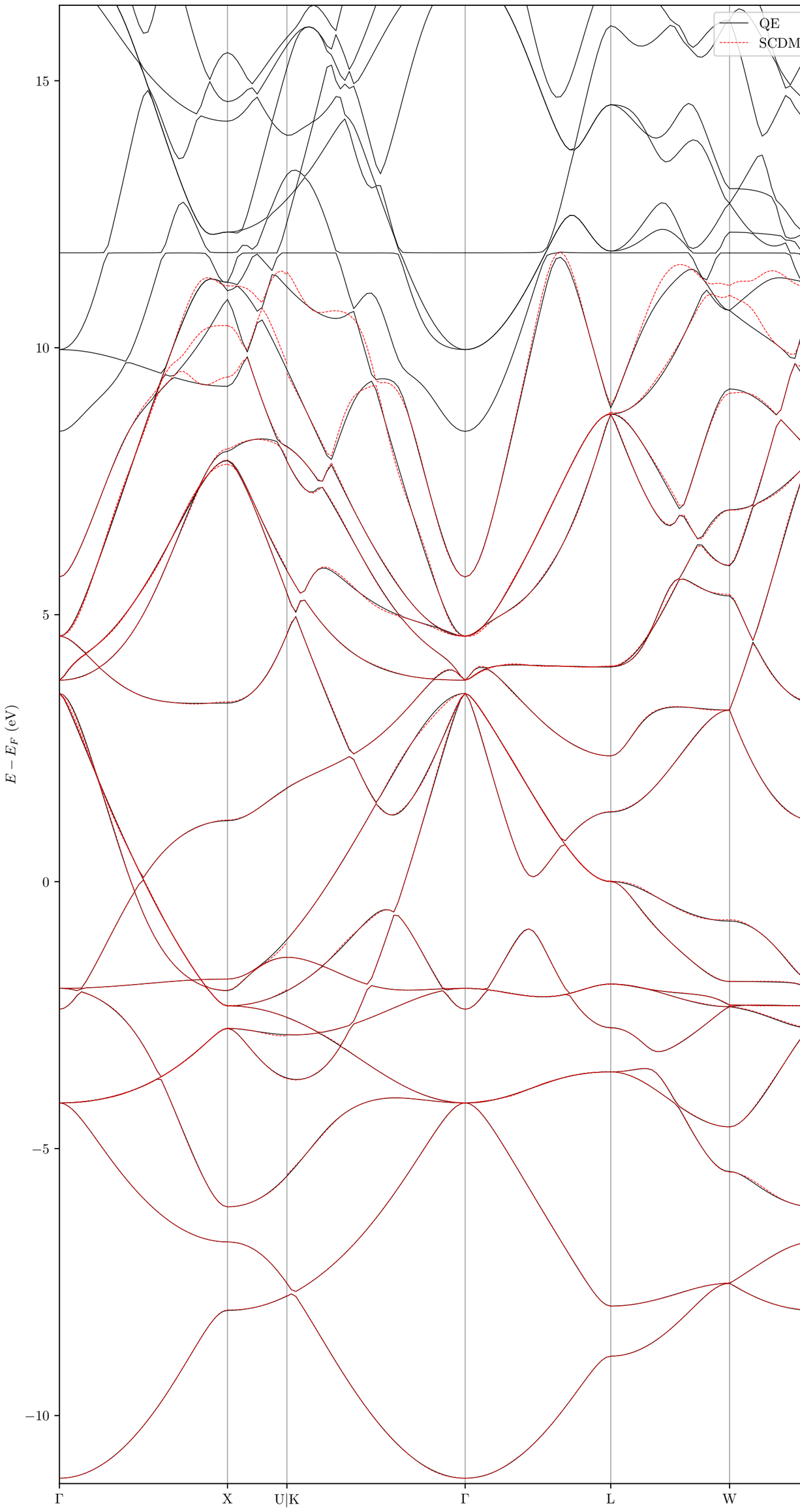
IrSn2 exclude semicore
PW=20f51459-c25b-4e87-8296-854c989c733c
W90=d568a63b-e2ee-428d-8b8d-e81746584a45




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.6 | 3.1 | 45.3 | 9.0 | 25.7 | 229.6 | 2.360 |

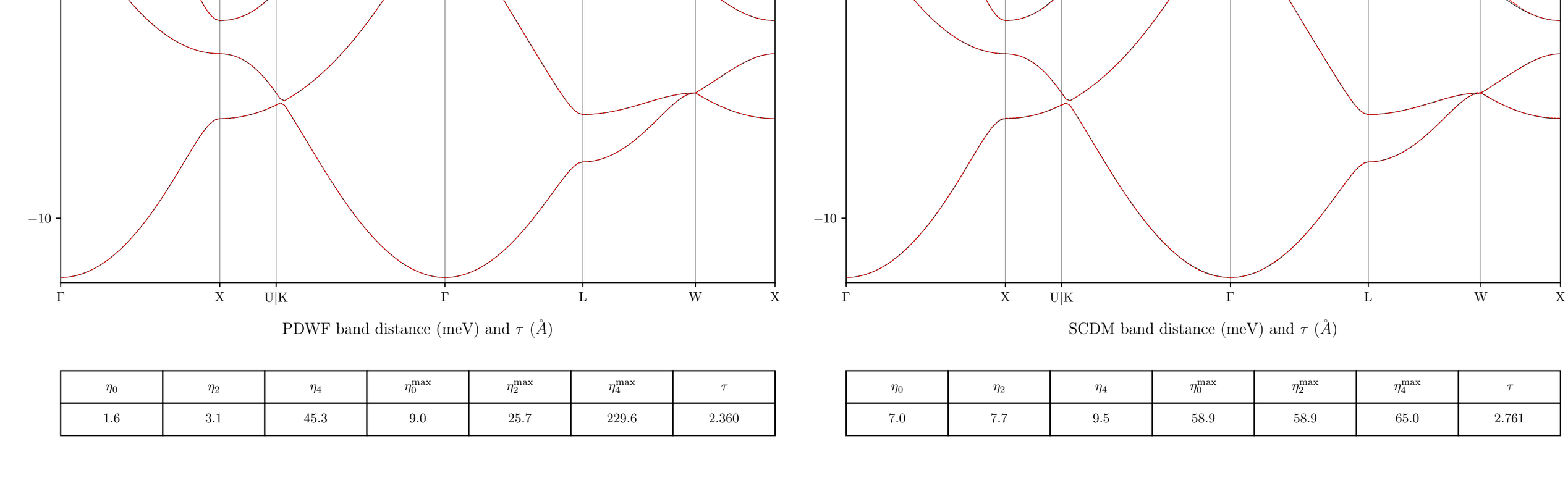
IrSn2 exclude semicore
PW=20f51459-c25b-4e87-8296-854c989c733c
W90=2fa4068b-76e5-4427-b69d-2f40c97cbe5f



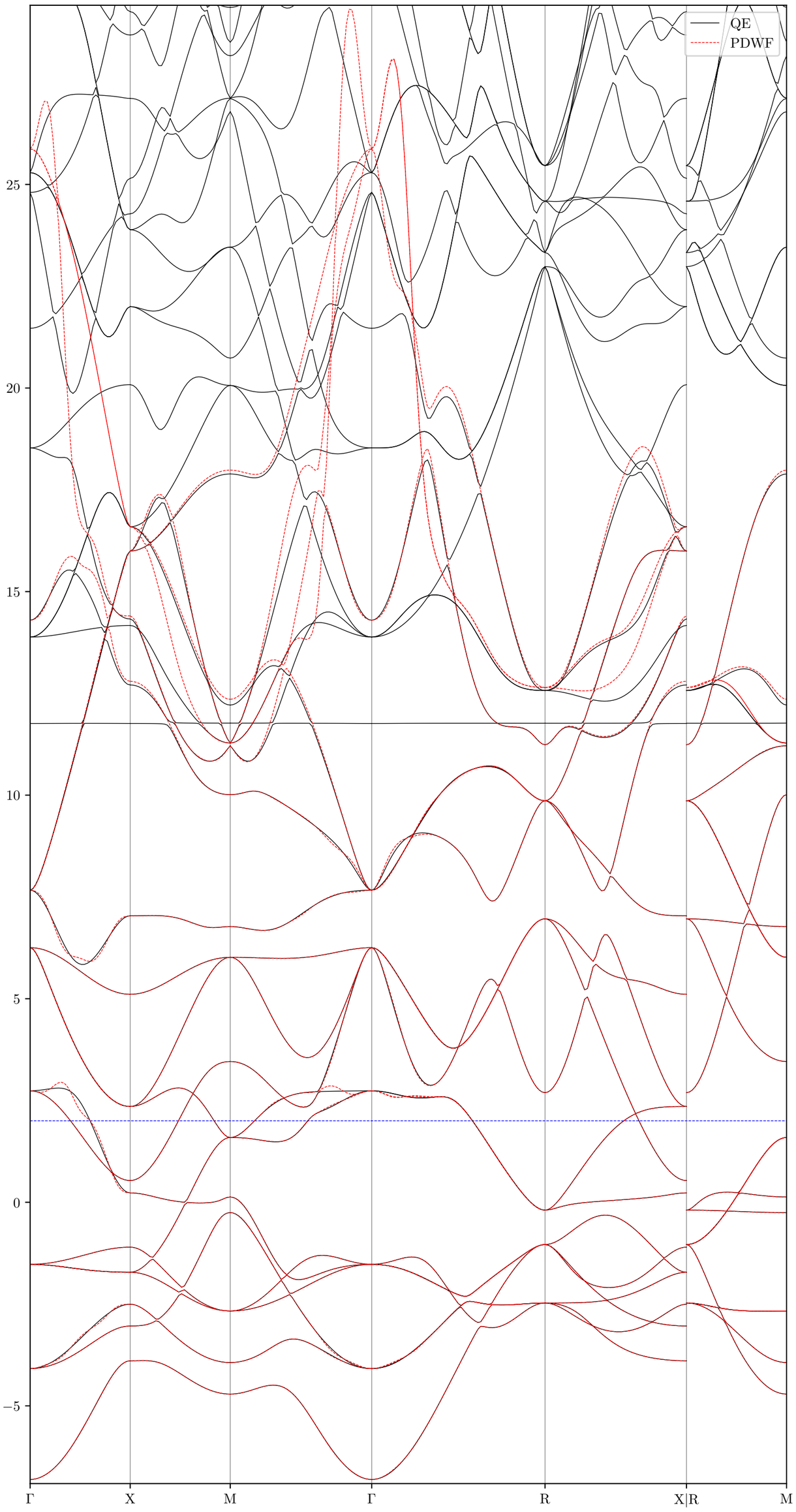

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.0 | 7.7 | 9.5 | 58.9 | 58.9 | 65.0 | 2.761 |

Hamiltonian decay



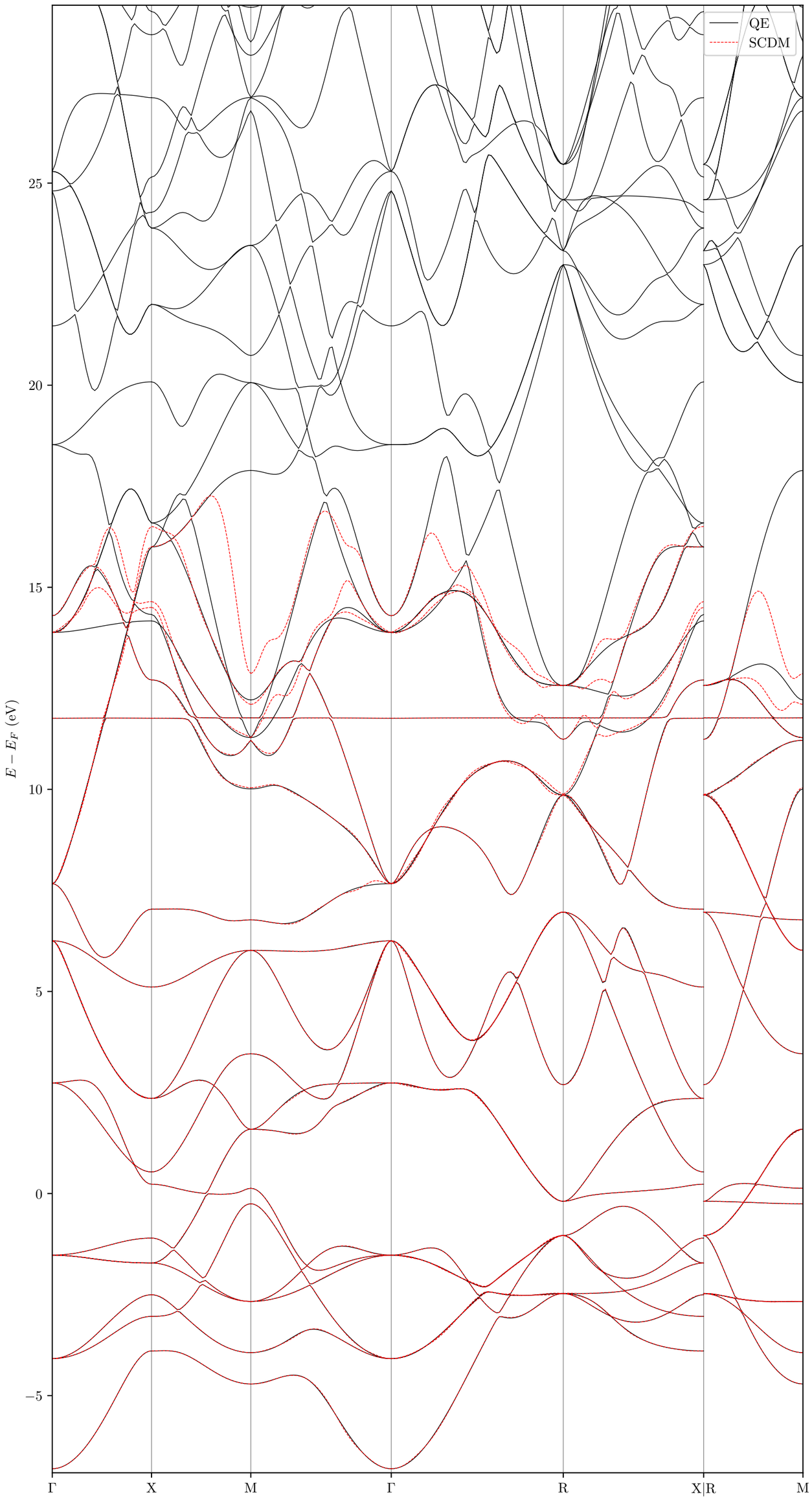
IrY exclude semicore
PW=26fe0ce6-d5da-4c61-b21e-95e7915988af
W90=ae6dac70-177d-49c9-8be1-f481a1bc1712




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.7 | 7.9 | 15.4 | 50.8 | 111.8 | 211.8 | 2.321 |

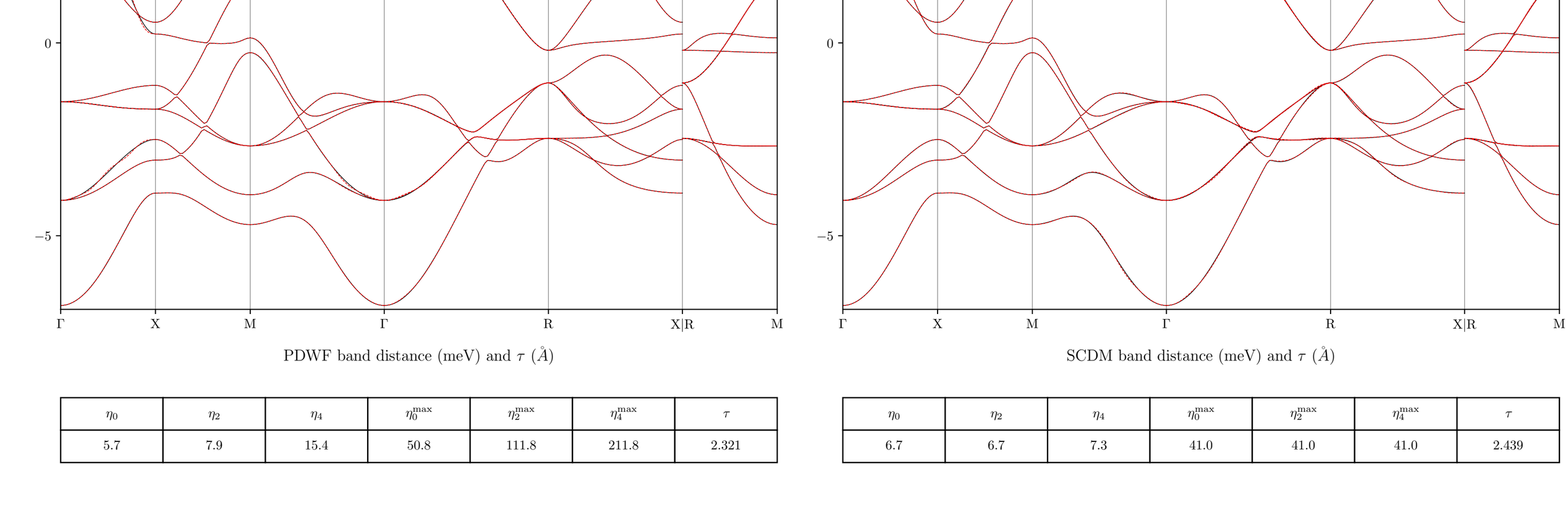
IrY exclude semicore
PW=26fe0ce6-d5da-4c61-b21e-95e7915988af
W90=c83ce0e6-1525-4c21-9ea9-a106e4100d21



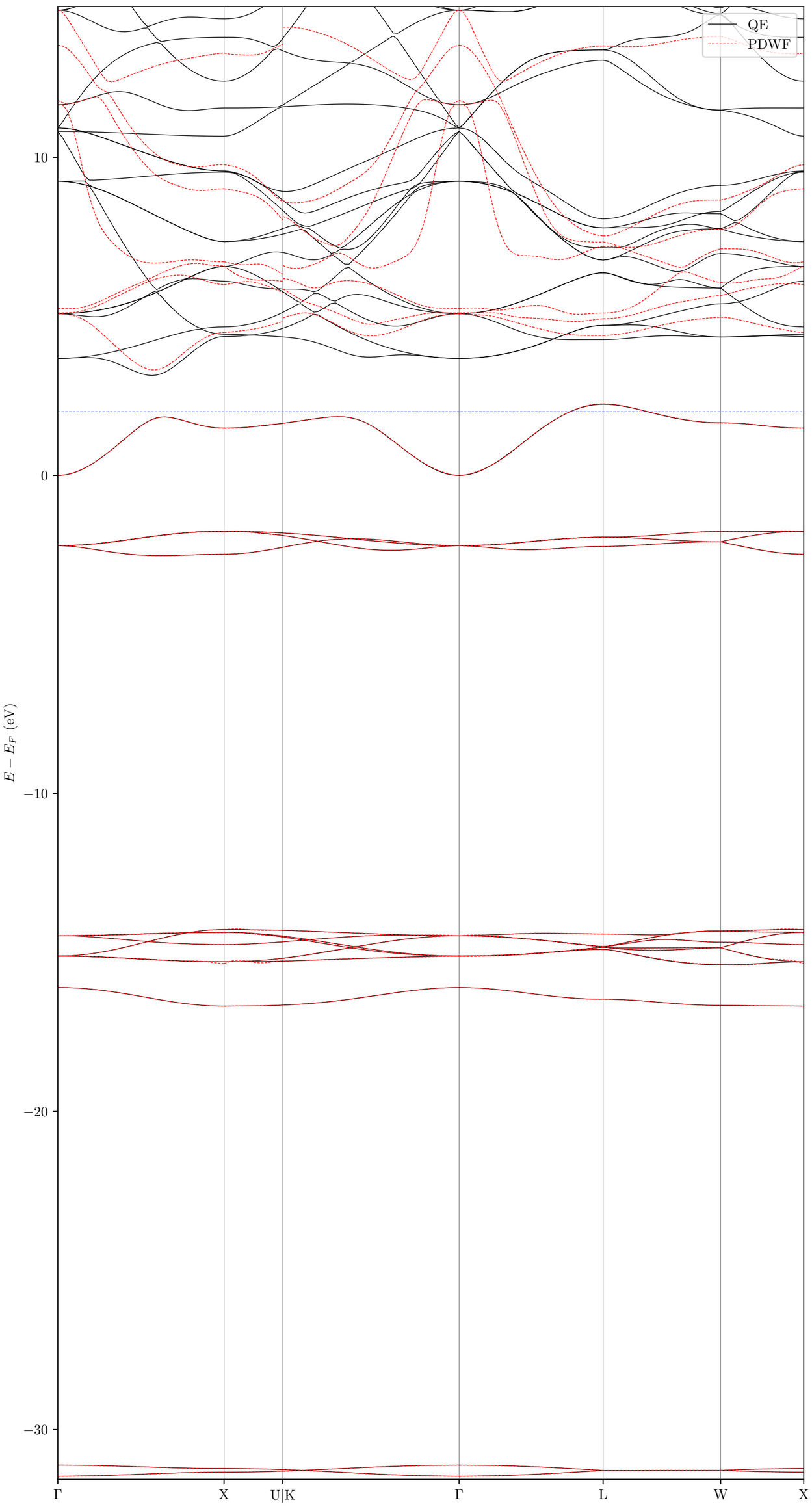

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.7 | 6.7 | 7.3 | 41.0 | 41.0 | 41.0 | 2.439 |

Hamiltonian decay



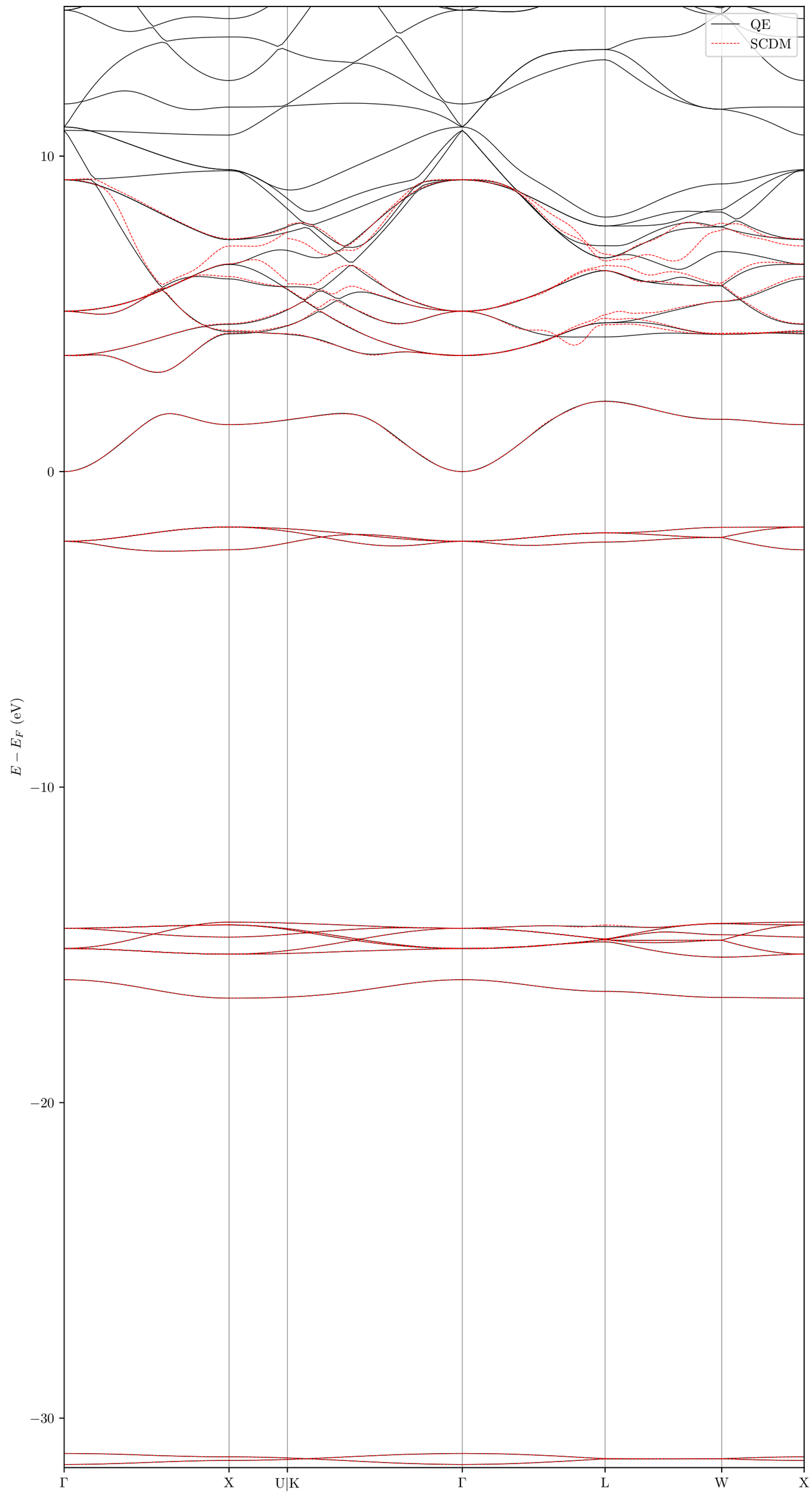
K2O **INCLUDE** semicore
PW=e366f2a4-4047-4b43-898b-2fdfe193ecbb
W90=a3296794-b739-4185-9c74-93982474832a




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.4 | 5.5 | 14.9 | 54.1 | 54.1 | 176.8 | 2.415 |

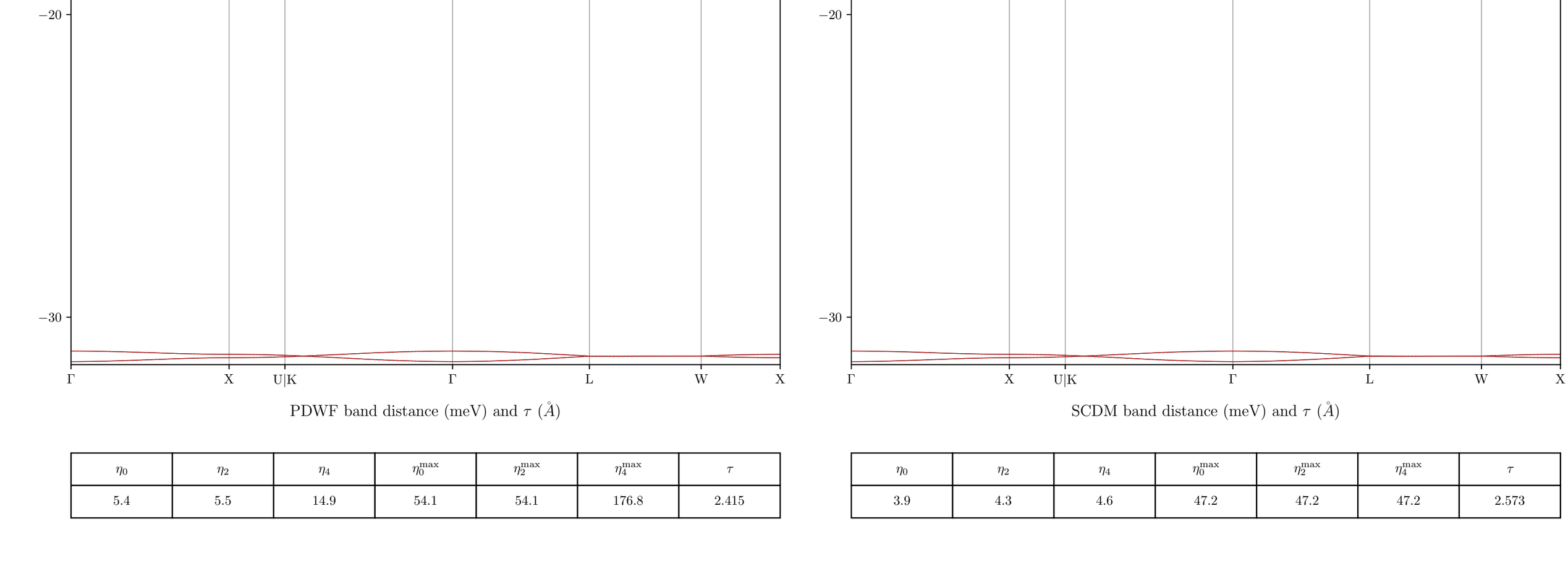
K2O **INCLUDE** semicore
PW=e366f2a4-4047-4b43-898b-2fdfe193ecbb
W90=a0c9447f-4ce3-4db0-ace1-39aaea119b3e



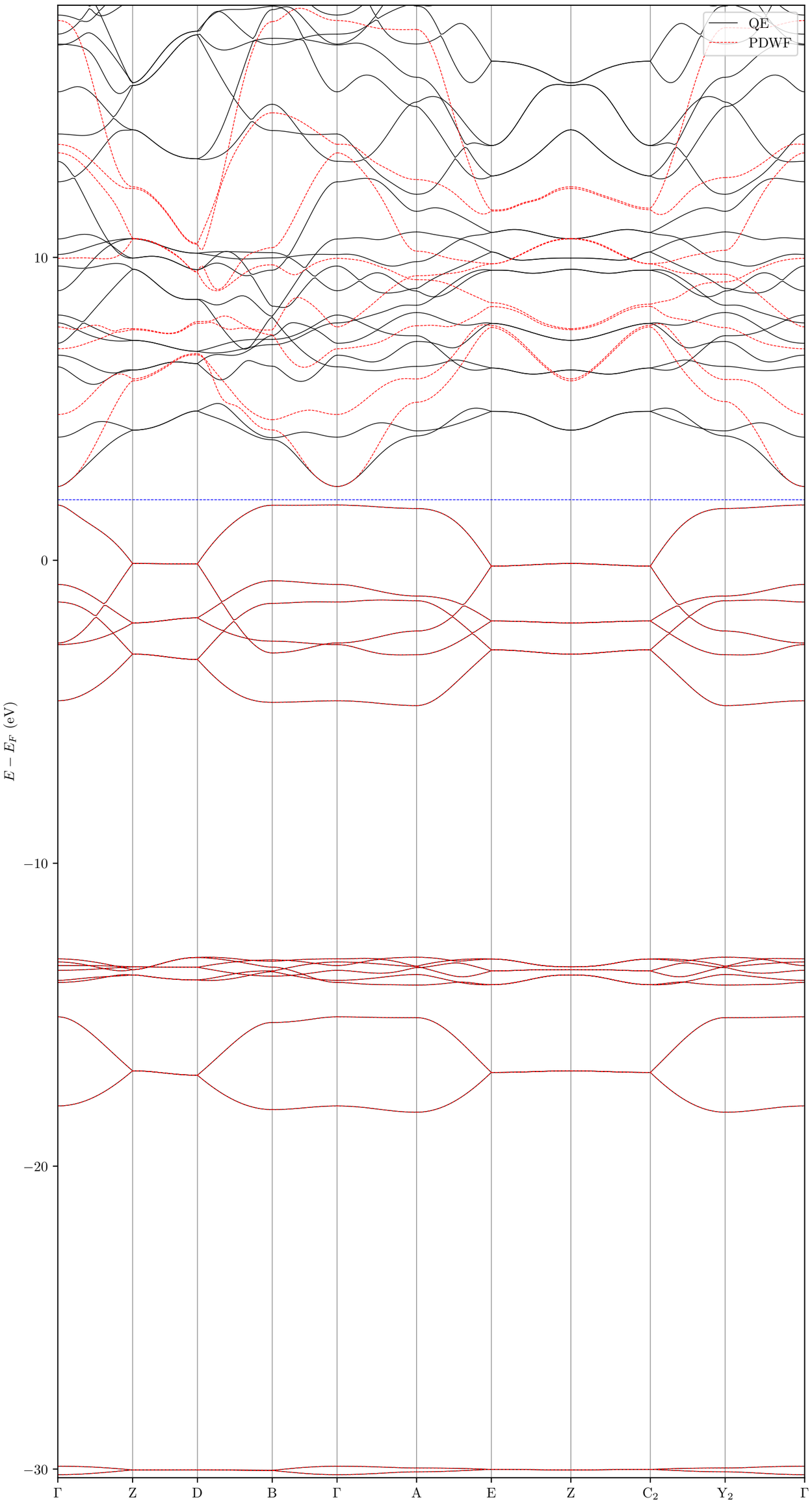

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.9 | 4.3 | 4.6 | 47.2 | 47.2 | 47.2 | 2.573 |

Hamiltonian decay



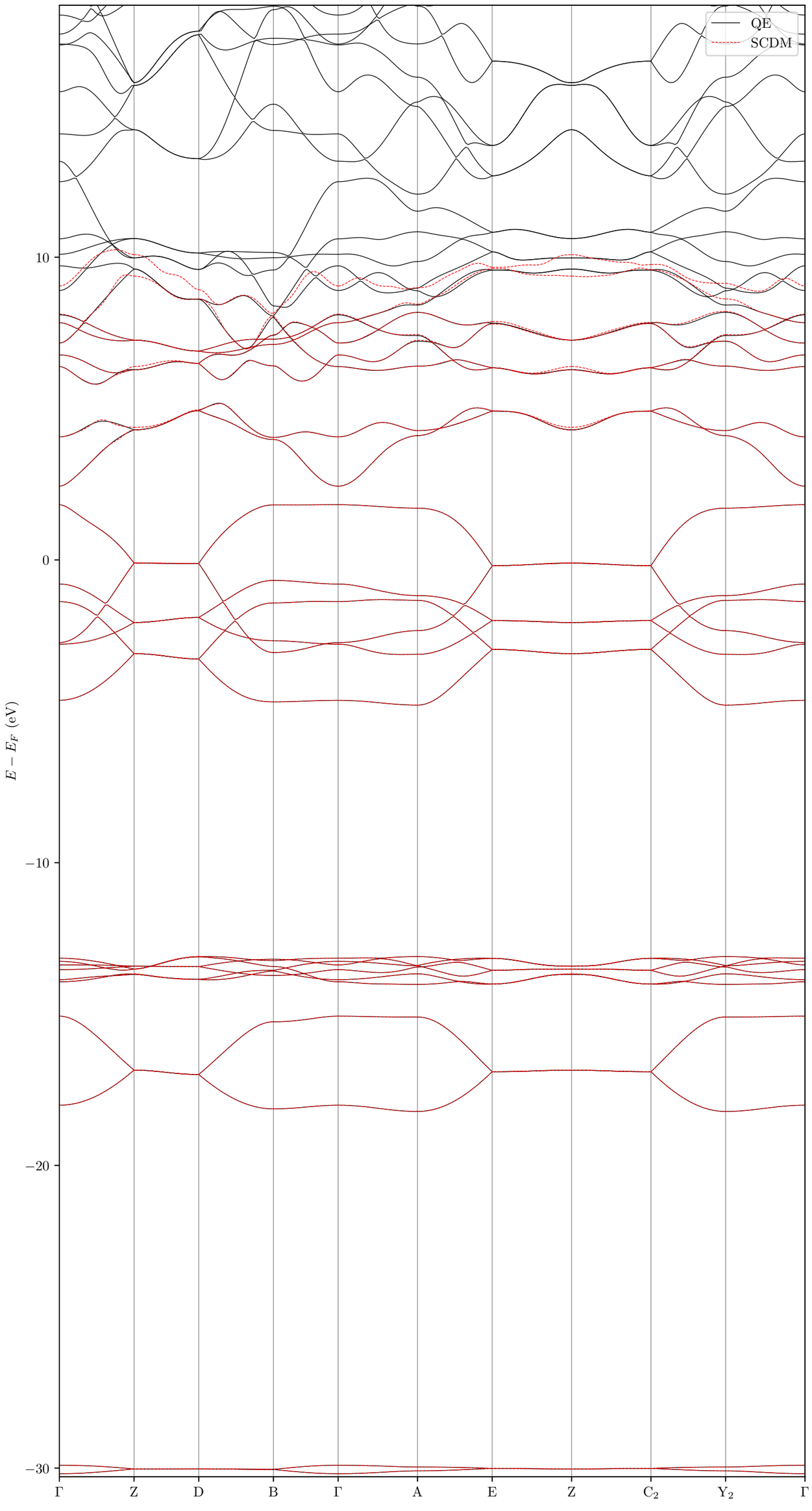
K2O2 **INCLUDE** semicore
PW=0be5eae4-e4c5-466e-bfc9-40a8fe932b36
W90=2bb89531-7ae1-4250-9dfc-3afc398f34e0




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.8 | 0.8 | 23.9 | 6.0 | 6.0 | 337.5 | 2.134 |

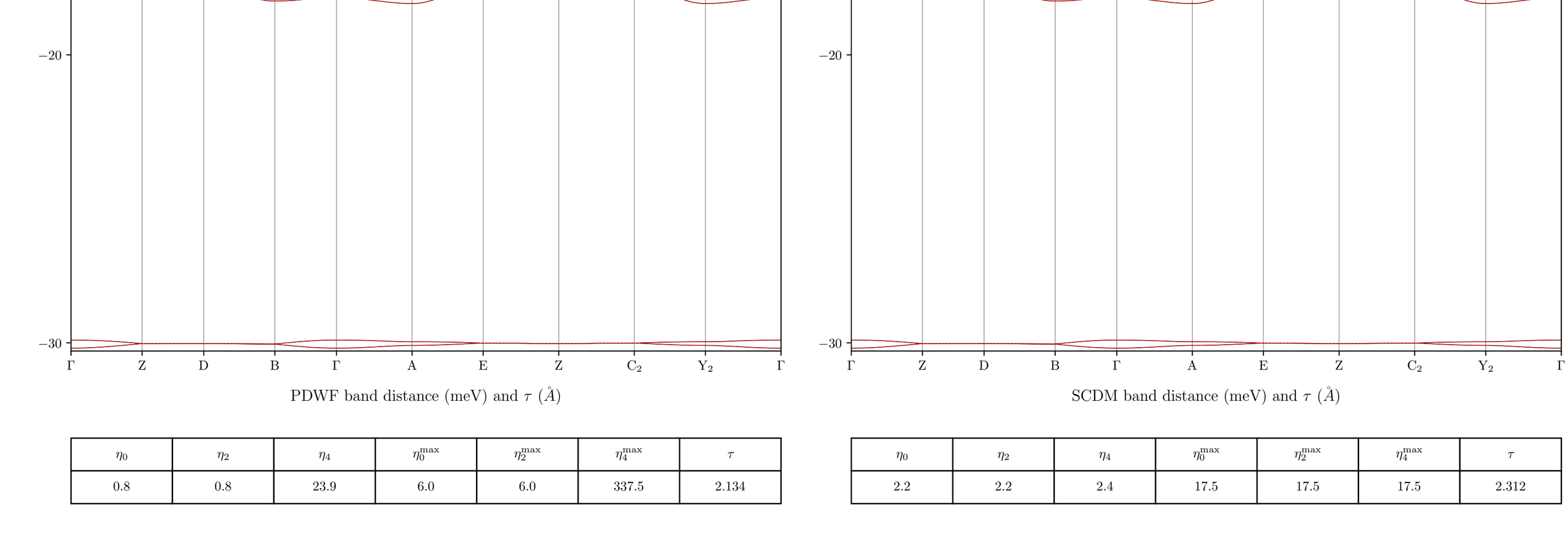
K2O2 **INCLUDE** semicore
PW=0be5eae4-e4c5-466e-bfc9-40a8fe932b36
W90=9feccd6a-7a7c-4078-802d-381ad7dbd99b

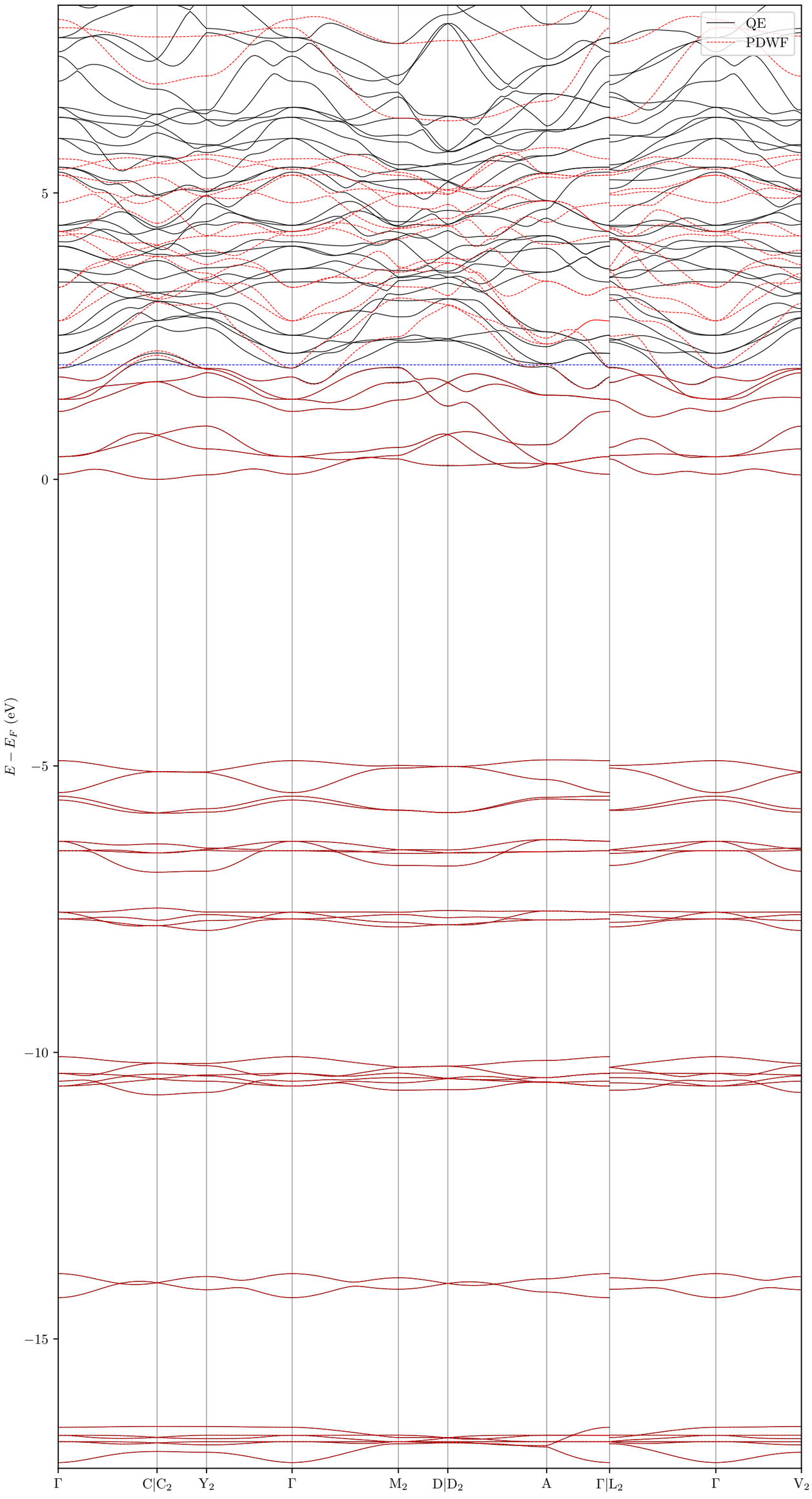



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.2 | 2.2 | 2.4 | 17.5 | 17.5 | 17.5 | 2.312 |

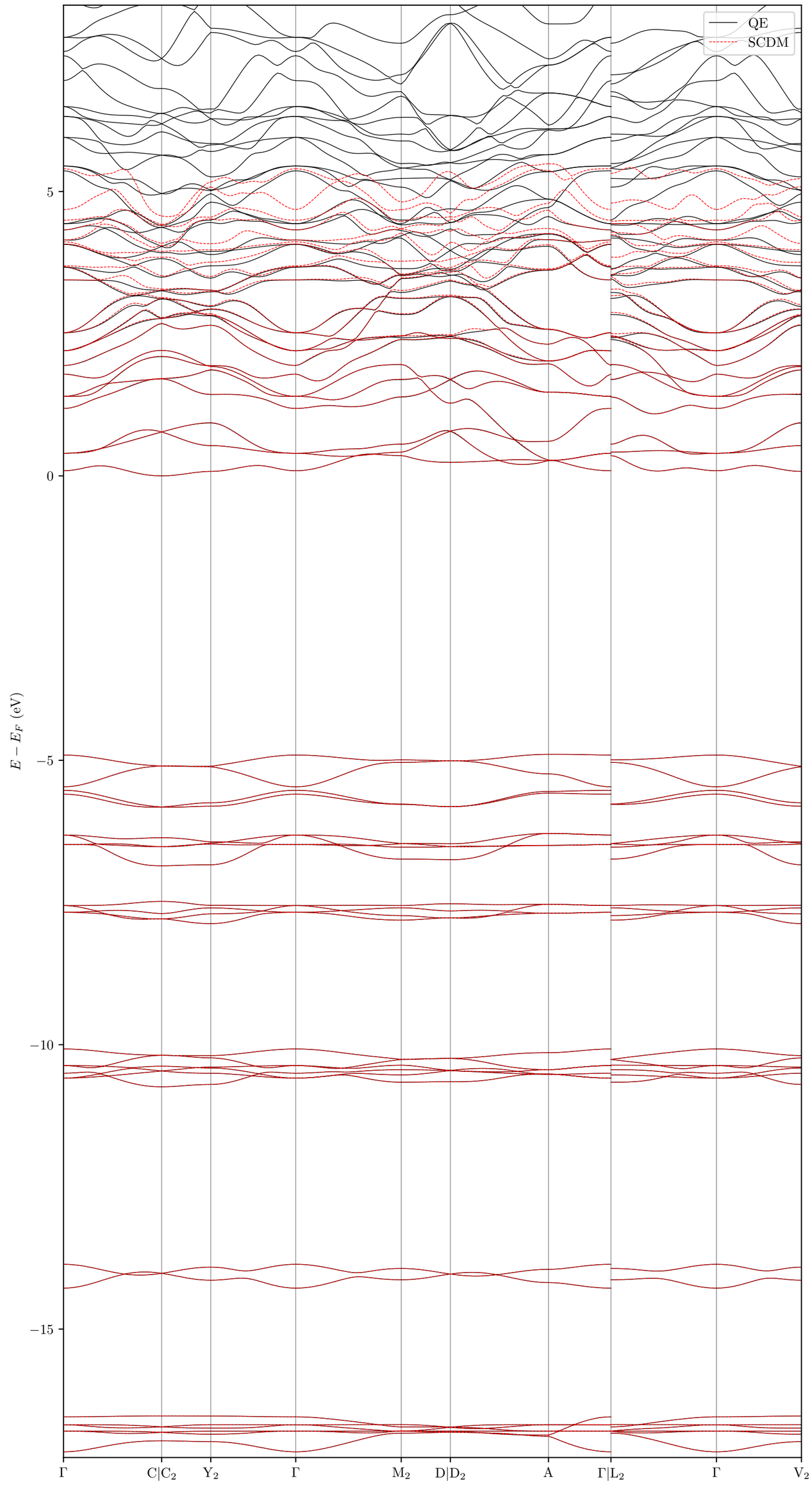
Hamiltonian decay





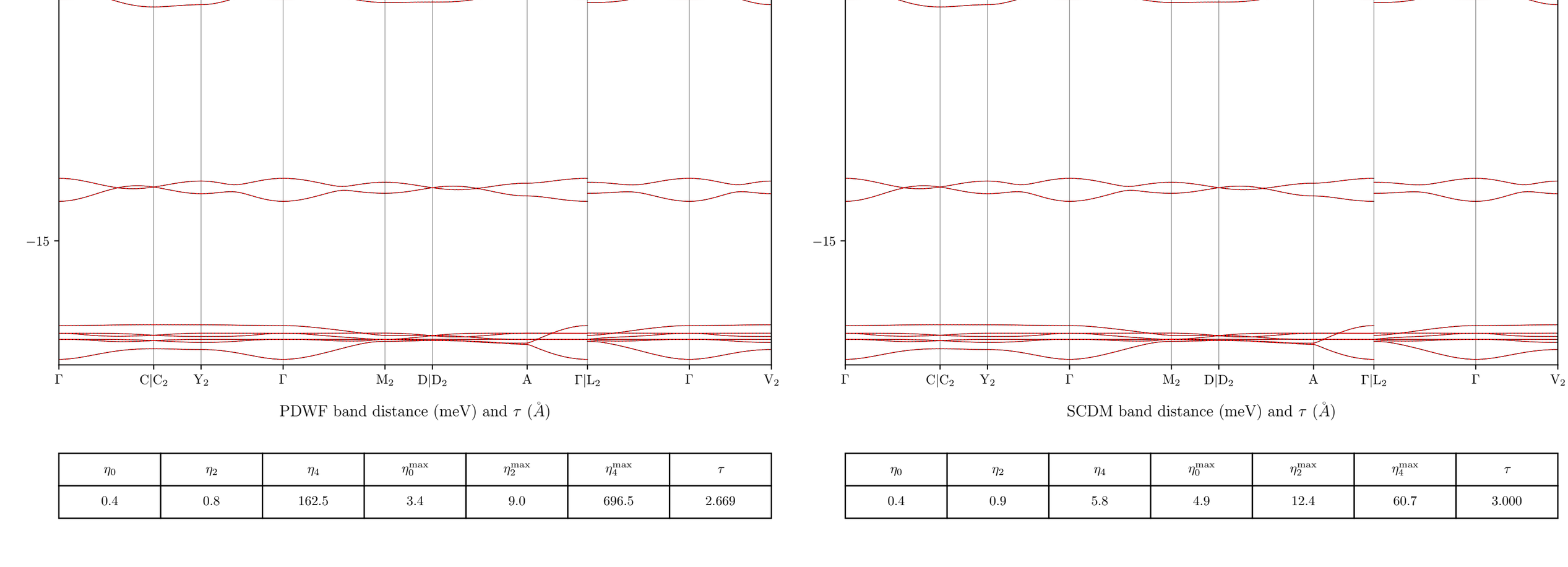

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

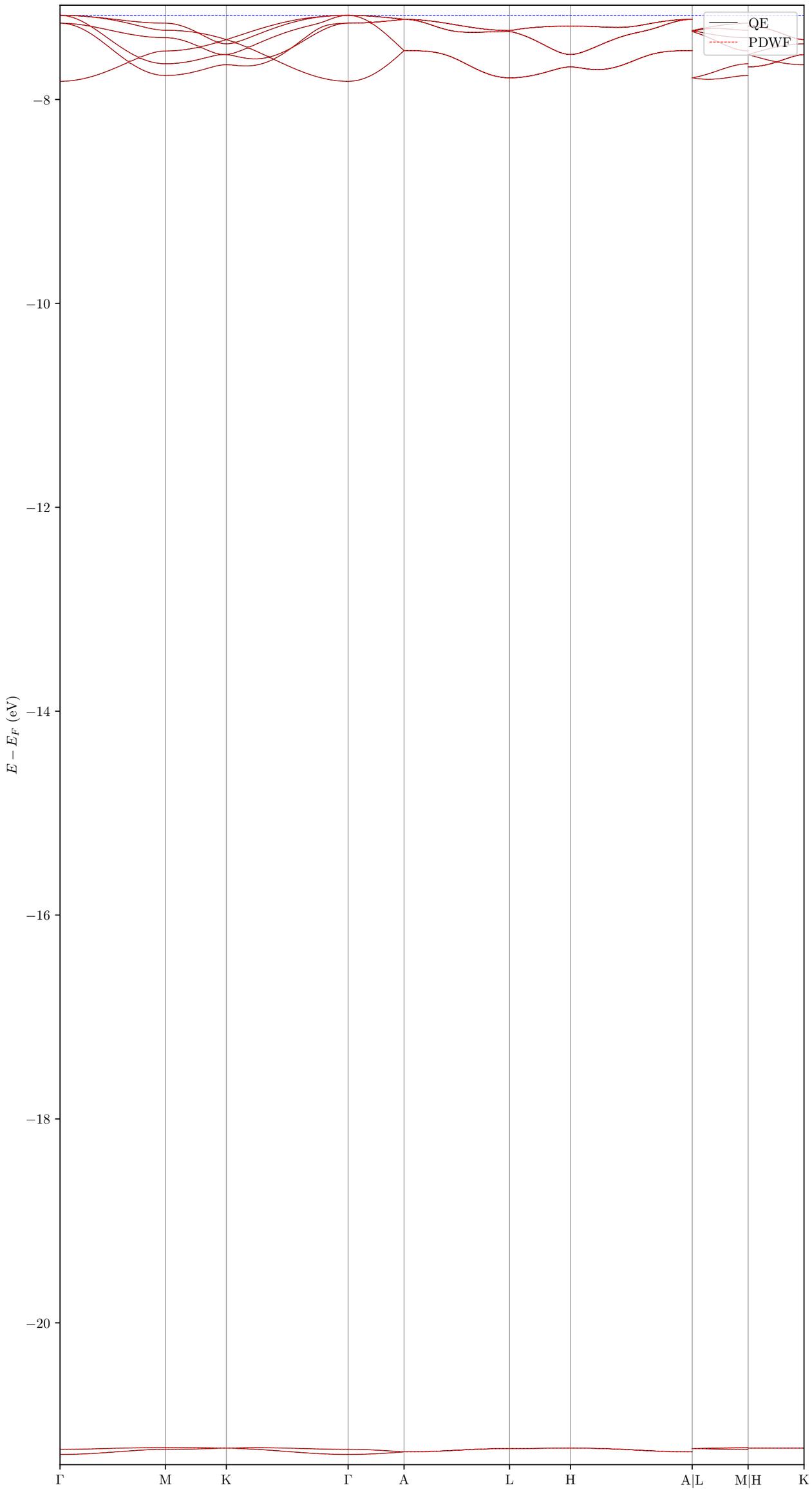
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.4 | 0.8 | 162.5 | 3.4 | 9.0 | 696.5 | 2.669 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

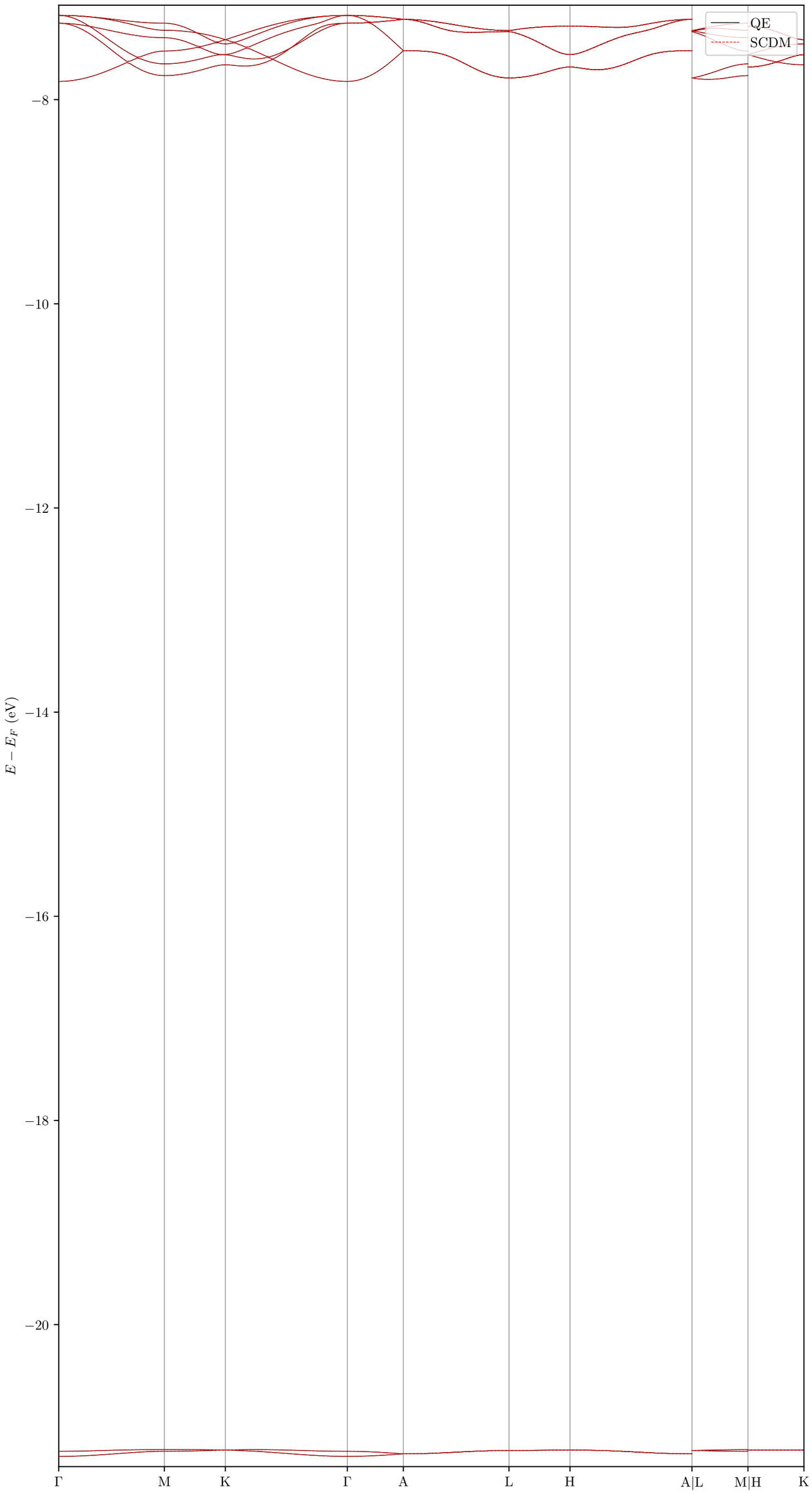
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.4 | 0.9 | 5.8 | 4.9 | 12.4 | 60.7 | 3.000 |





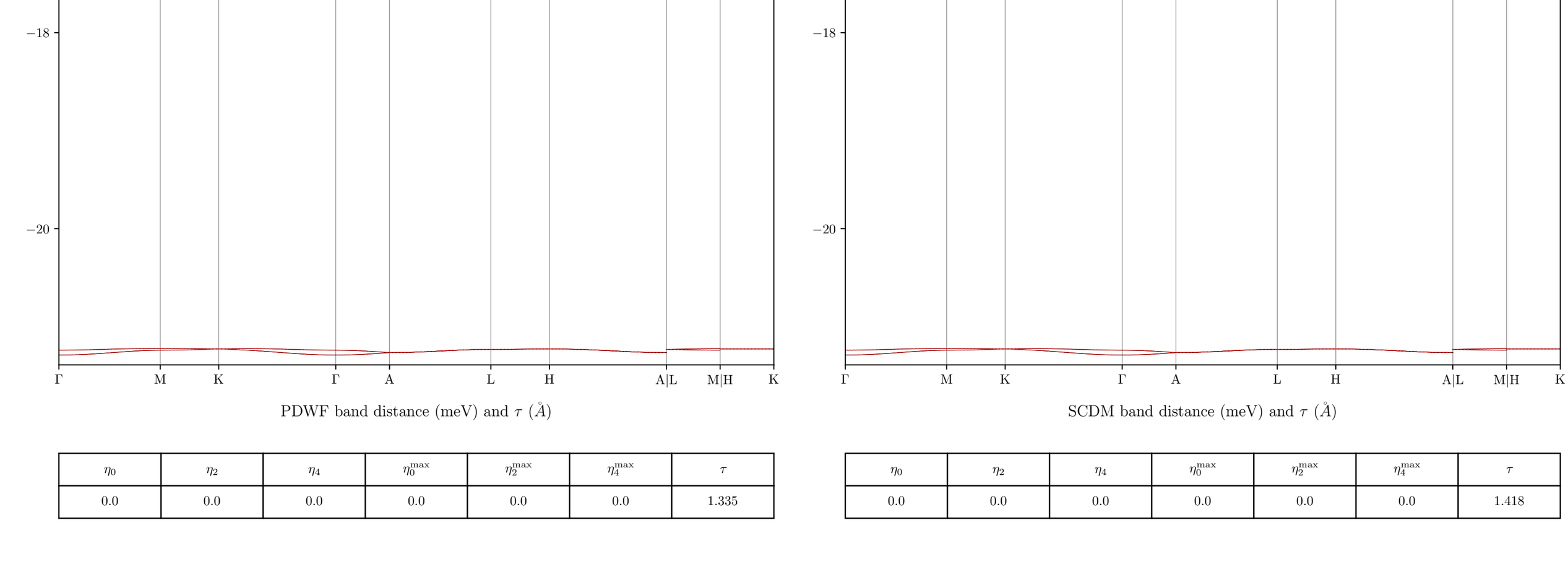

PDWF band distance (meV) and $\tau$ ($\AA$)

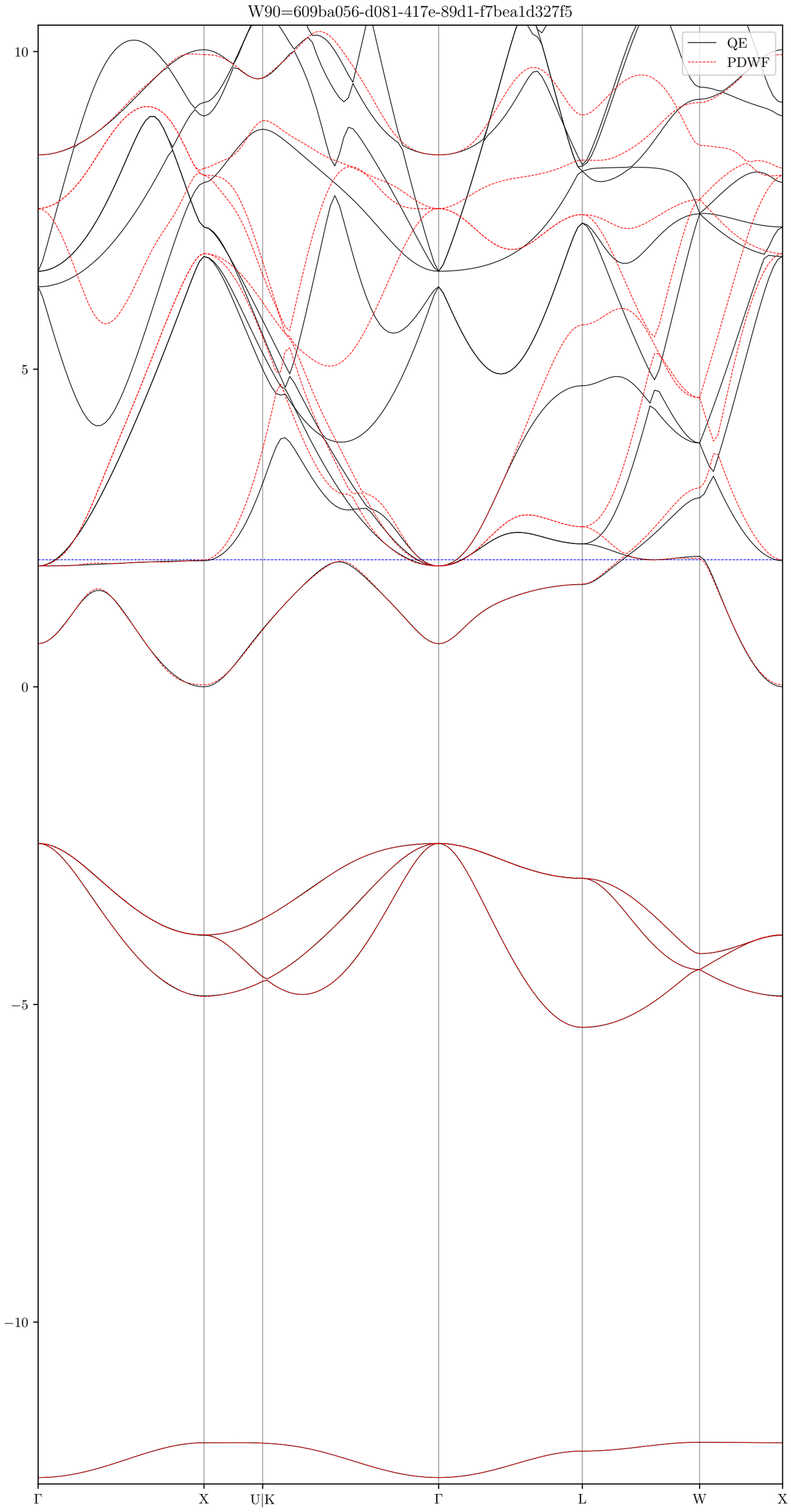
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 1.335 |




SCDM band distance (meV) and $\tau$ ($\AA$)

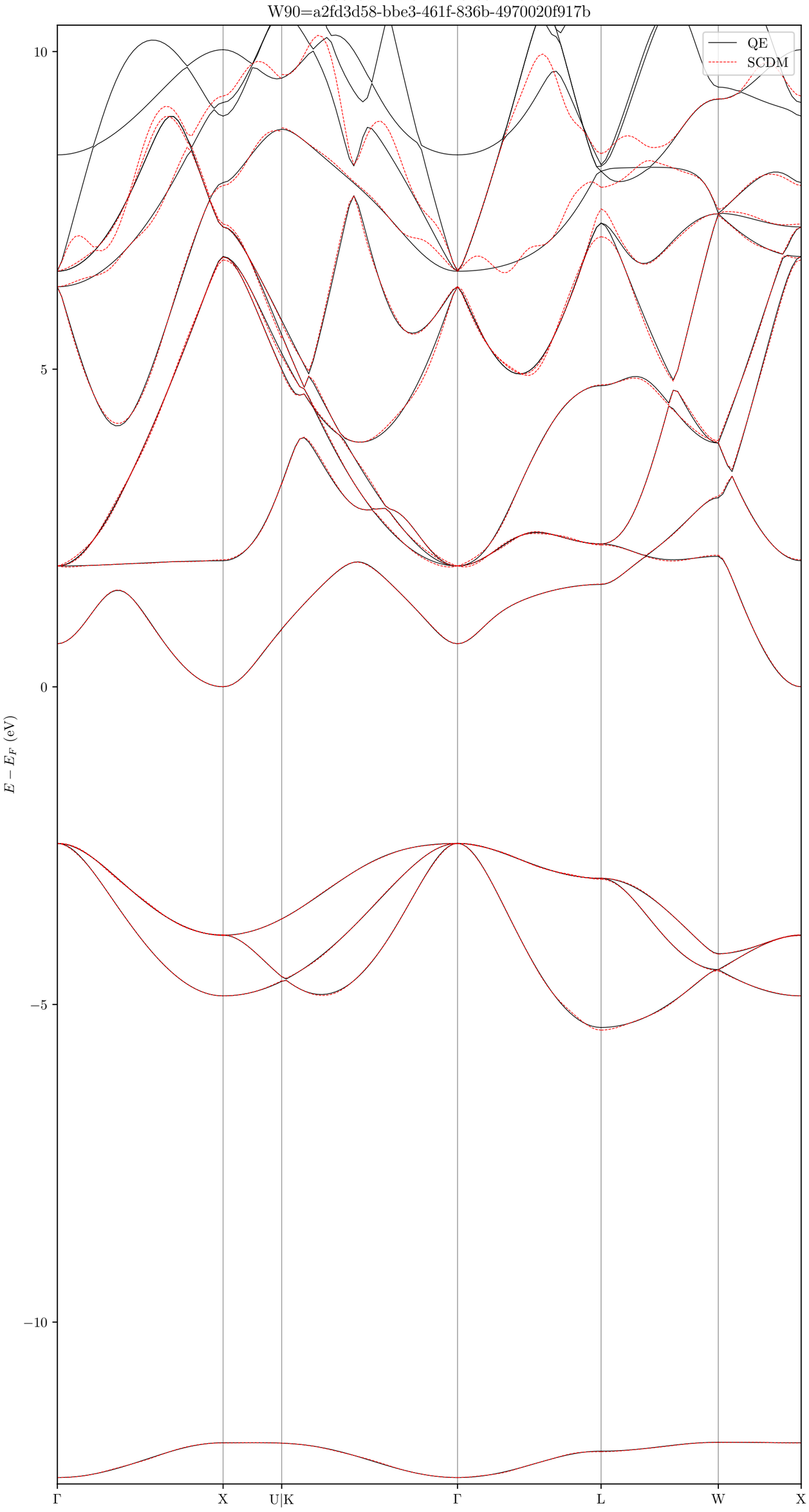
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 1.418 |





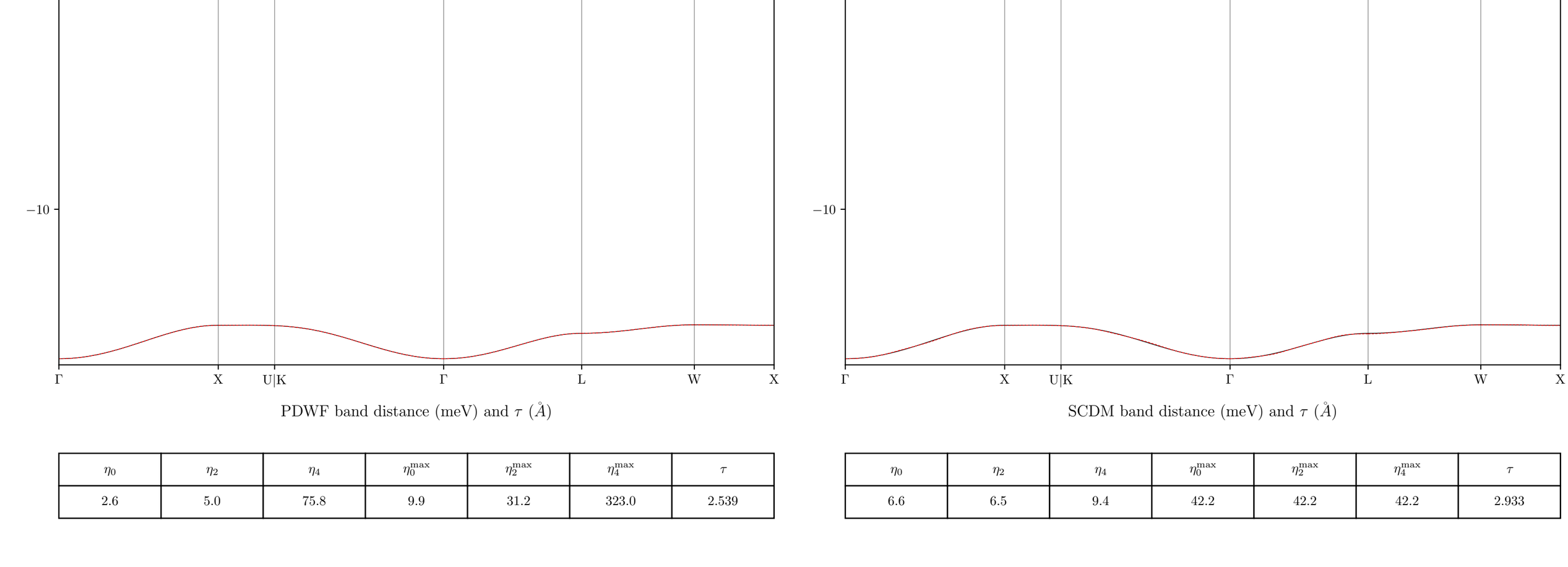

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.6 | 5.0 | 75.8 | 9.9 | 31.2 | 323.0 | 2.539 |

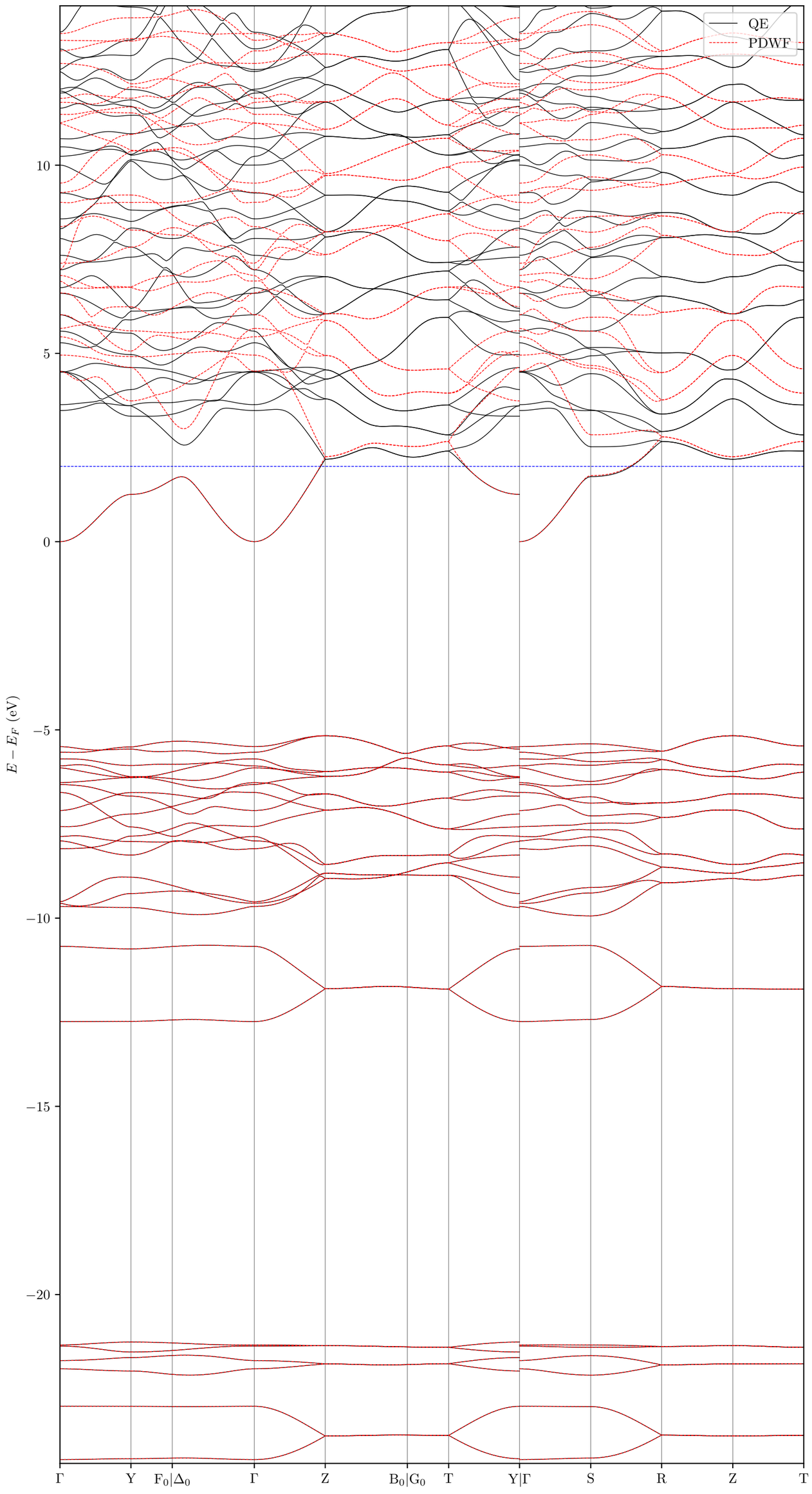



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.6 | 6.5 | 9.4 | 42.2 | 42.2 | 42.2 | 2.933 |



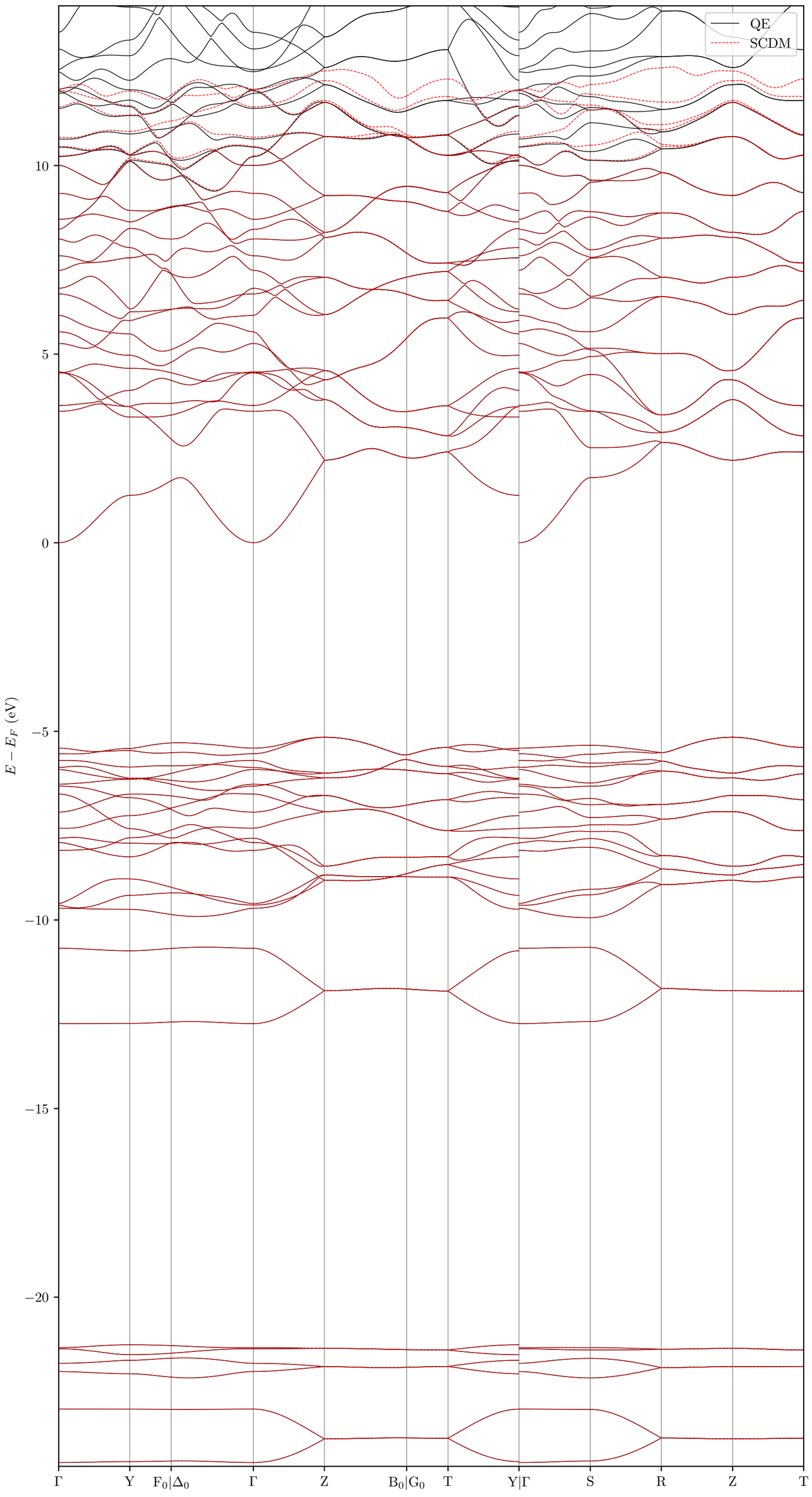
Li4O6Si2 exclude semicore
PW=a9640577-bdfc-4016-9f70-ffa311d3f244
W90=932ea85f-98b1-4018-b2cb-067a3dc8ae9a




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 0.8 | 62.7 | 5.3 | 11.8 | 655.6 | 2.300 |

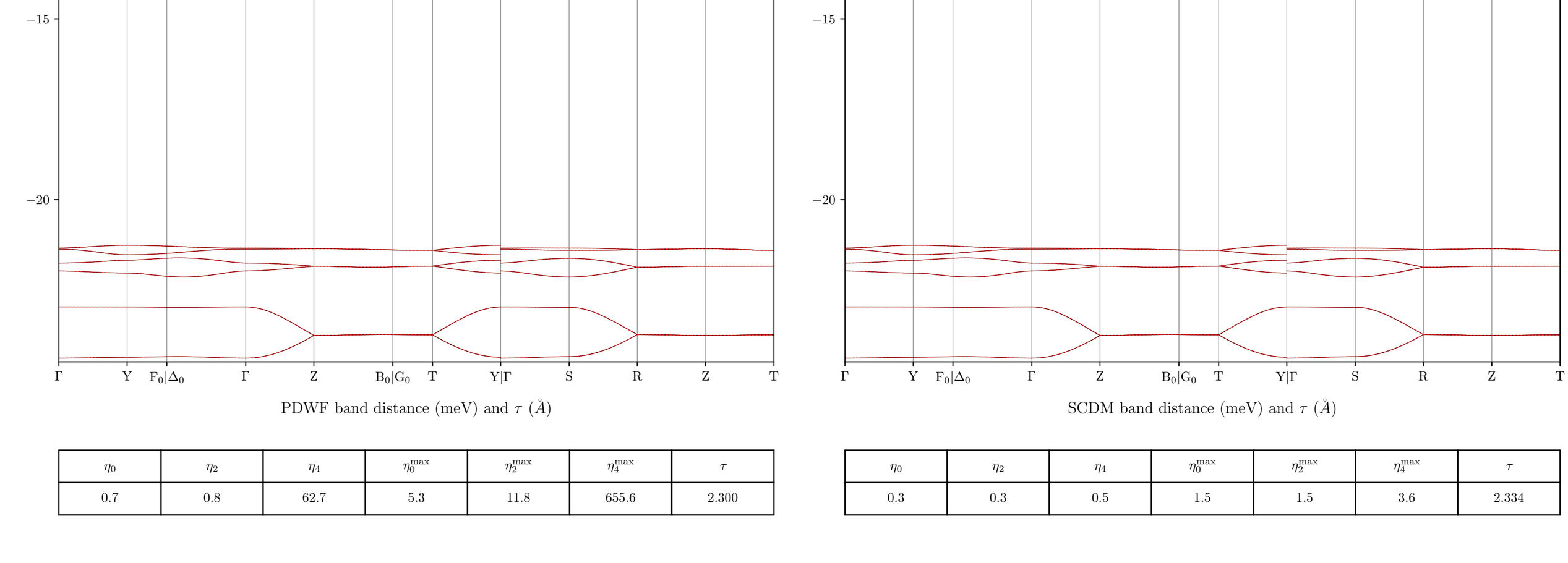
Li4O6Si2 exclude semicore
PW=a9640577-bdfc-4016-9f70-ffa311d3f244
W90=aaf395cd-4adb-468a-8dc9-3df69d3eef23



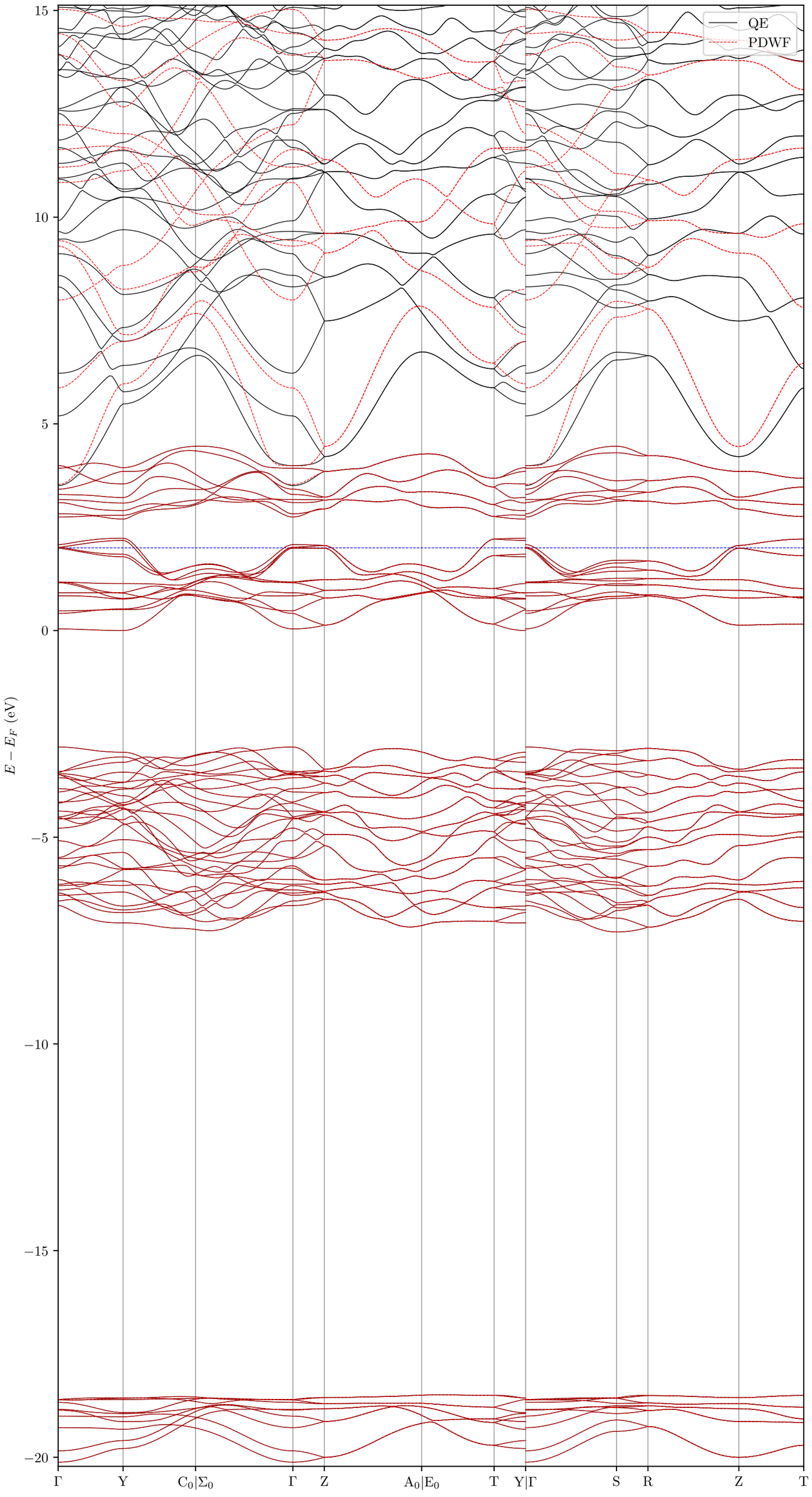

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.3 | 0.5 | 1.5 | 1.5 | 3.6 | 2.334 |

Hamiltonian decay



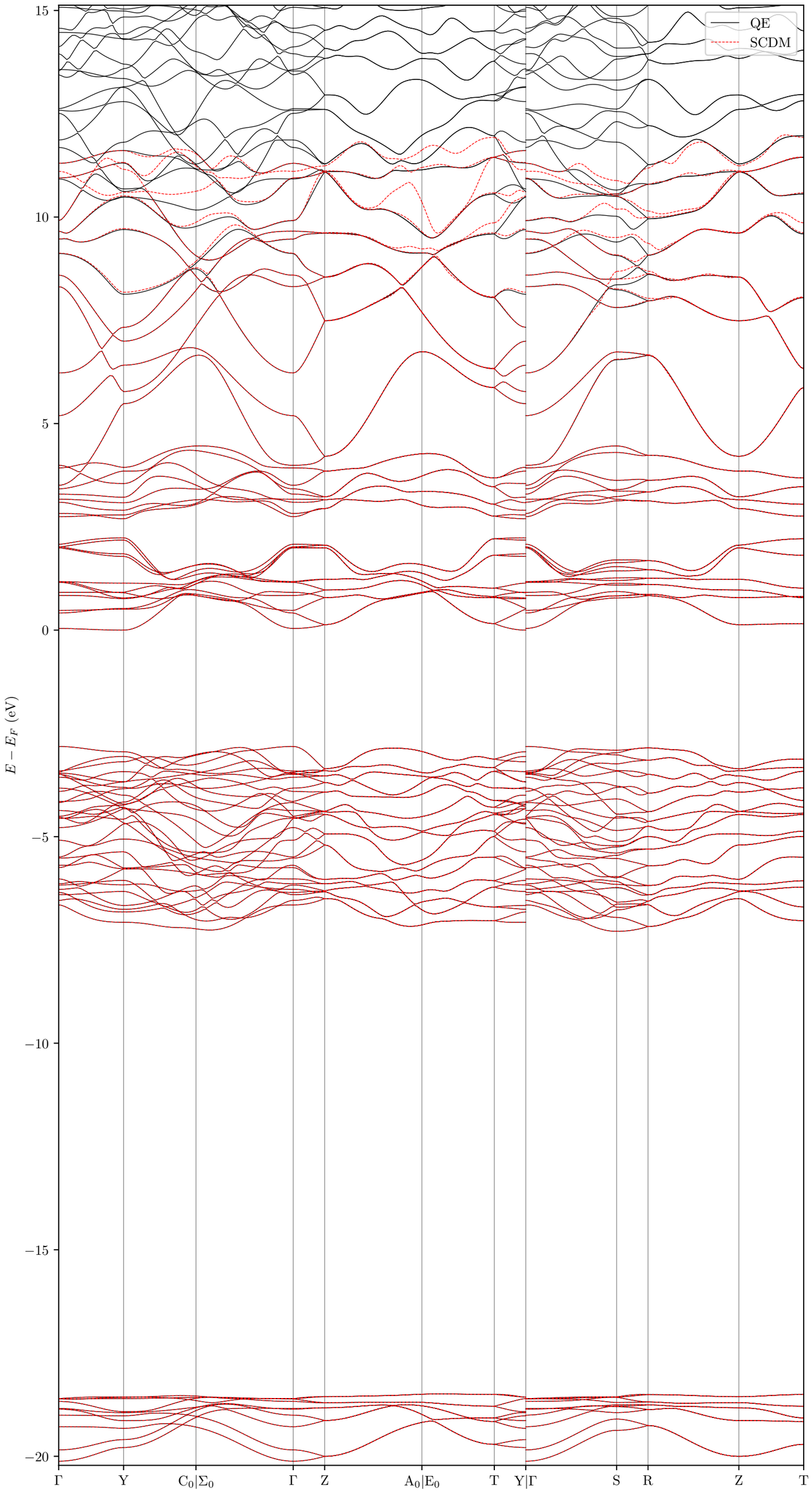
Mg2O10Ti4 exclude semicore
PW=da5a1e37-81d2-44ed-a899-4afbd43dff2f
W90=567269f5-8f97-44b0-bda2-8f7e0f0cd521




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.1 | 0.2 | 1.8 | 1.8 | 4.2 | 2.422 |

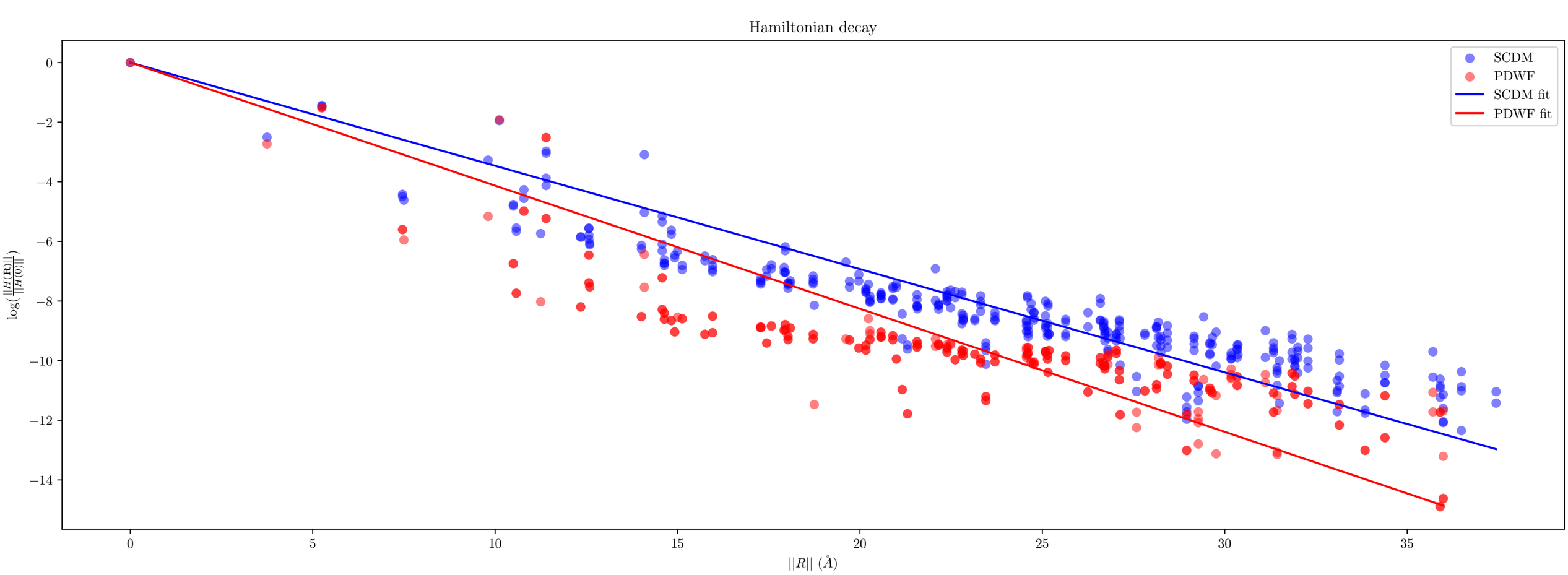
Mg2O10Ti4 exclude semicore
PW=da5a1e37-81d2-44ed-a899-4afbd43dff2f
W90=072c622a-bcd1-48b2-9352-bb029db1a052



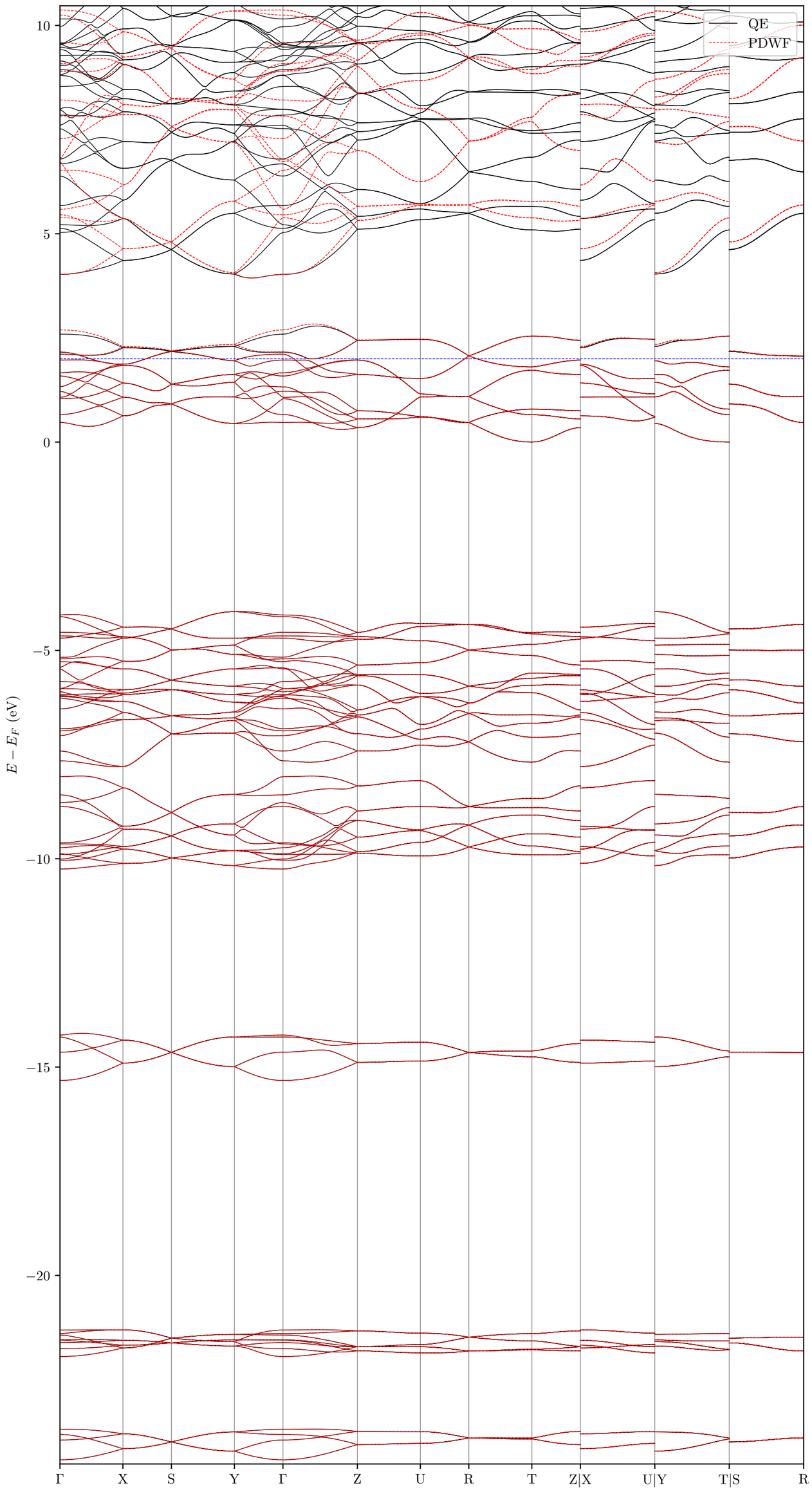

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 0.5 | 10.4 | 10.4 | 10.4 | 2.887 |

Hamiltonian decay



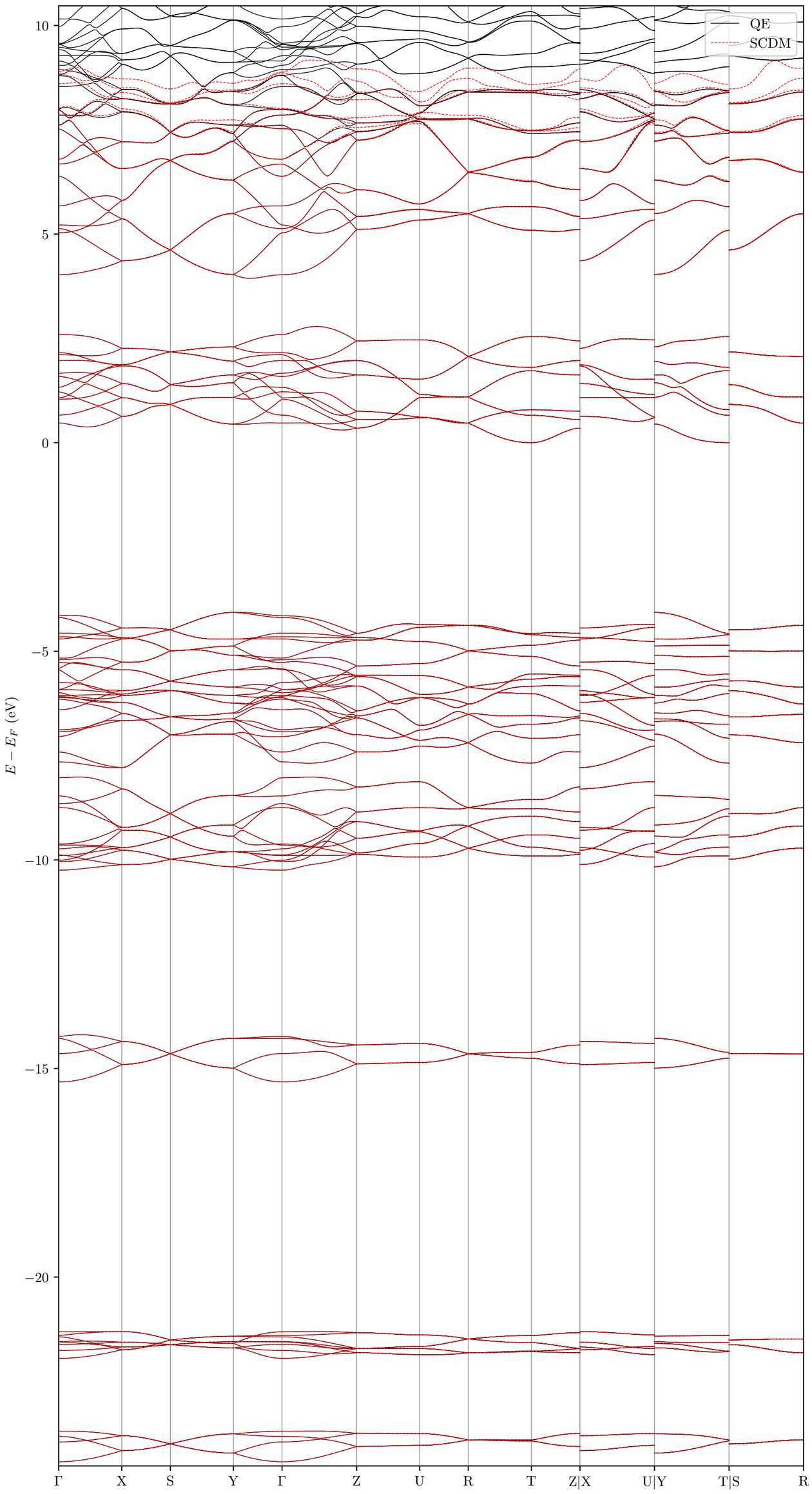
Mg4O12Se4 exclude semicore
PW=e89ad87d-1331-4513-9aff-04b14649c941
W90=46aa381a-d4e6-4cc2-82d6-c2a1f30078a9




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.1 | 0.1 | 0.9 | 1.3 | 1.3 | 5.5 | 2.396 |

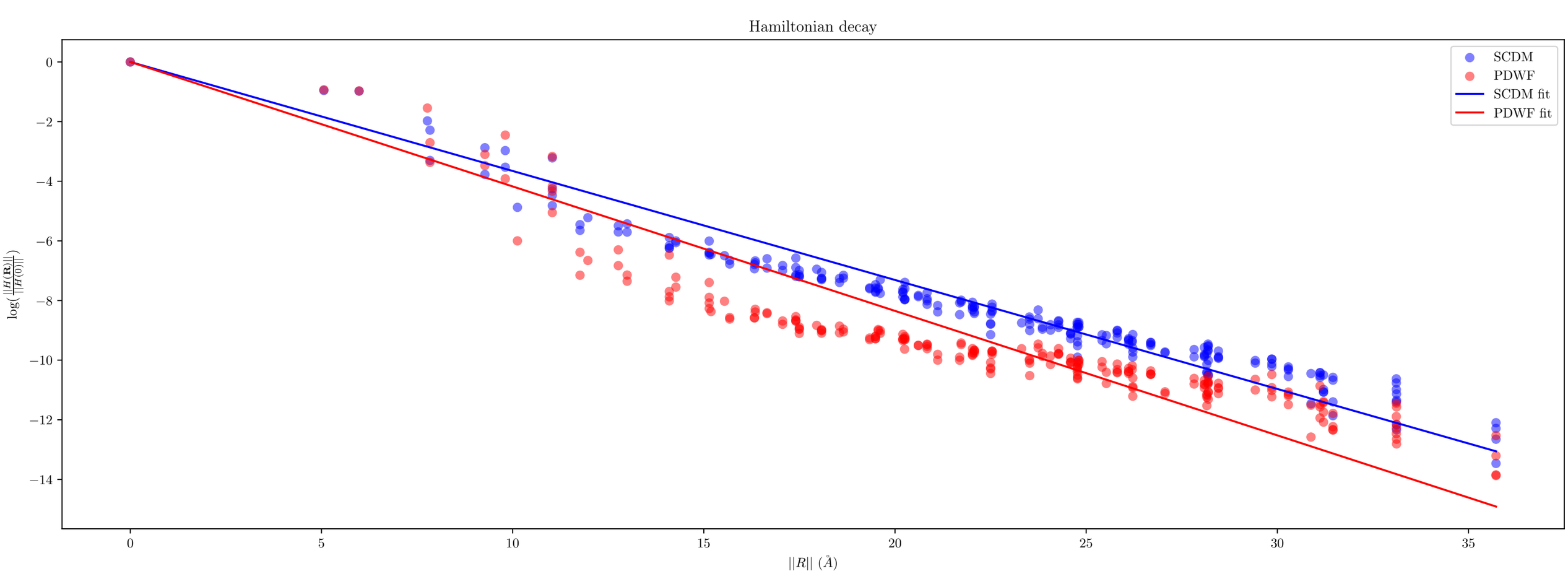
Mg4O12Se4 exclude semicore
PW=e89ad87d-1331-4513-9aff-04b14649c941
W90=b97a285c-1c24-44fe-af45-ecfb666639f5

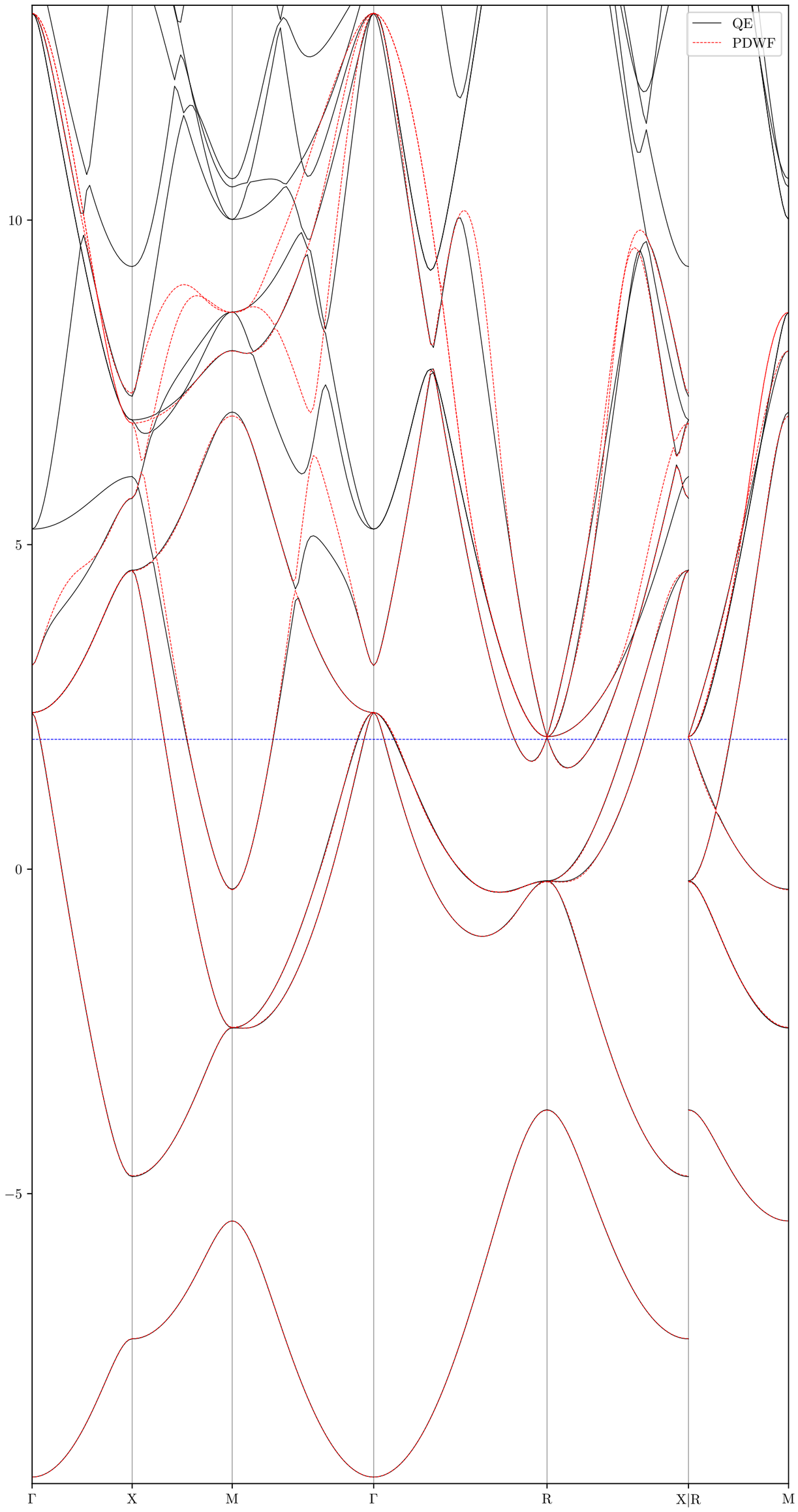



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 0.7 | 5.9 | 5.9 | 6.0 | 2.736 |

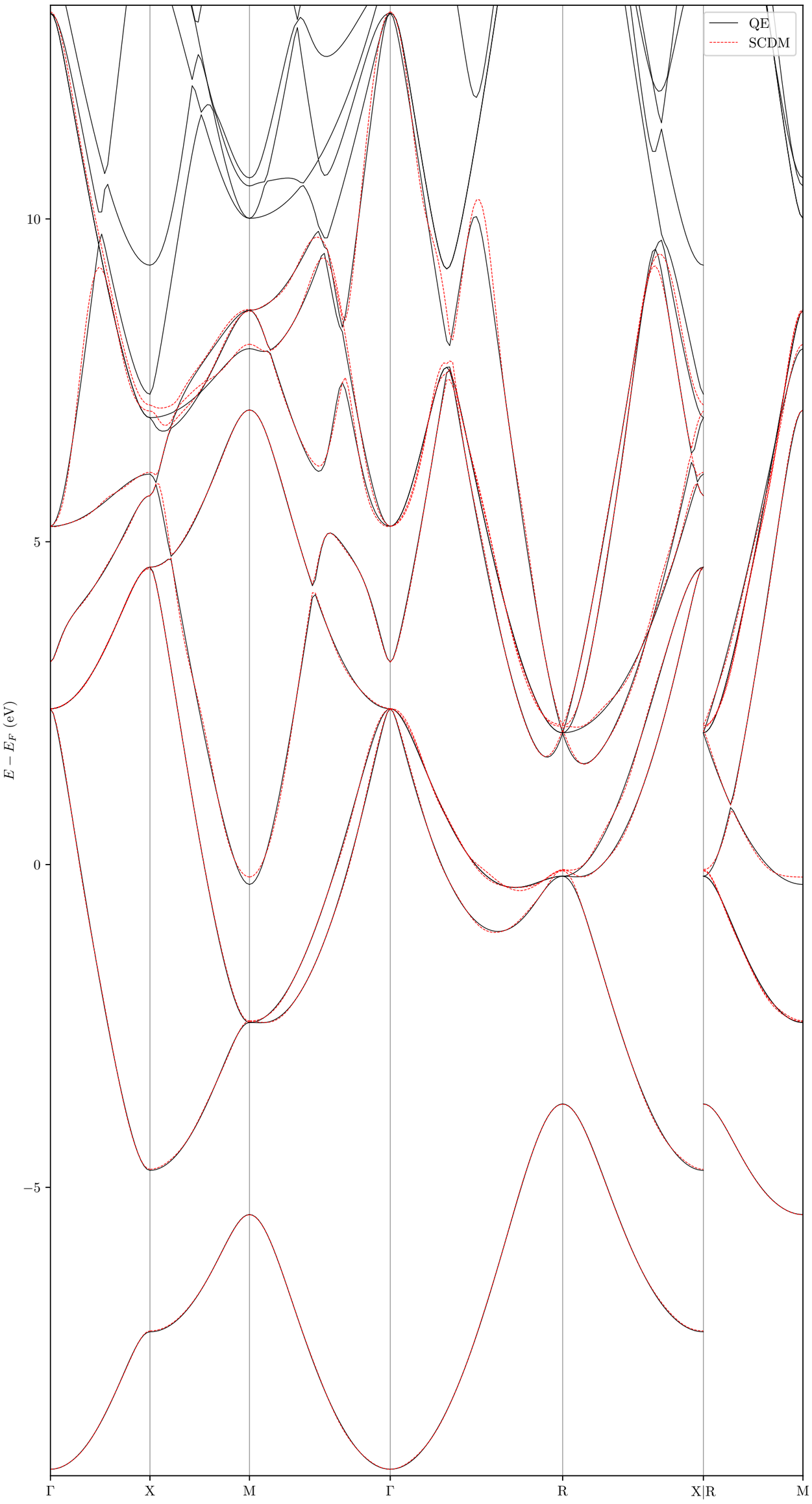
Hamiltonian decay





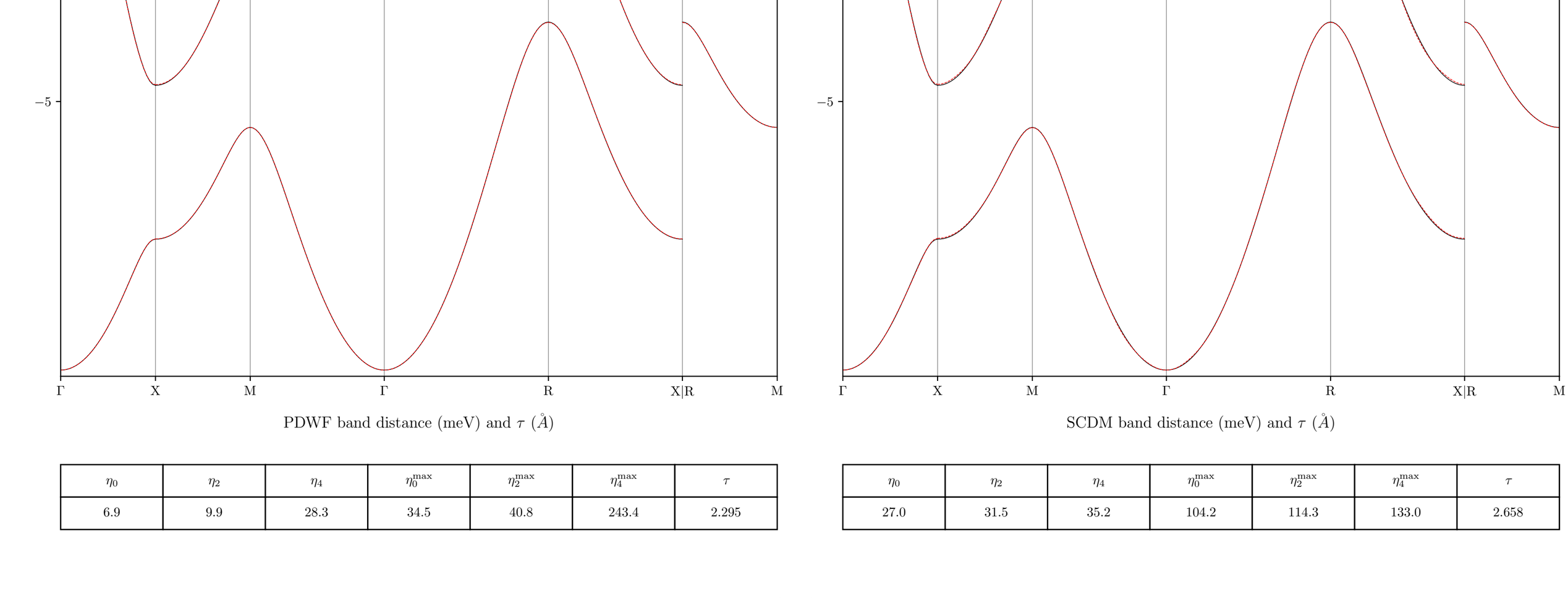

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

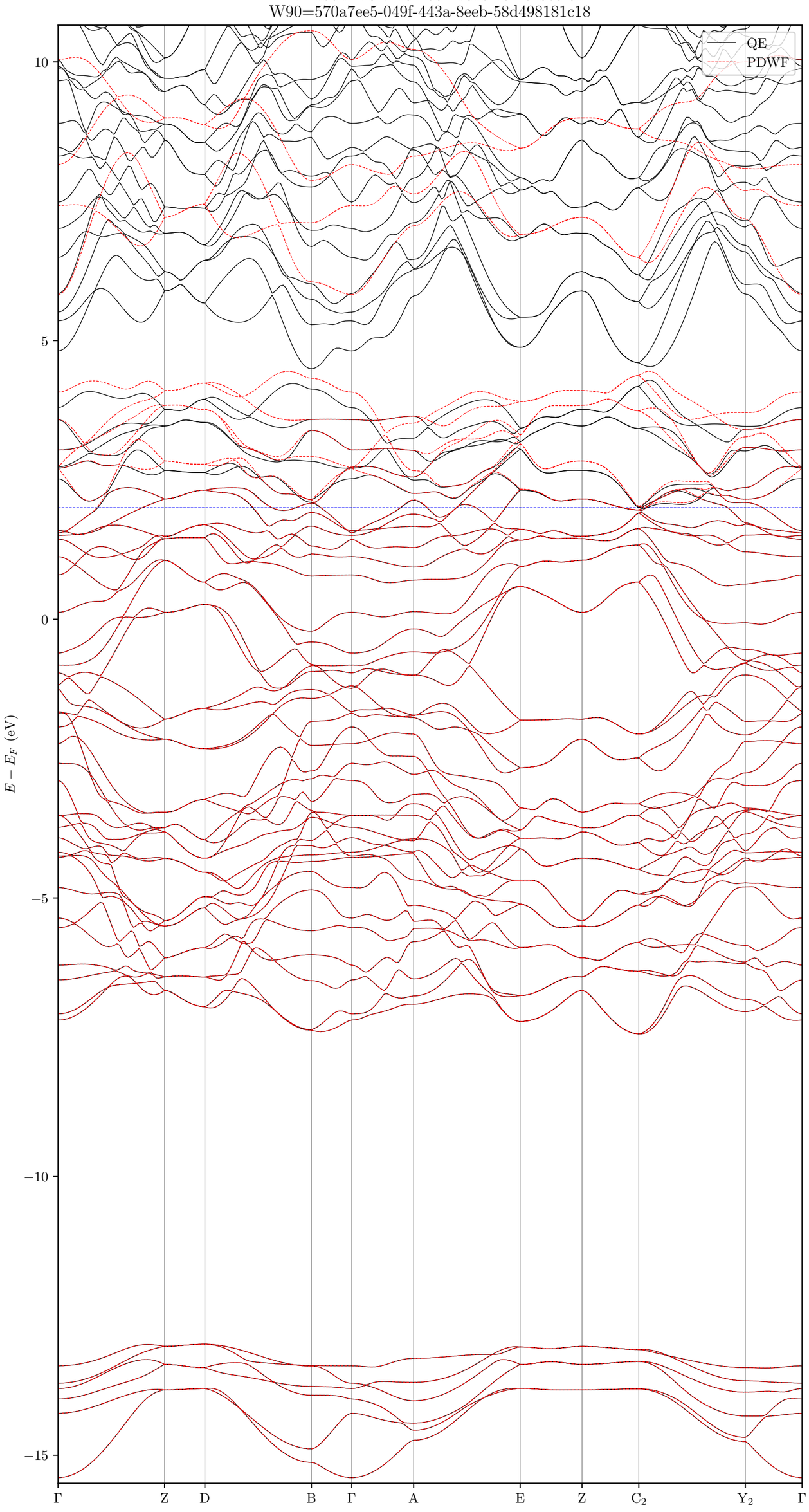
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.9 | 9.9 | 28.3 | 34.5 | 40.8 | 243.4 | 2.295 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

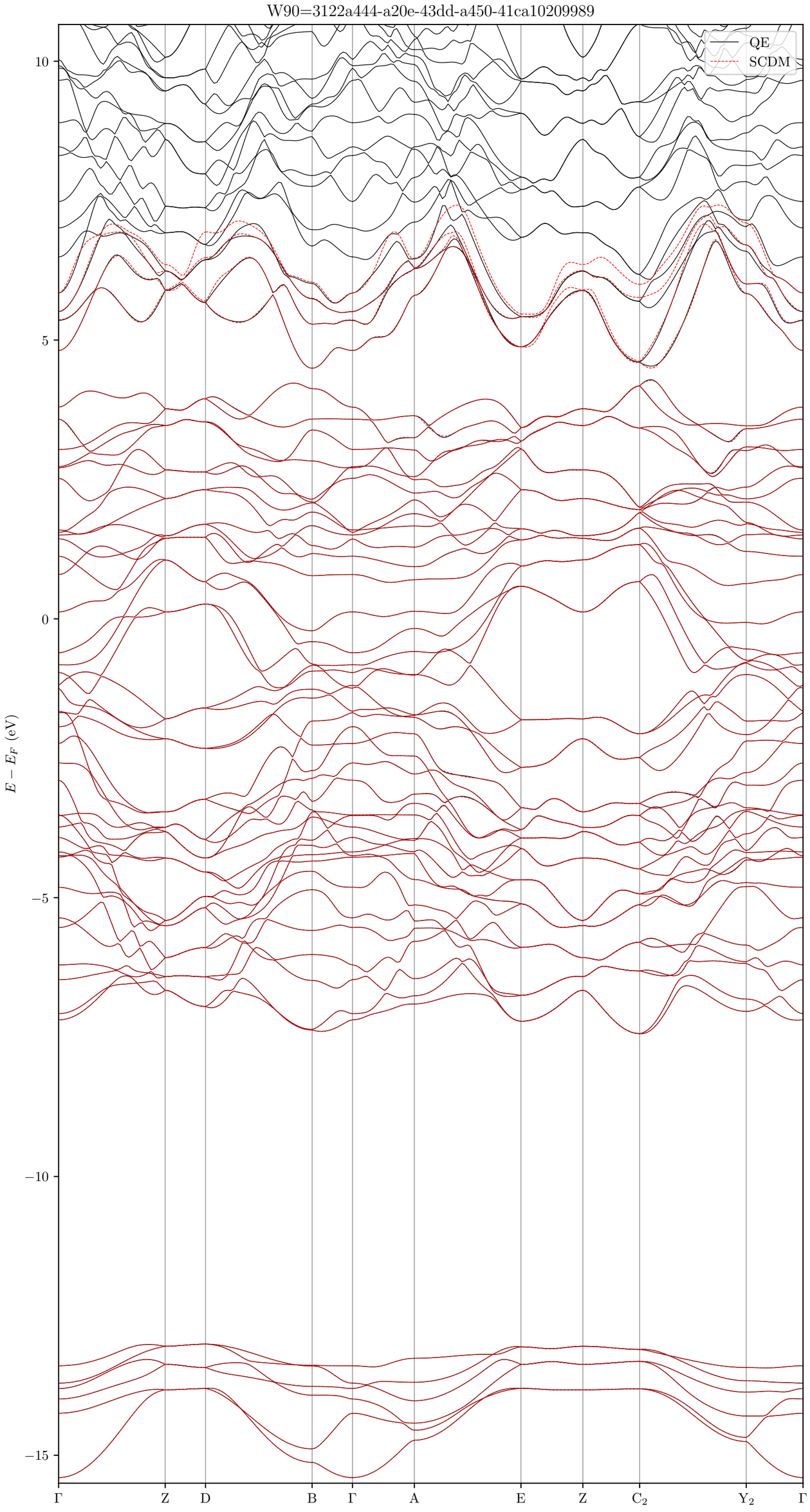
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 27.0 | 31.5 | 35.2 | 104.2 | 114.3 | 133.0 | 2.658 |





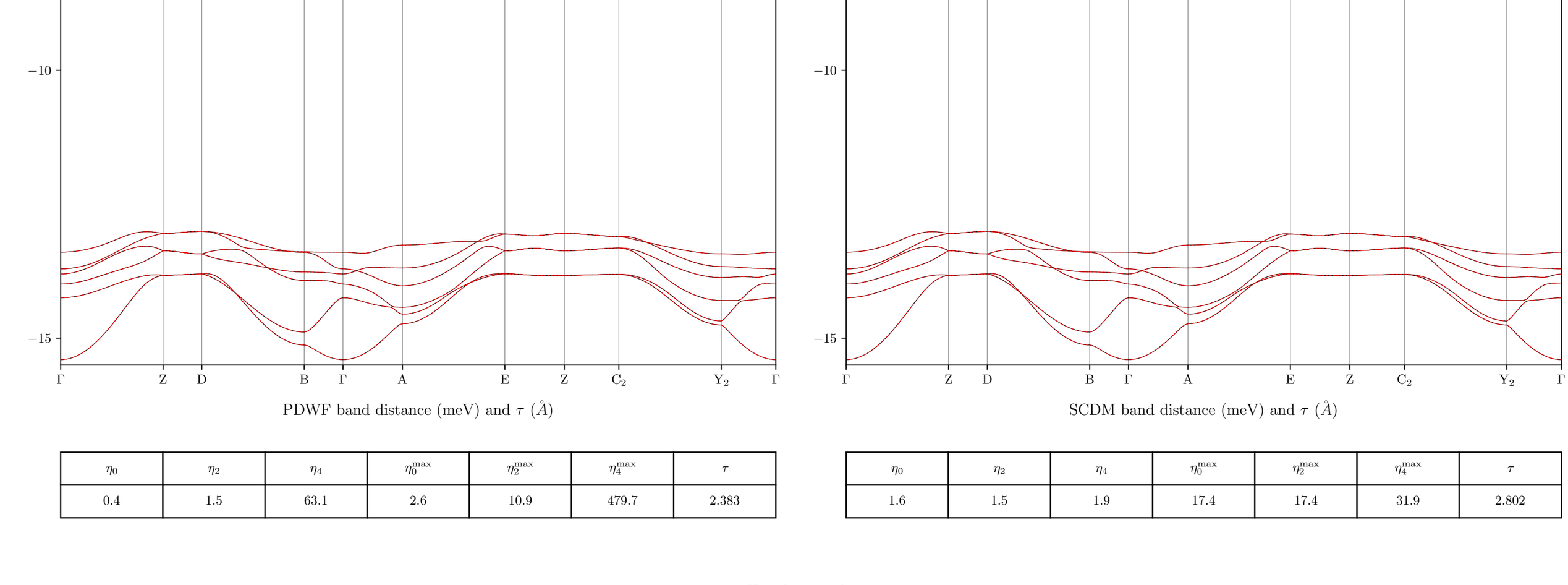

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

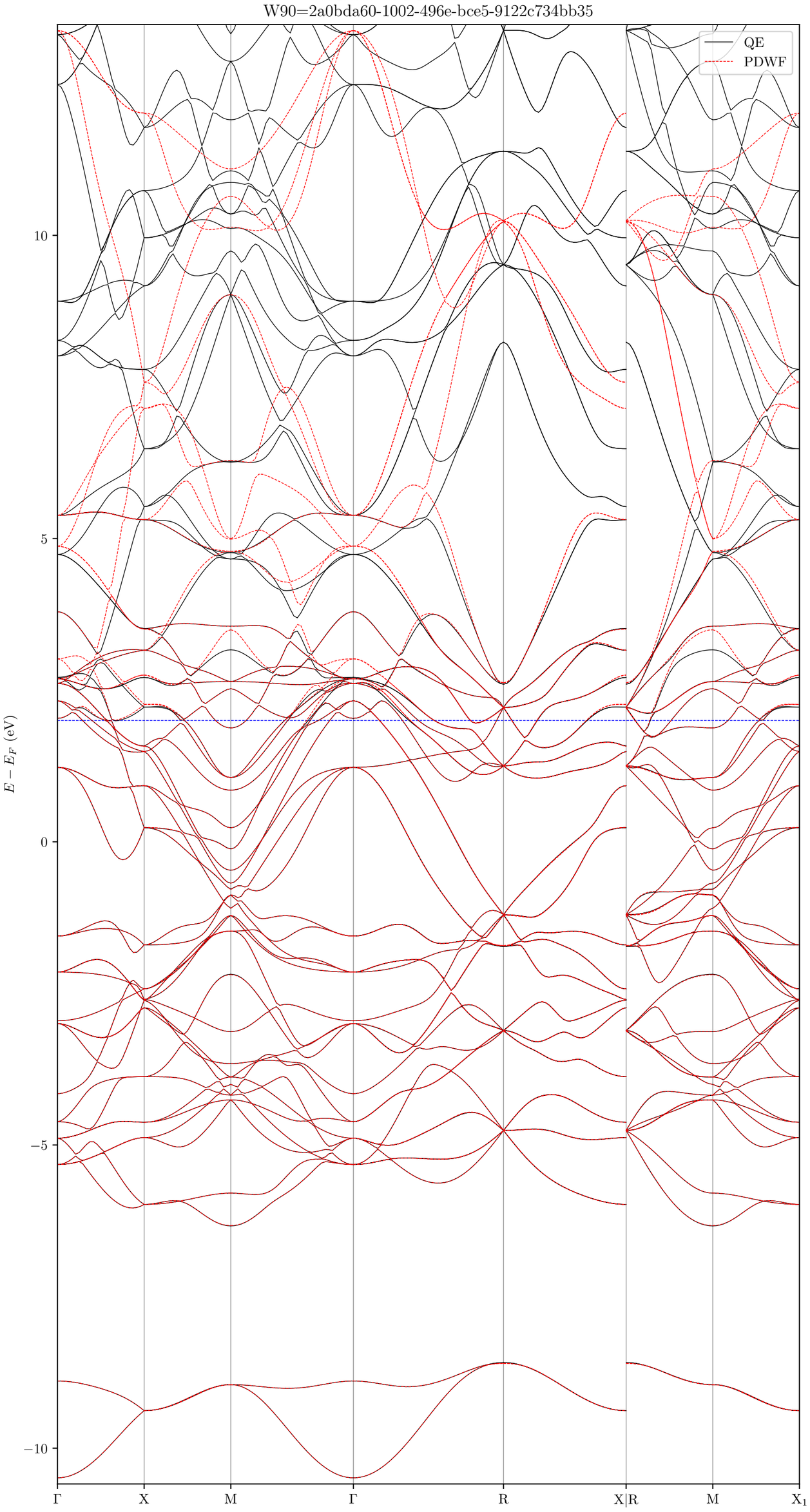
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.4 | 1.5 | 63.1 | 2.6 | 10.9 | 479.7 | 2.383 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

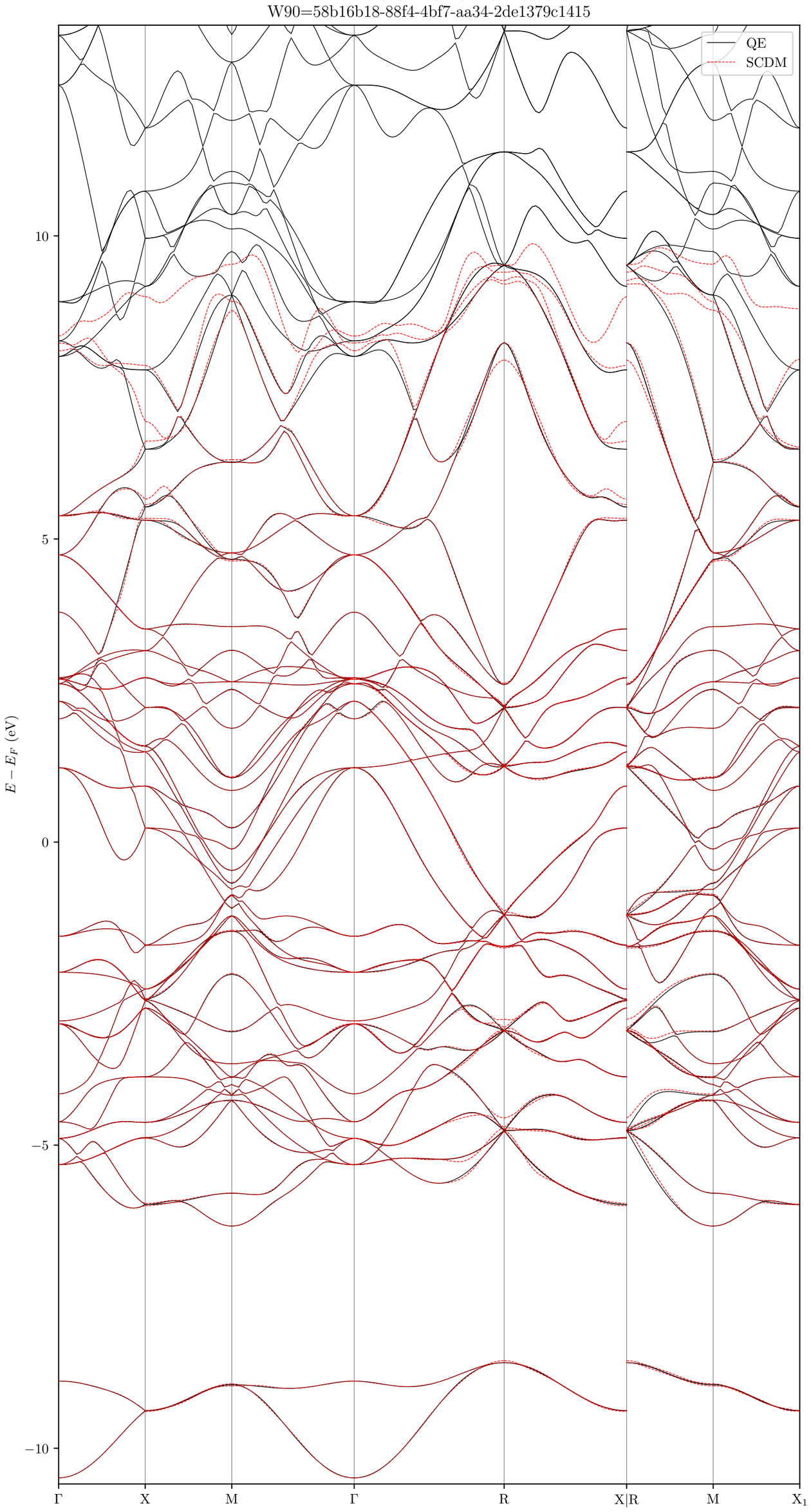
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.6 | 1.5 | 1.9 | 17.4 | 17.4 | 31.9 | 2.802 |





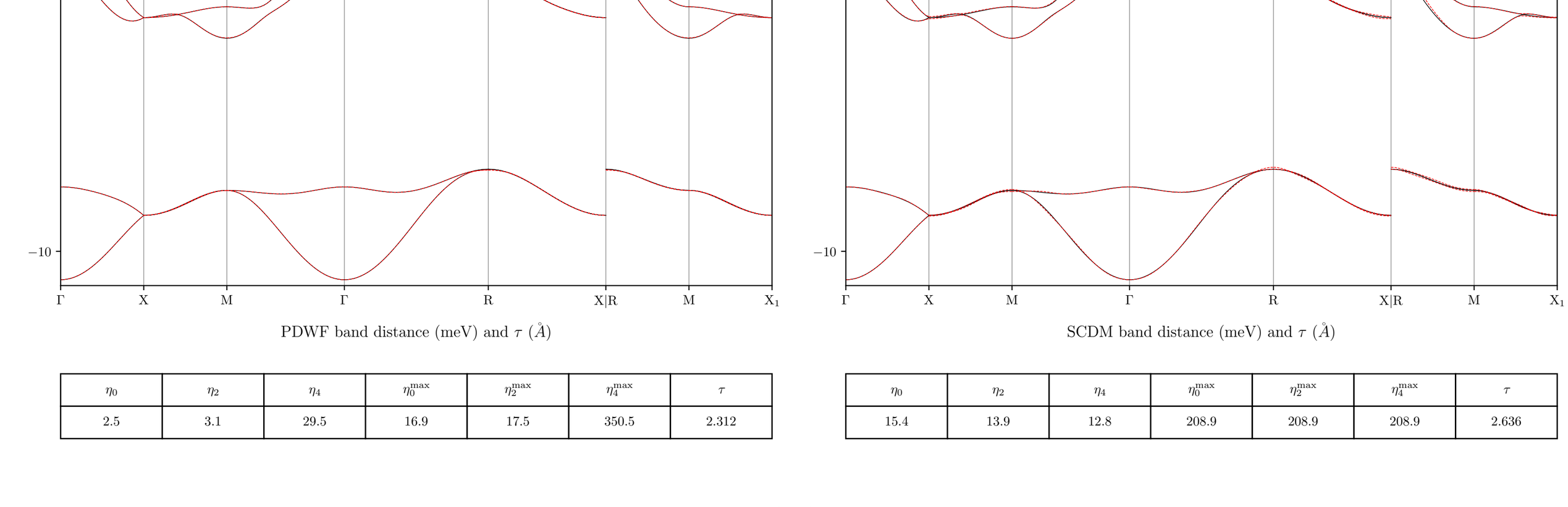

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.5 | 3.1 | 29.5 | 16.9 | 17.5 | 350.5 | 2.312 |

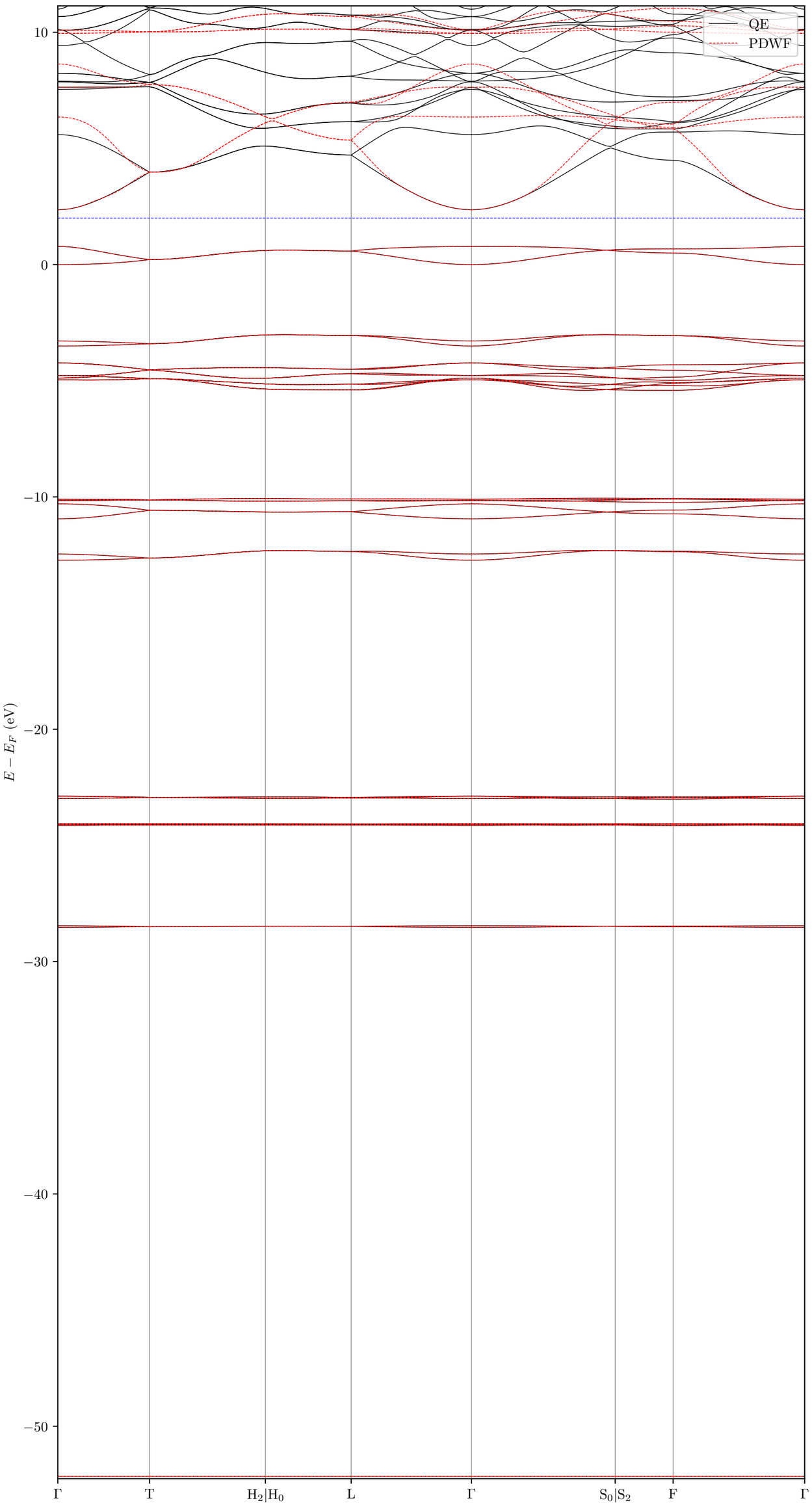



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 15.4 | 13.9 | 12.8 | 208.9 | 208.9 | 208.9 | 2.636 |



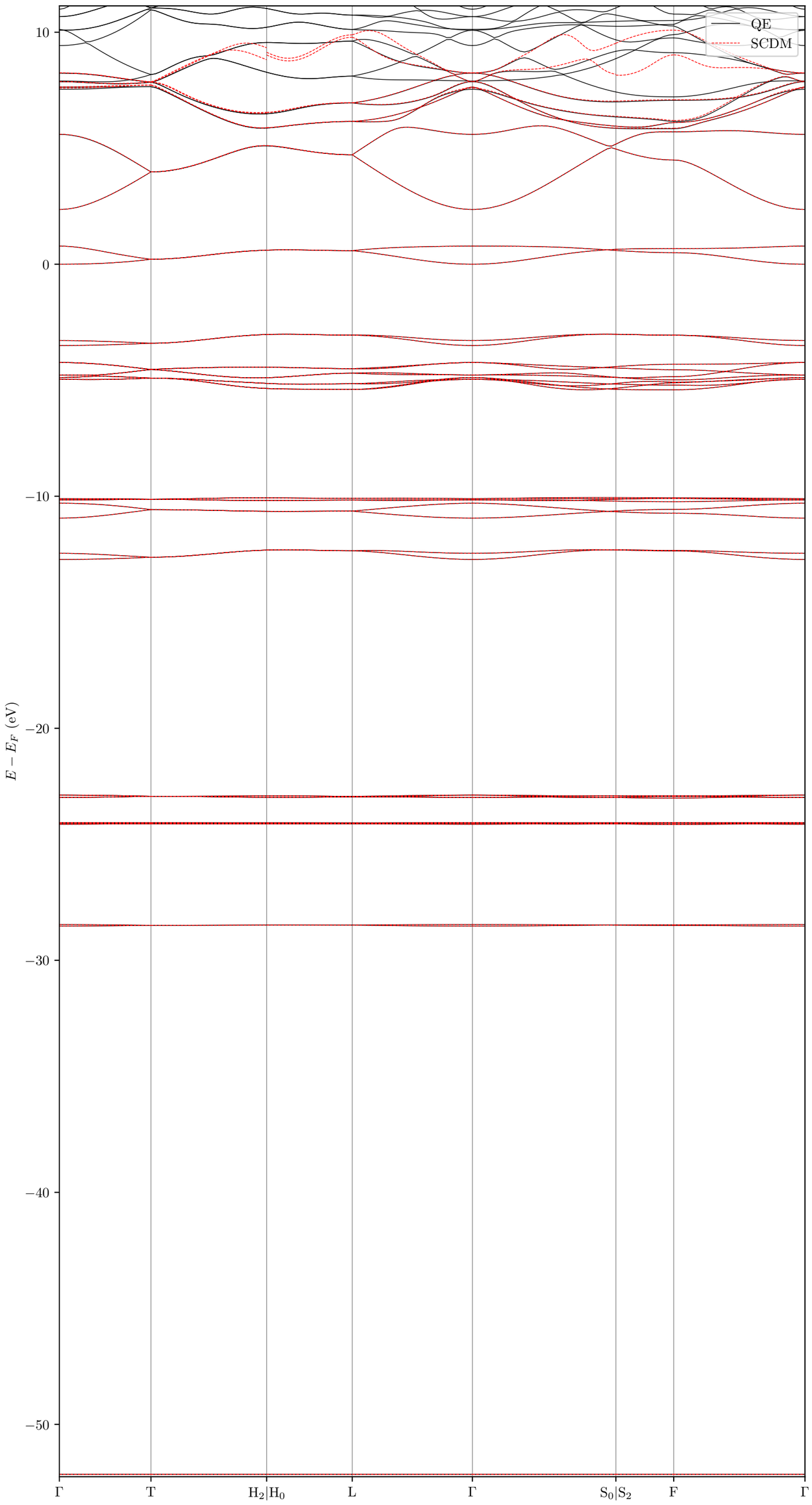
N2Na2O6 **INCLUDE** semicore
PW=464df8c9-7fea-42d7-adb8-a918f0f84099
W90=63b318d9-33e3-4c2c-9315-53f50bdd50a6




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.2 | 1.7 | 1.1 | 1.1 | 28.8 | 2.431 |

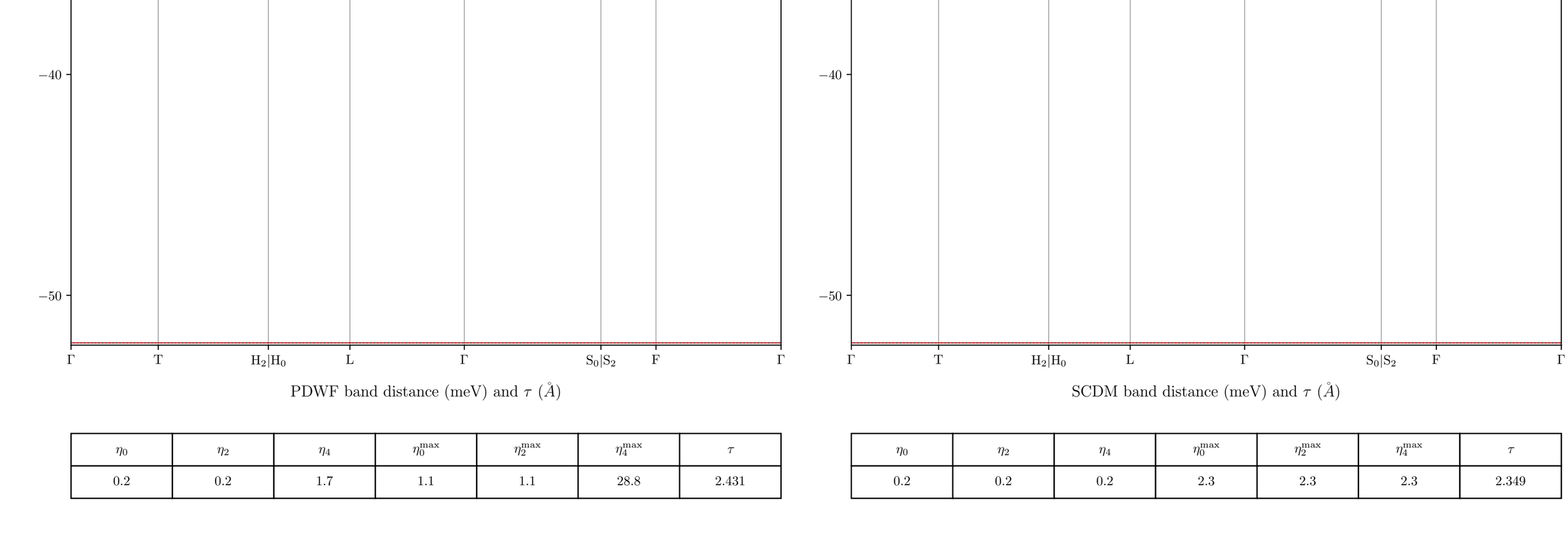
N2Na2O6 **INCLUDE** semicore
PW=464df8c9-7fea-42d7-adb8-a918f0f84099
W90=fc84f724-38c6-40c9-88ac-4a069e3d951d

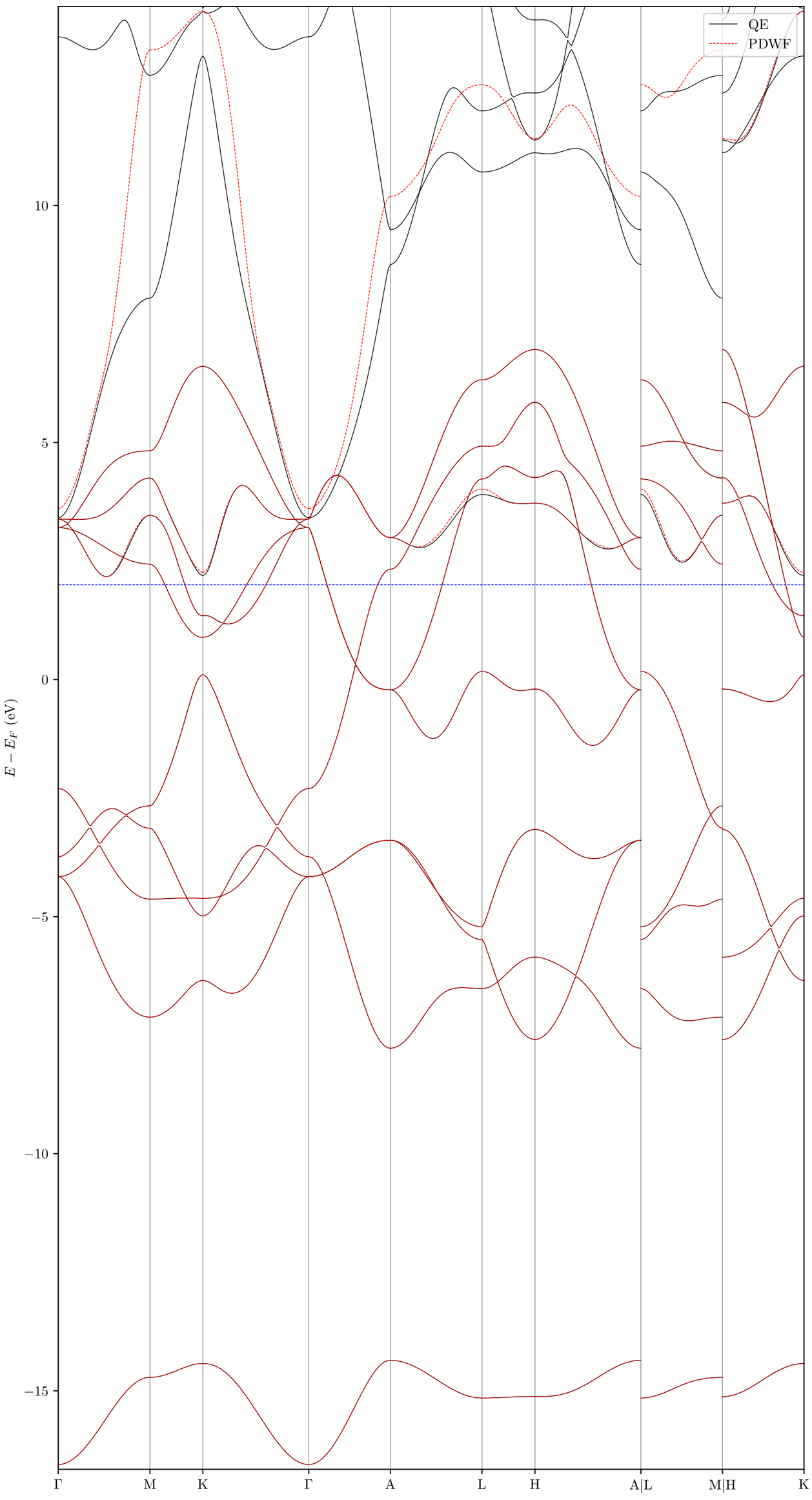



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.2 | 0.2 | 2.3 | 2.3 | 2.3 | 2.349 |

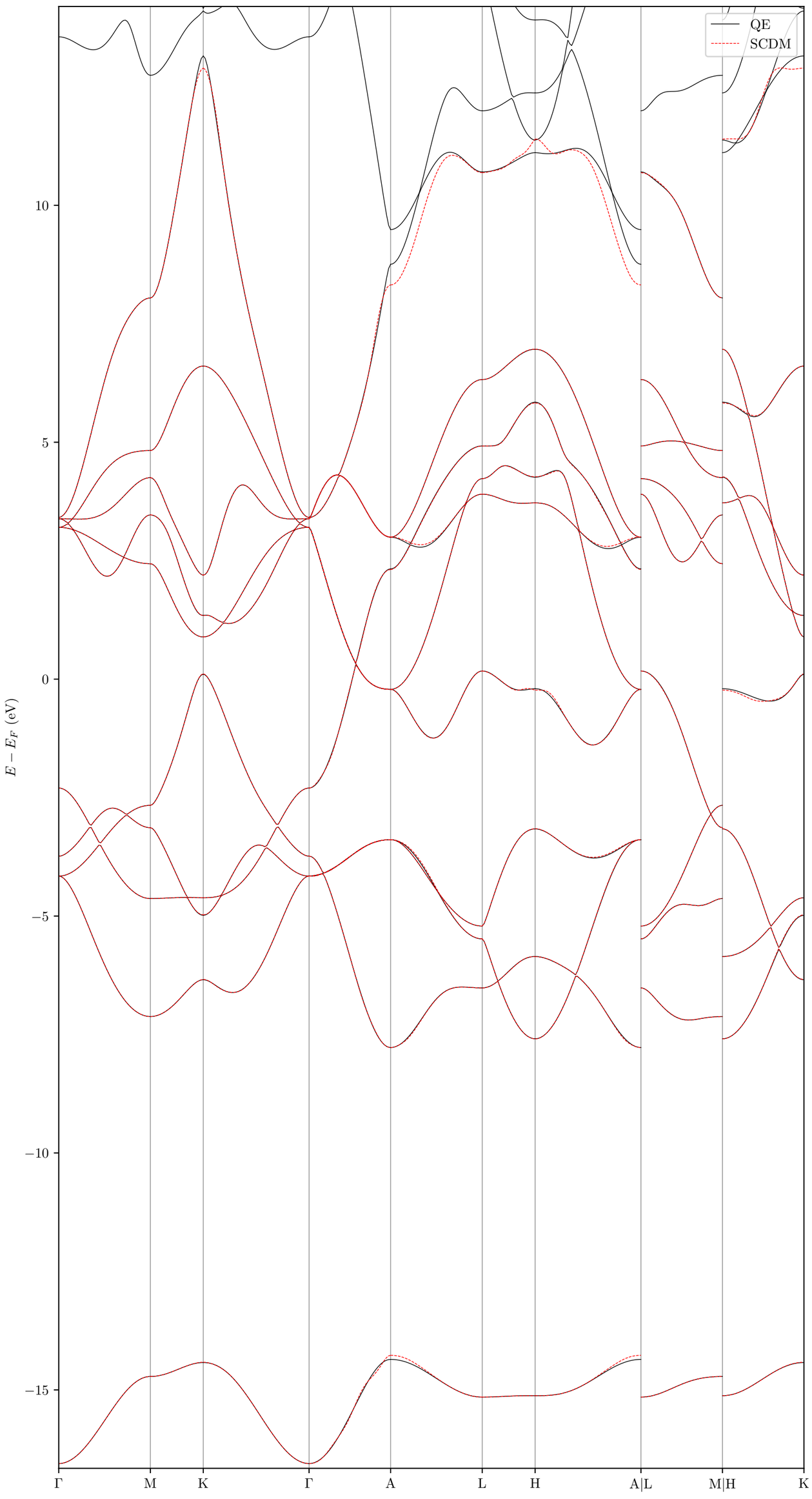
Hamiltonian decay





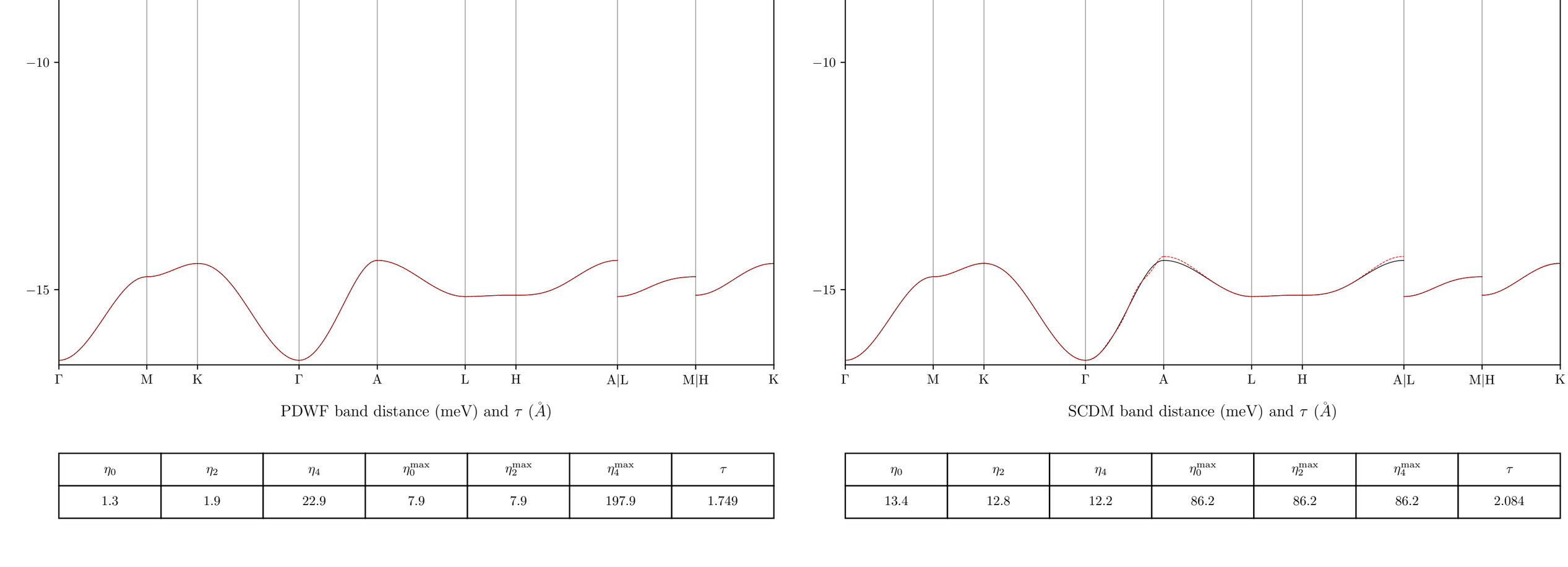

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.3 | 1.9 | 22.9 | 7.9 | 7.9 | 197.9 | 1.749 |

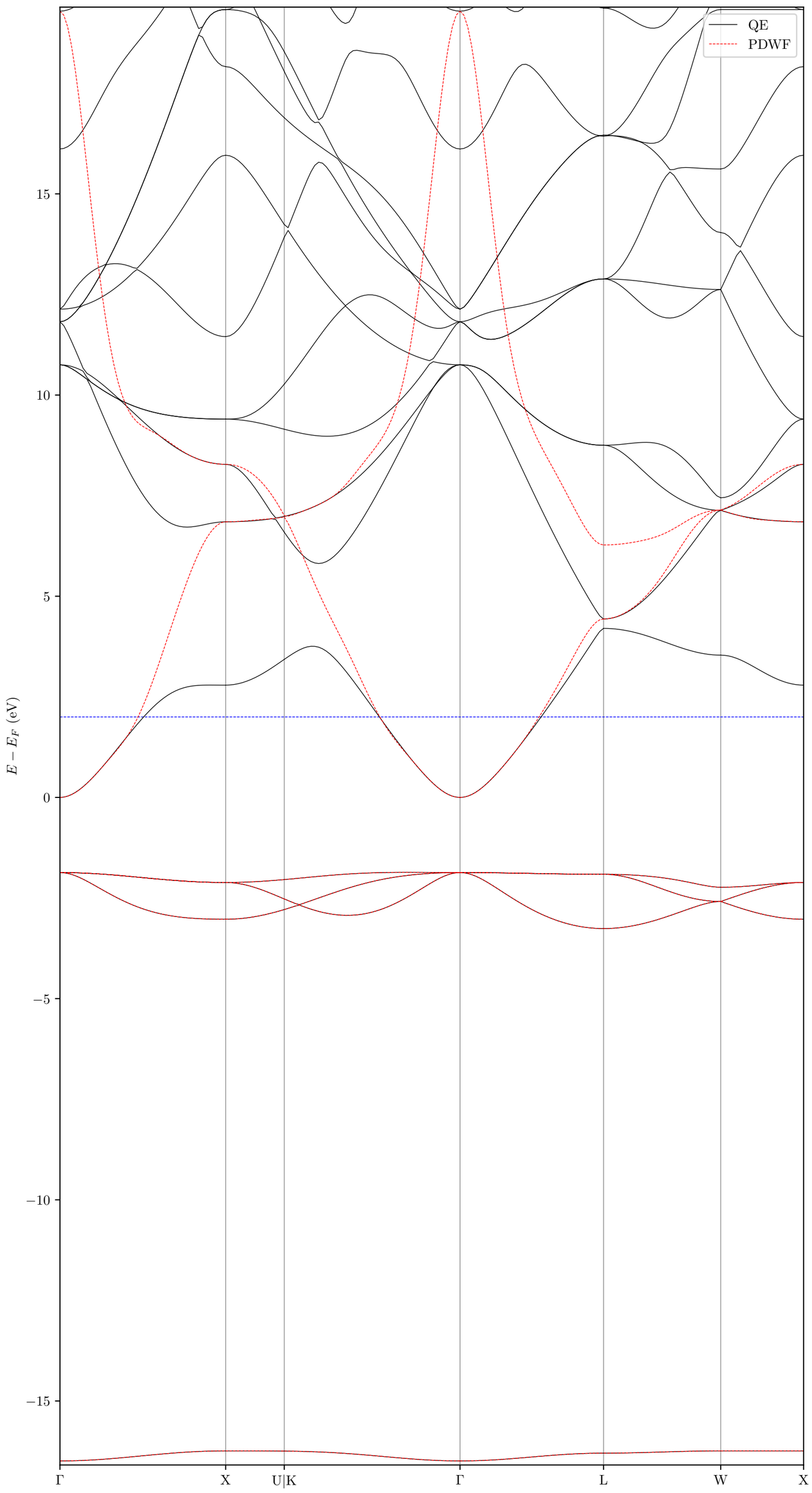



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 13.4 | 12.8 | 12.2 | 86.2 | 86.2 | 86.2 | 2.084 |



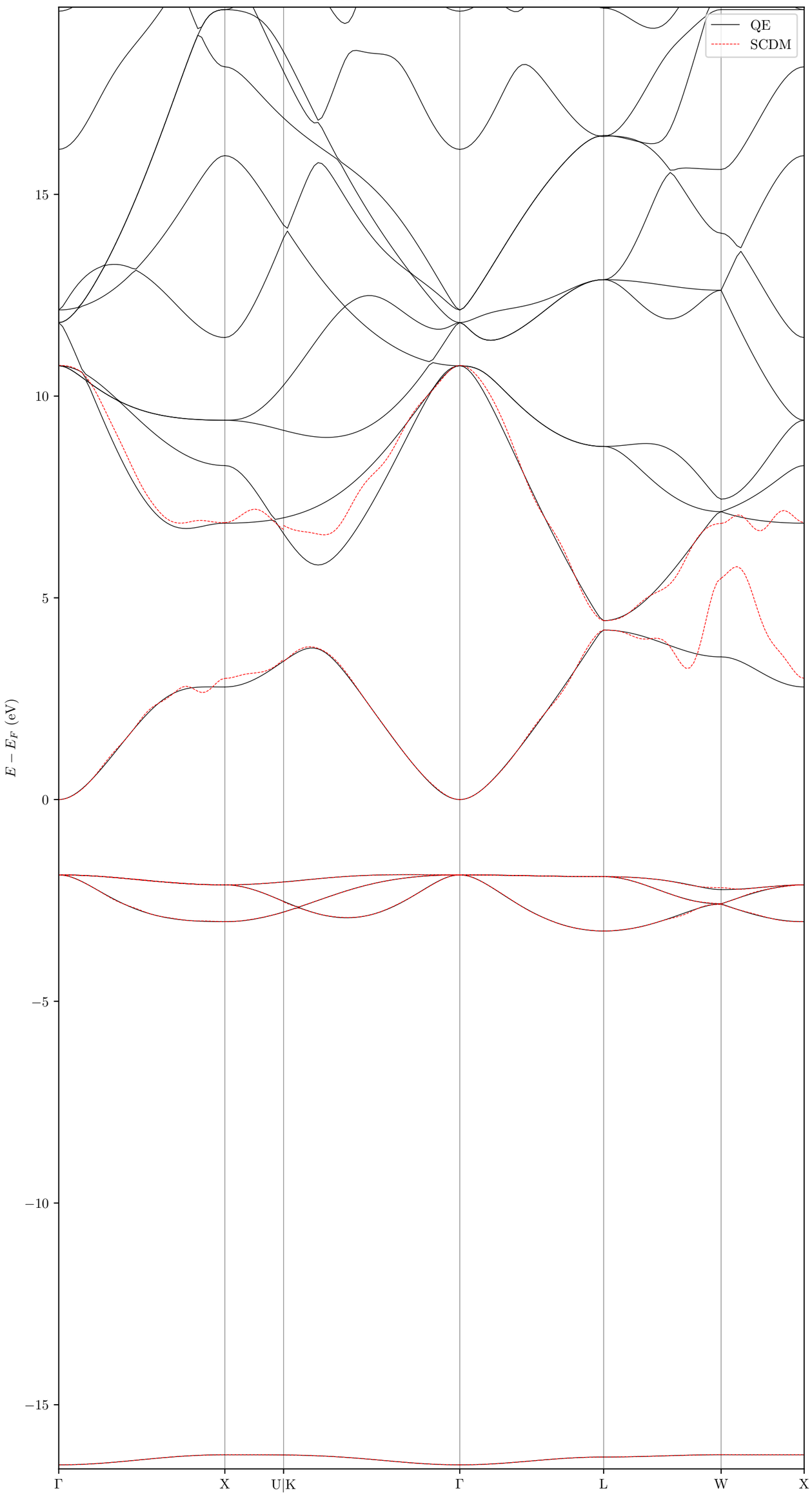
Na2O exclude semicore
PW=a155443e-19dc-48bc-af13-669185c87557
W90=61187a6d-465d-4fdb-806e-359e73103736




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.8 | 42.5 | 1.4 | 5.2 | 524.5 | 2.105 |

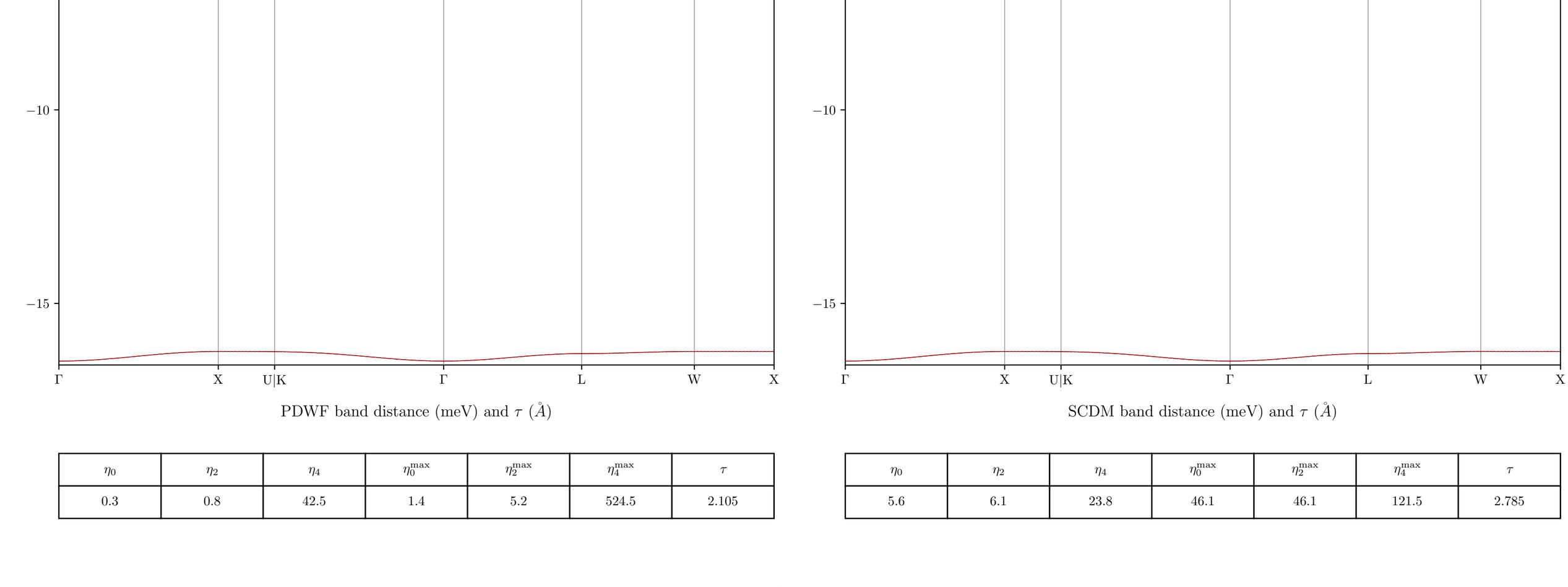
Na2O exclude semicore
PW=a155443e-19dc-48bc-af13-669185c87557
W90=e30e2566-3841-4cd7-885c-823de28e1786

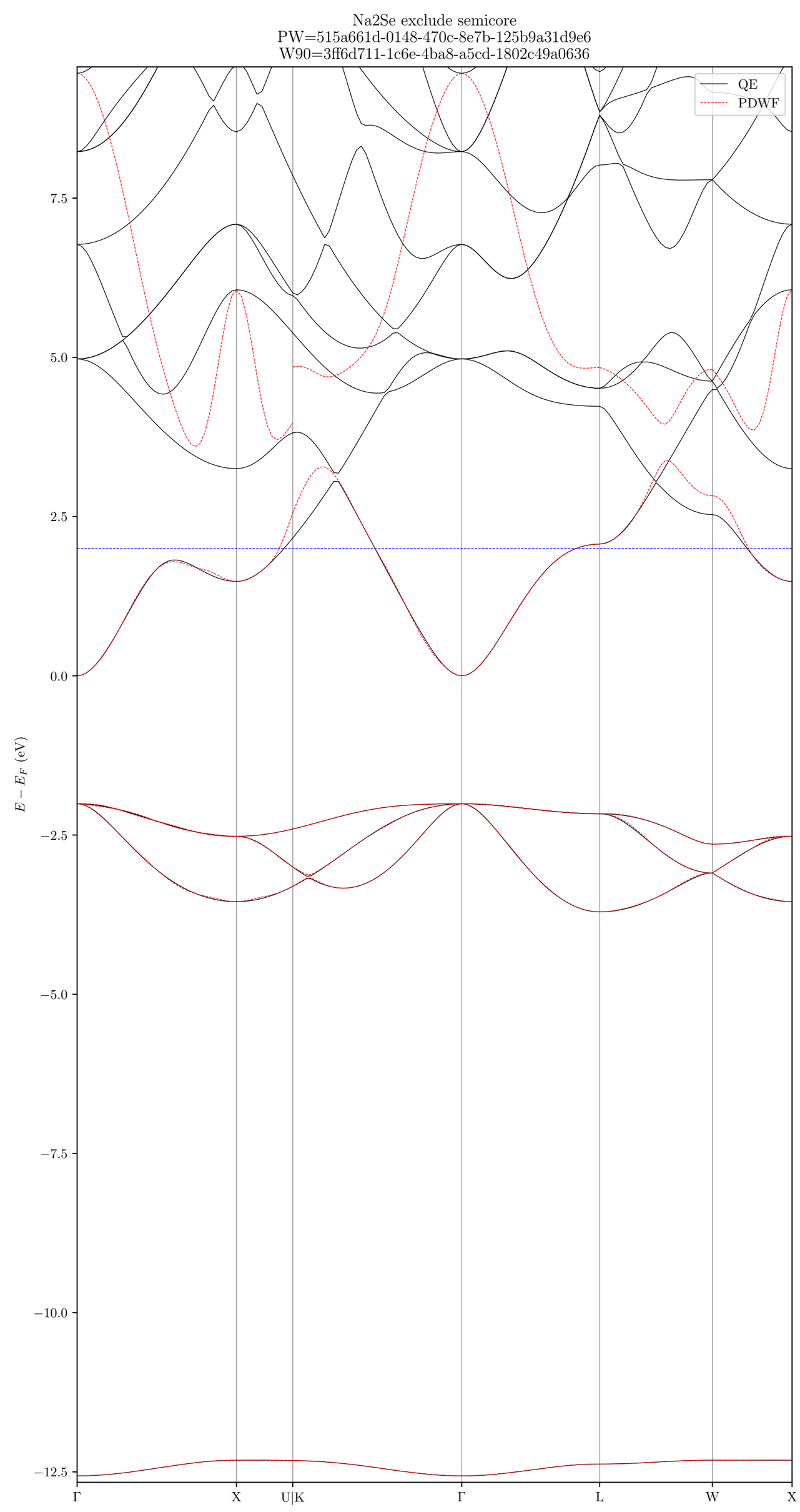



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.6 | 6.1 | 23.8 | 46.1 | 46.1 | 121.5 | 2.785 |

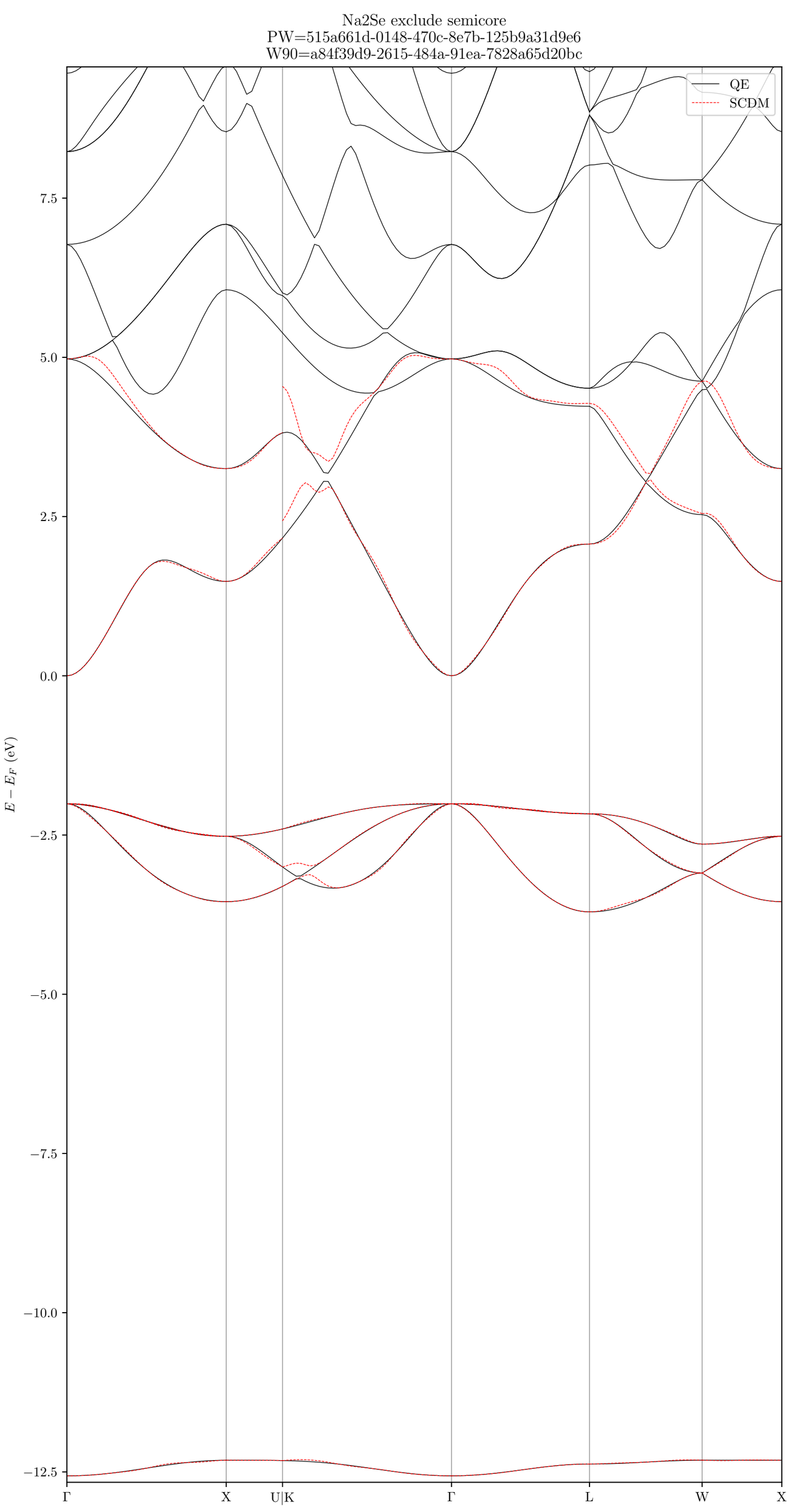
Hamiltonian decay





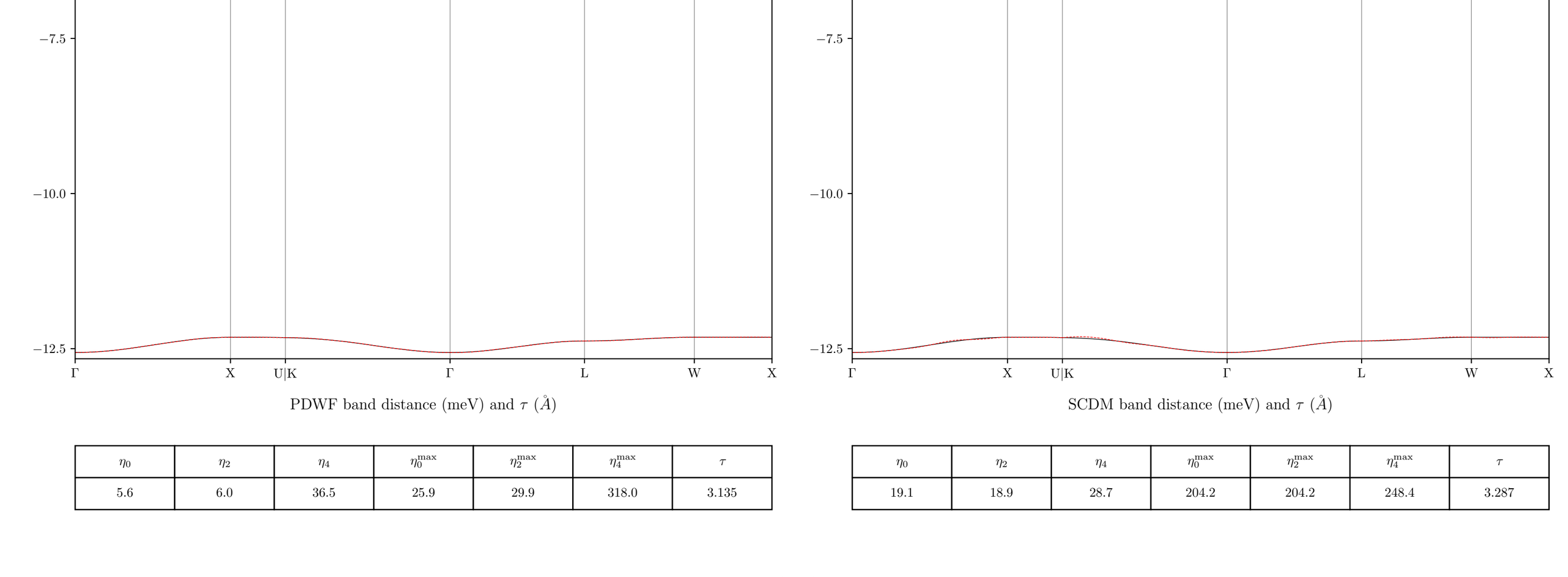

PDWF band distance (meV) and $\tau$ ($\AA$)

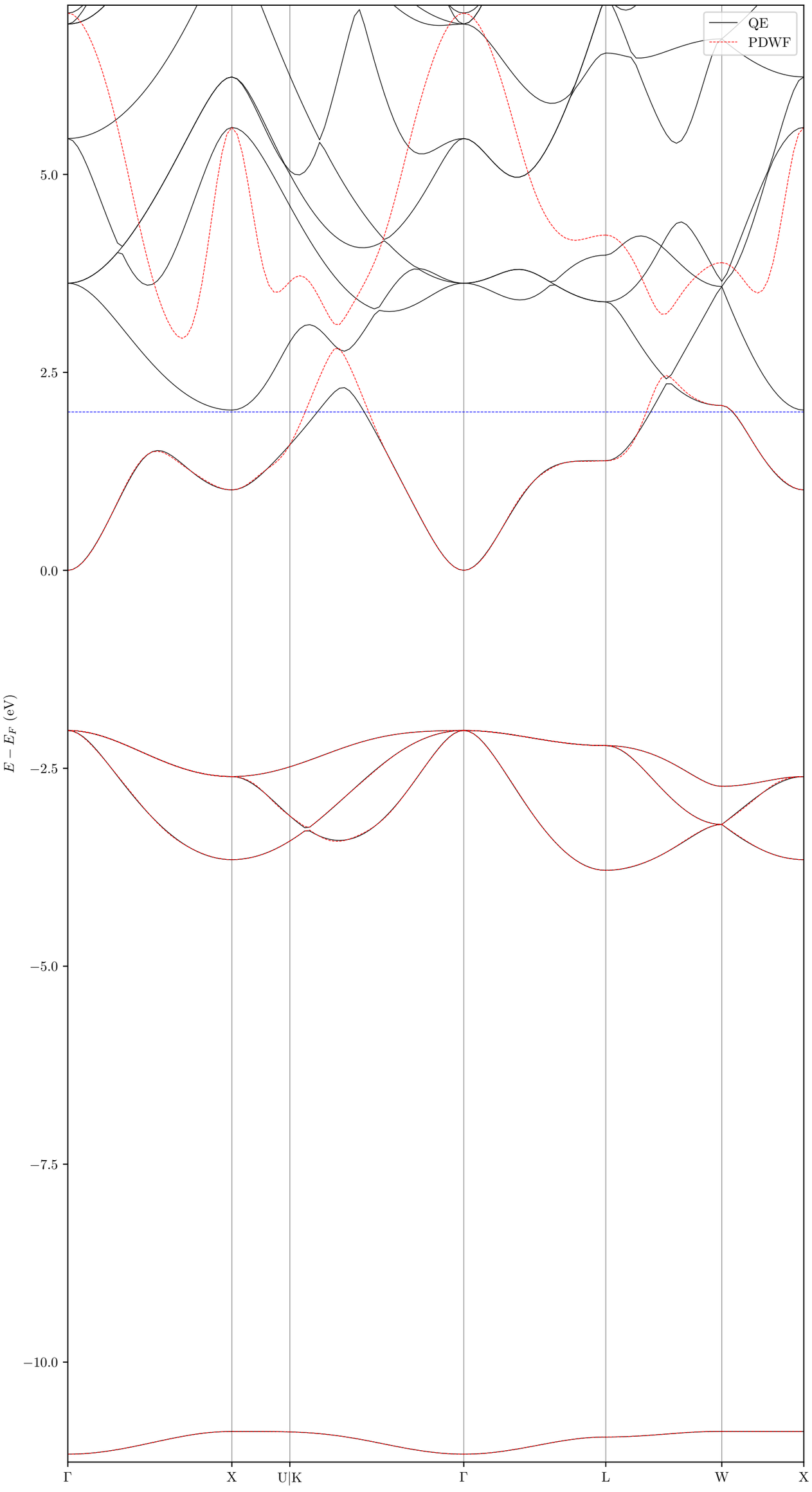
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.6 | 6.0 | 36.5 | 25.9 | 29.9 | 318.0 | 3.135 |




SCDM band distance (meV) and $\tau$ ($\AA$)

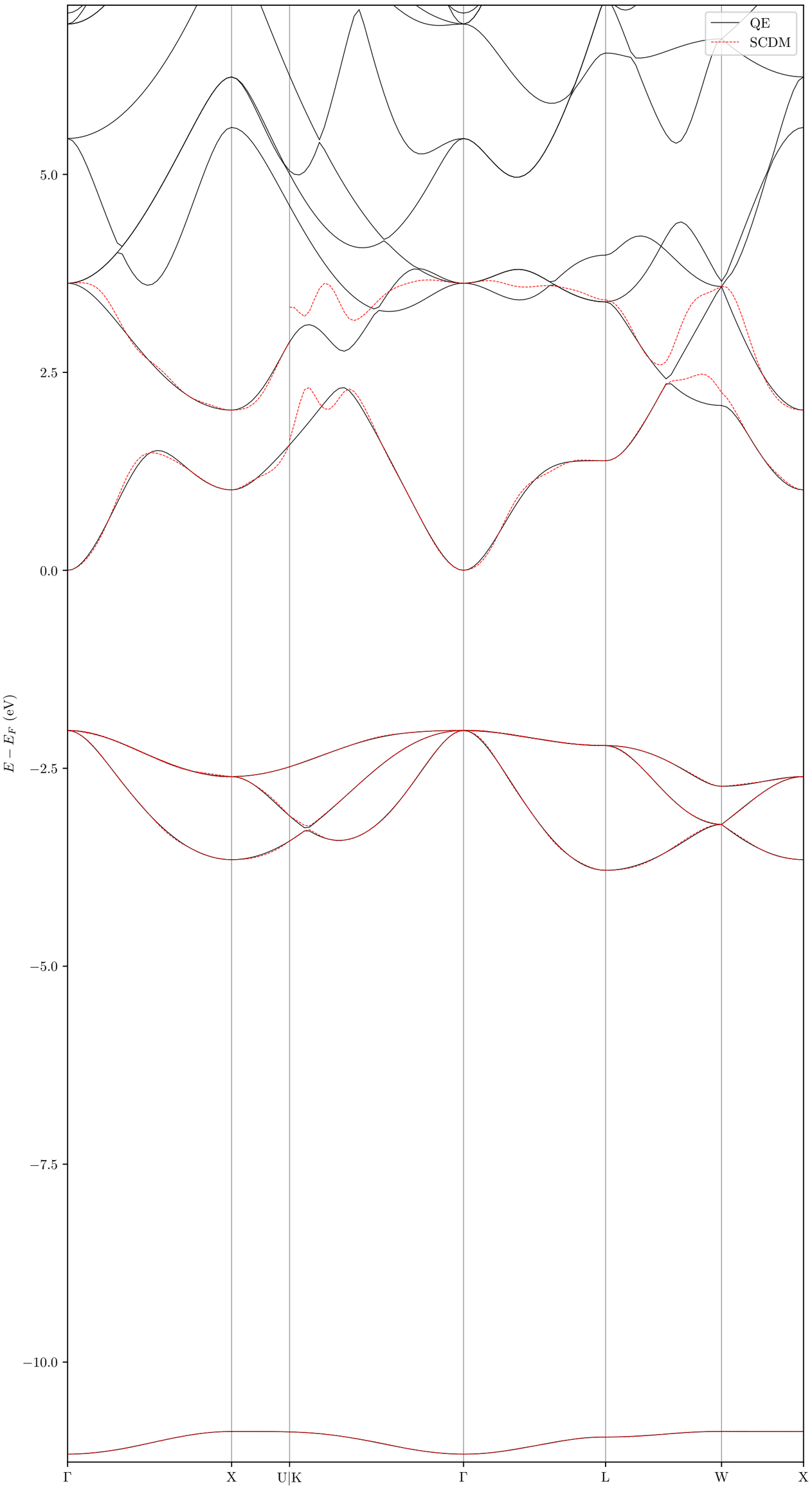
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 19.1 | 18.9 | 28.7 | 204.2 | 204.2 | 248.4 | 3.287 |





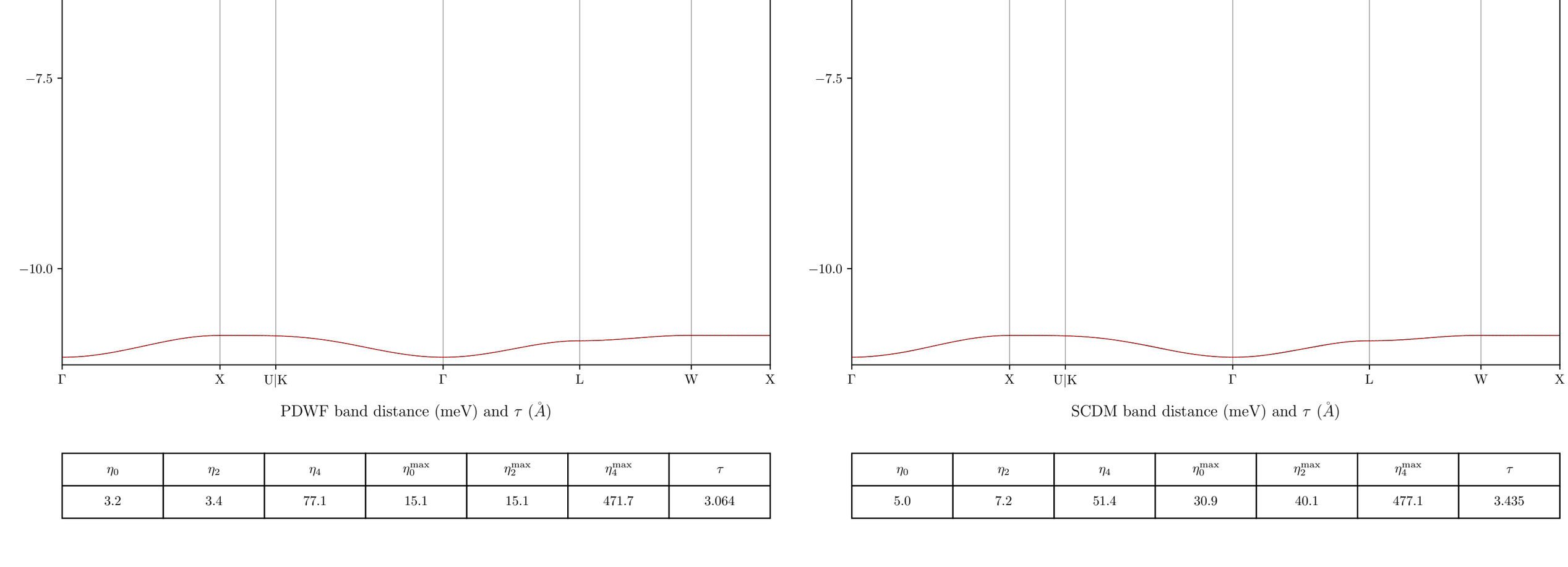

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.2 | 3.4 | 77.1 | 15.1 | 15.1 | 471.7 | 3.064 |

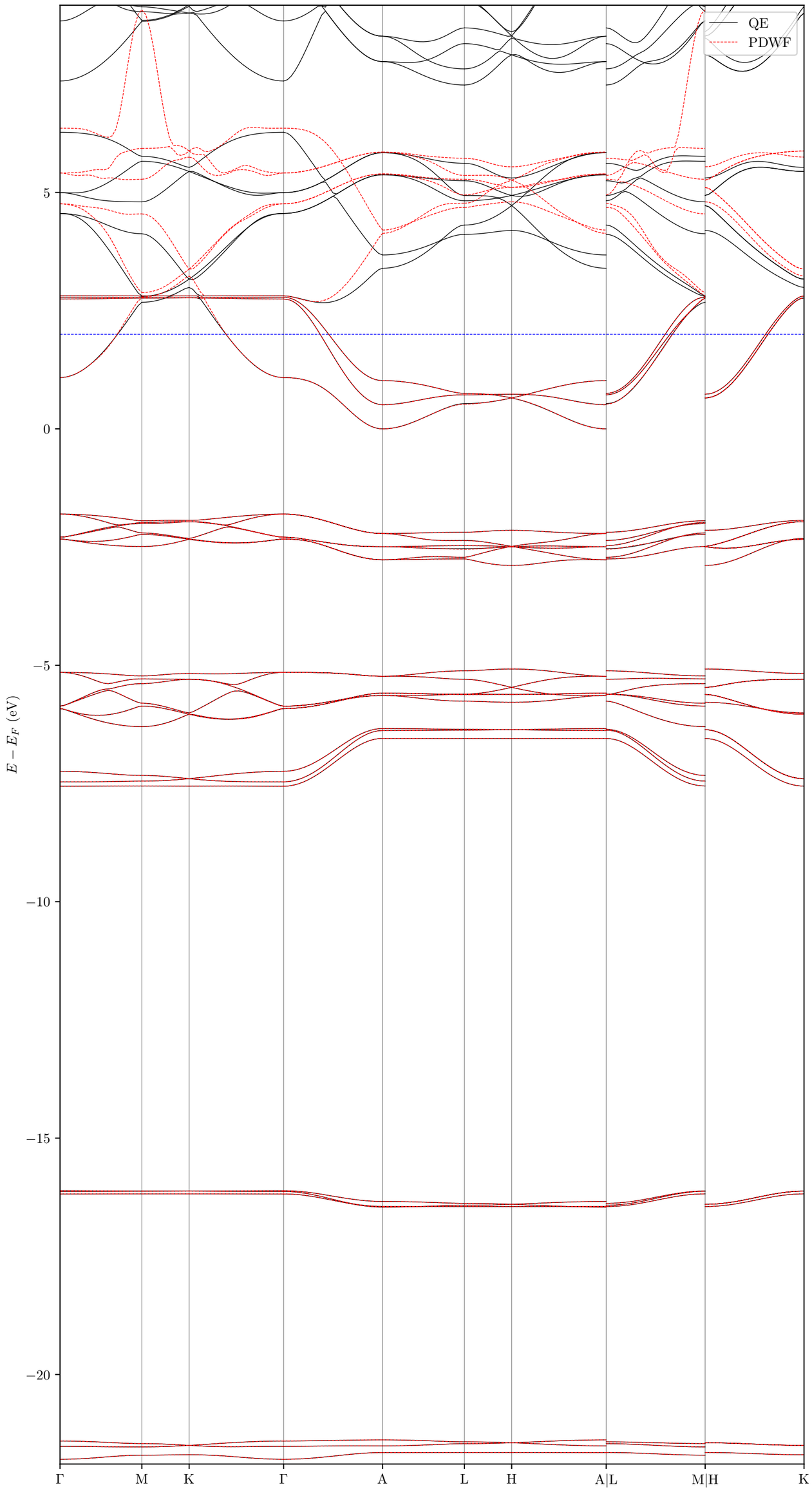



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.0 | 7.2 | 51.4 | 30.9 | 40.1 | 477.1 | 3.435 |



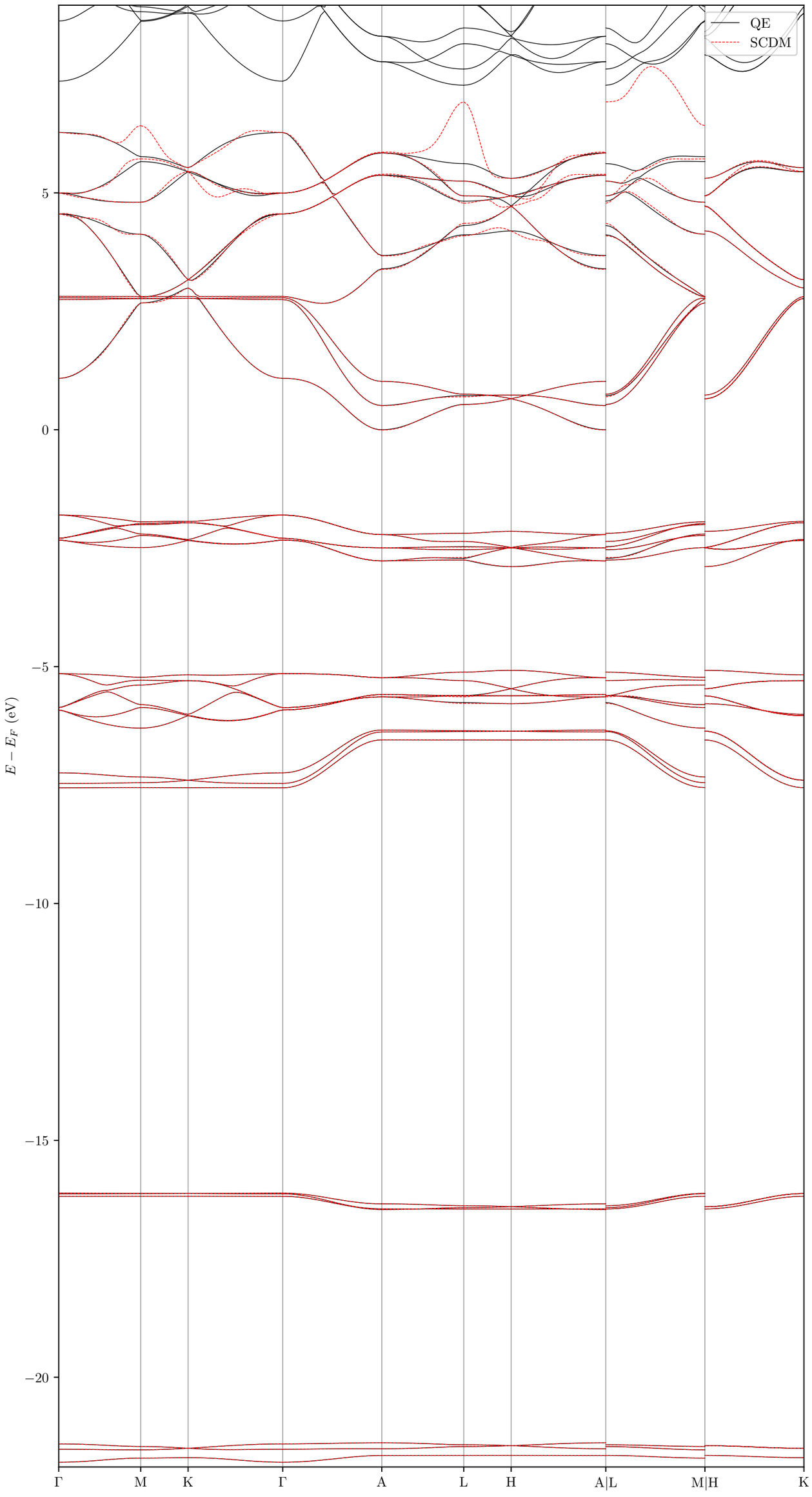
Na6O6 exclude semicore
PW=83a3a9ca-617d-48bb-9023-75c263e1b84c
W90=ec2c7767-a0d0-416b-a18f-e60ef92f775c




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.3 | 11.4 | 13.3 | 13.3 | 134.2 | 2.650 |

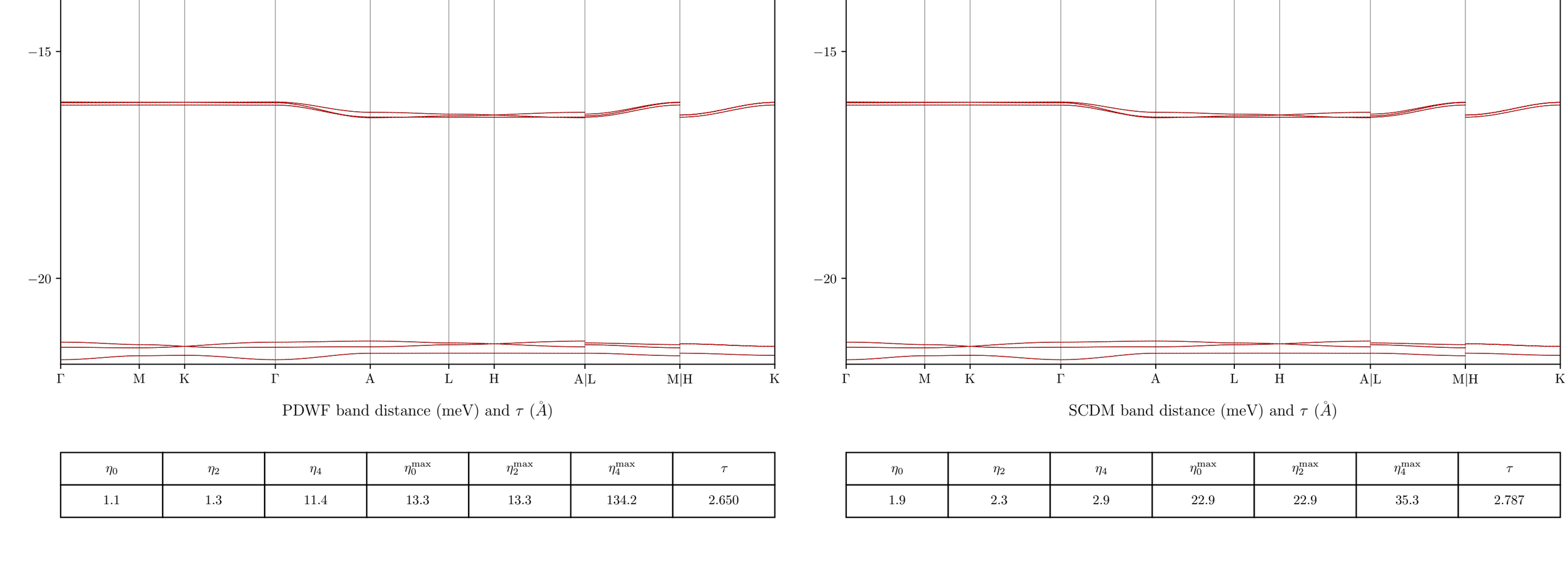
Na6O6 exclude semicore
PW=83a3a9ca-617d-48bb-9023-75c263e1b84c
W90=afc9ddf6-b711-4b71-8fde-584ba8787df5

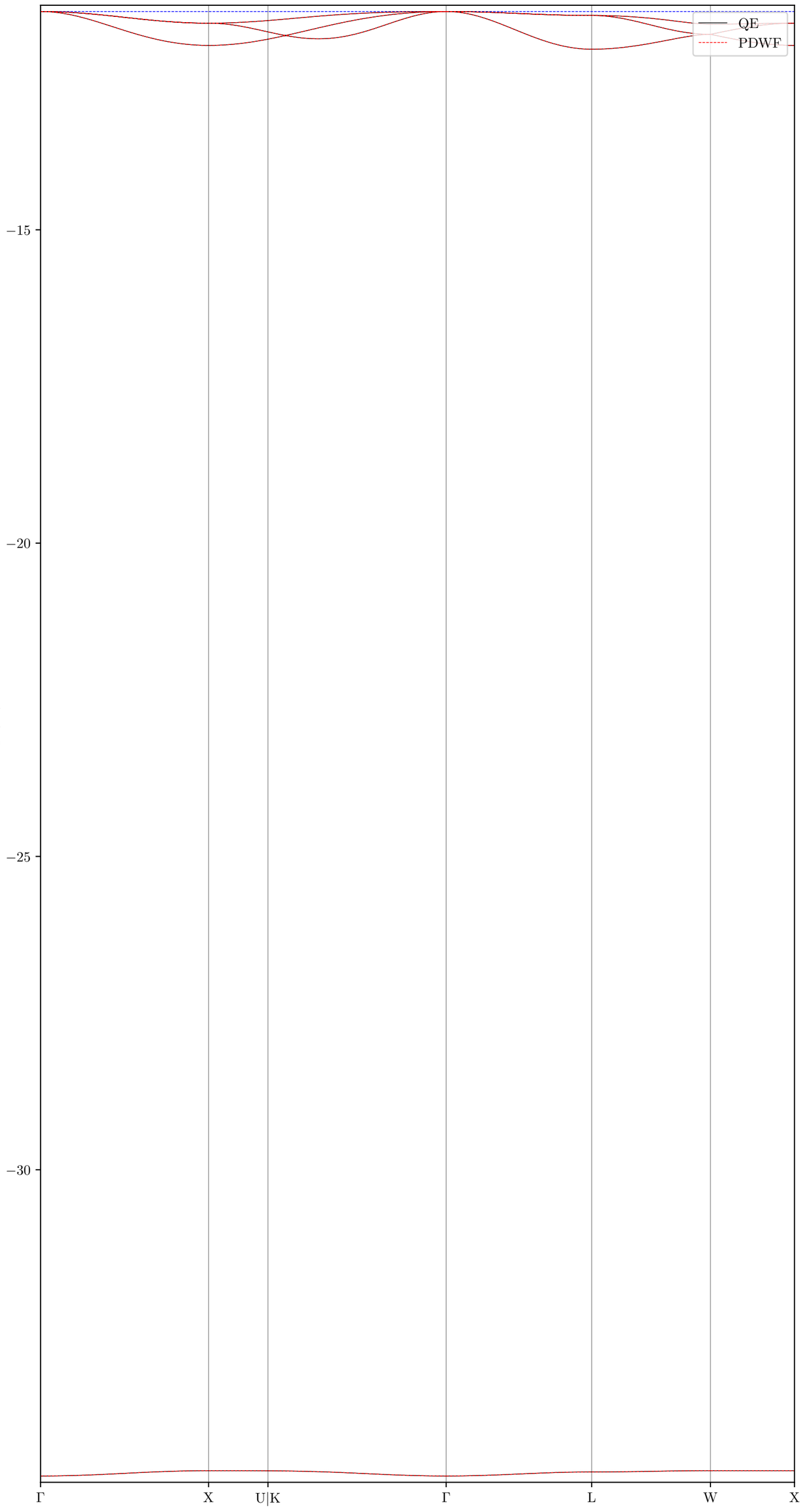



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.9 | 2.3 | 2.9 | 22.9 | 22.9 | 35.3 | 2.787 |

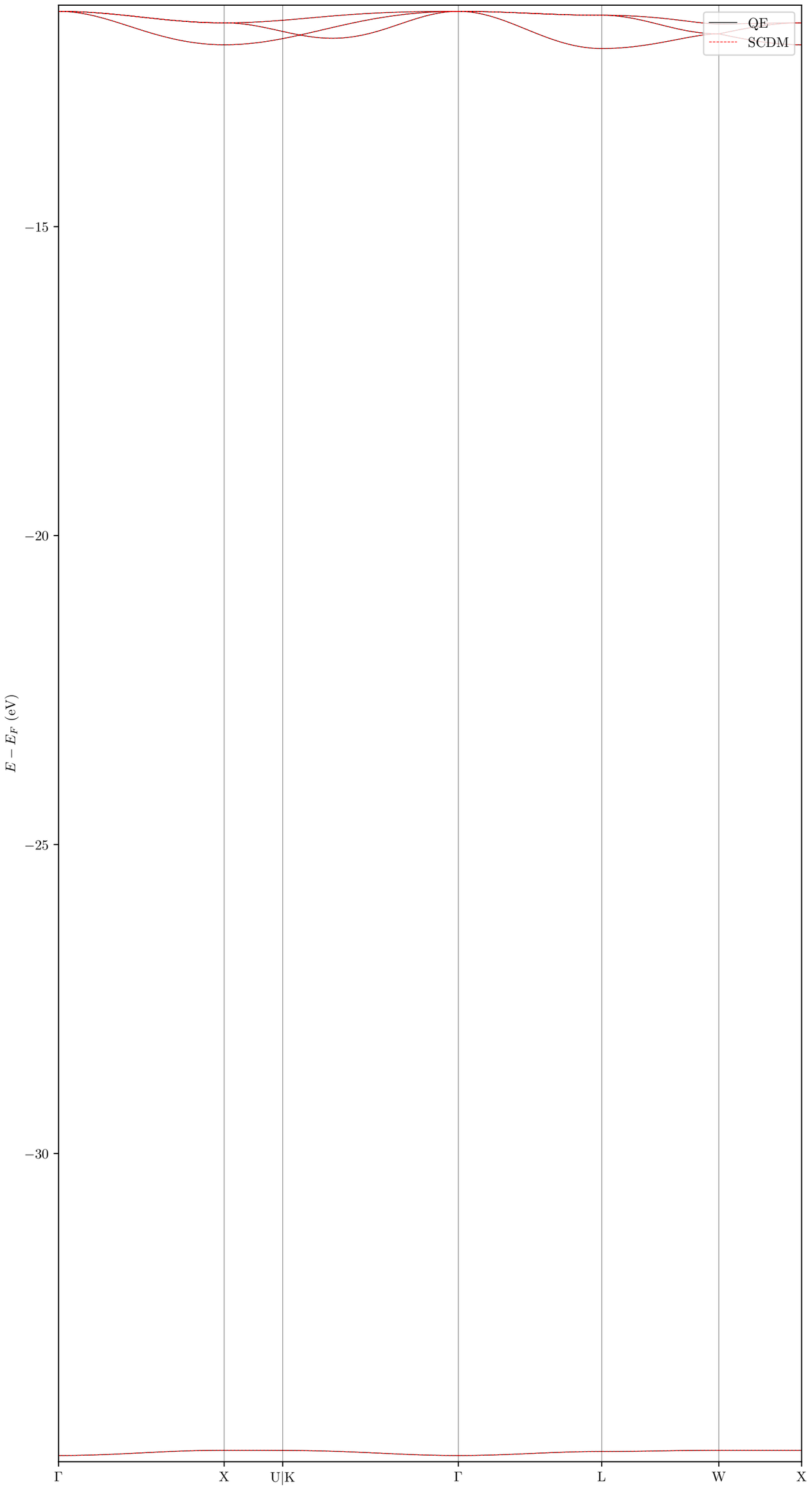
Hamiltonian decay





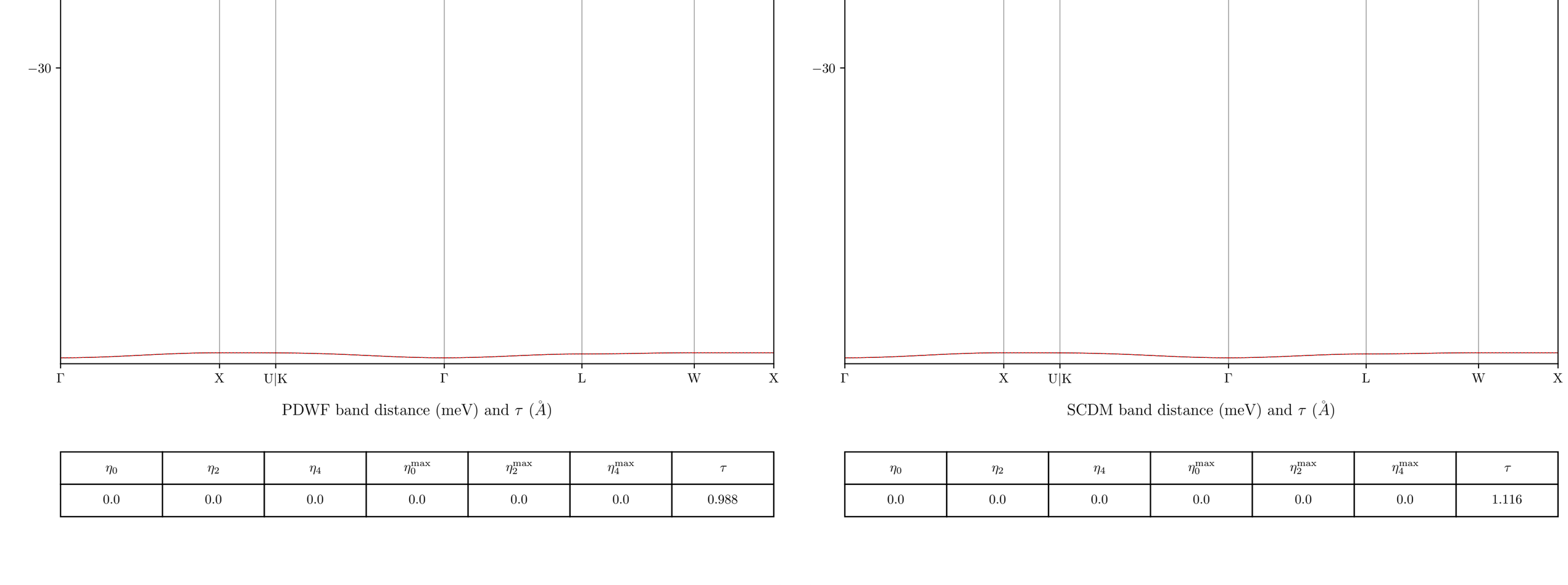

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.988 |

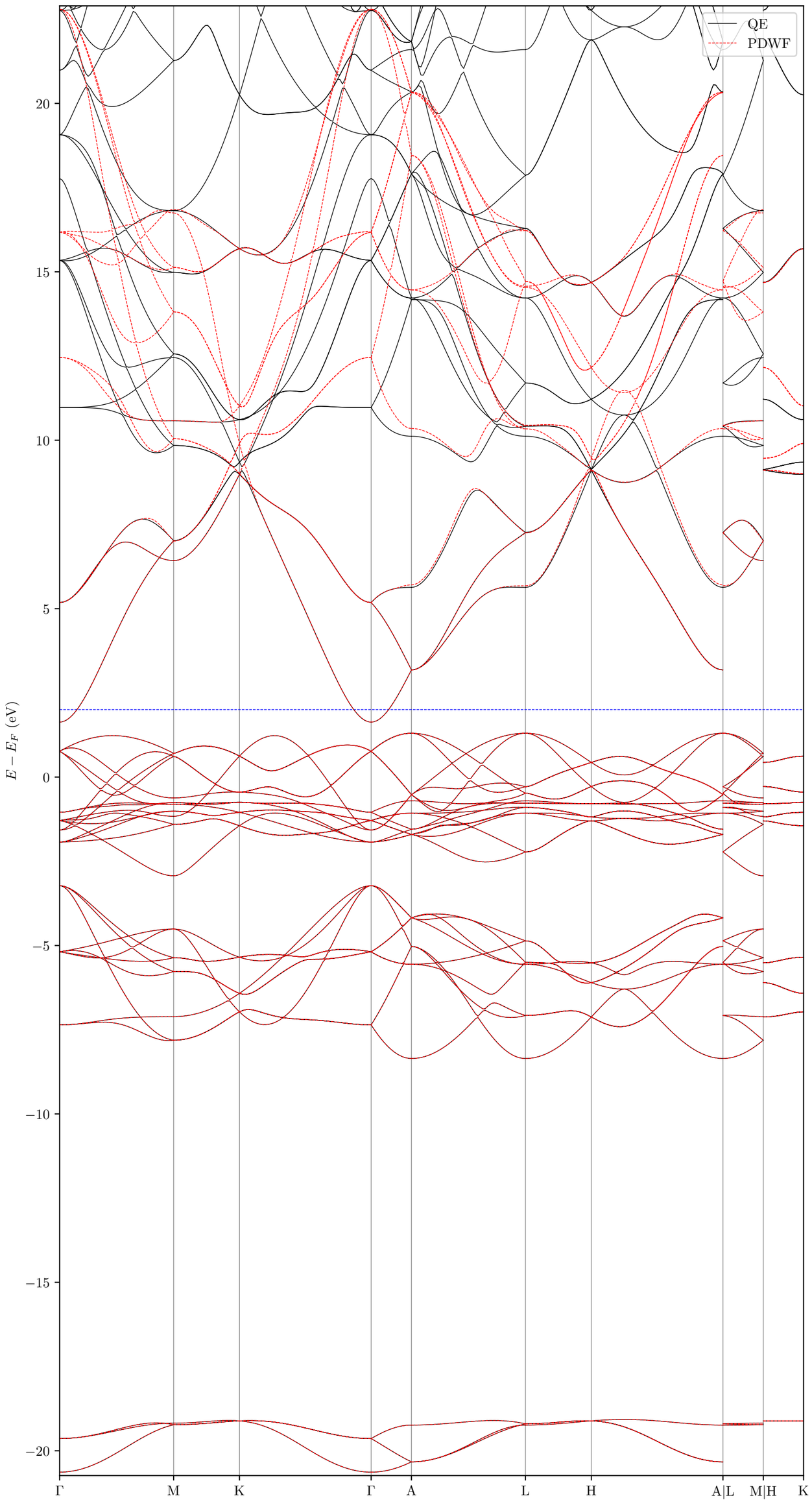



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 1.116 |



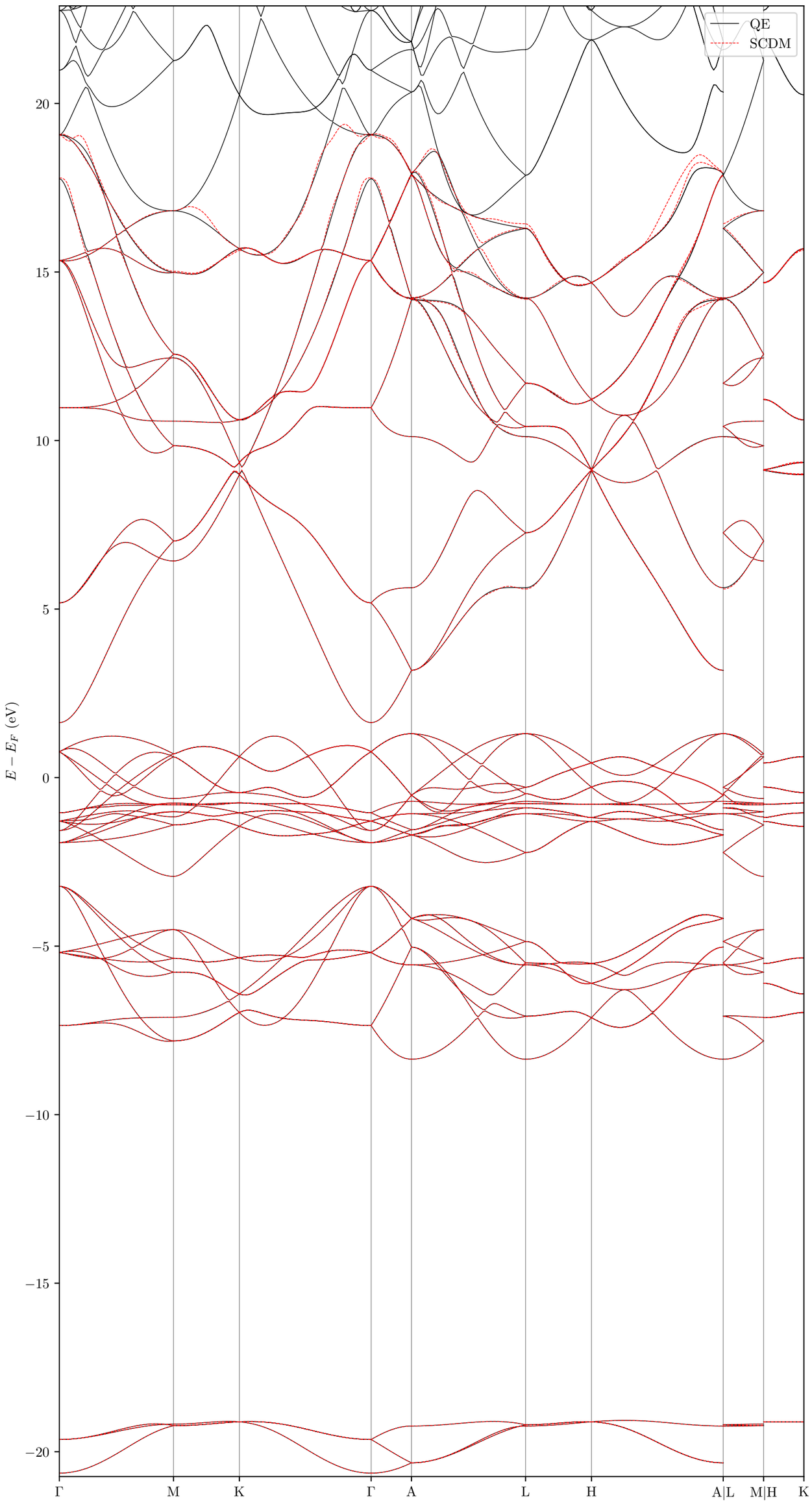
Ni3O3 exclude semicore
PW=def9a65e-4973-4c9e-8ad7-19125966c092
W90=d69752de-2c08-49a0-bf0b-43569e769a70




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 0.7 | 6.9 | 6.9 | 6.9 | 2.172 |

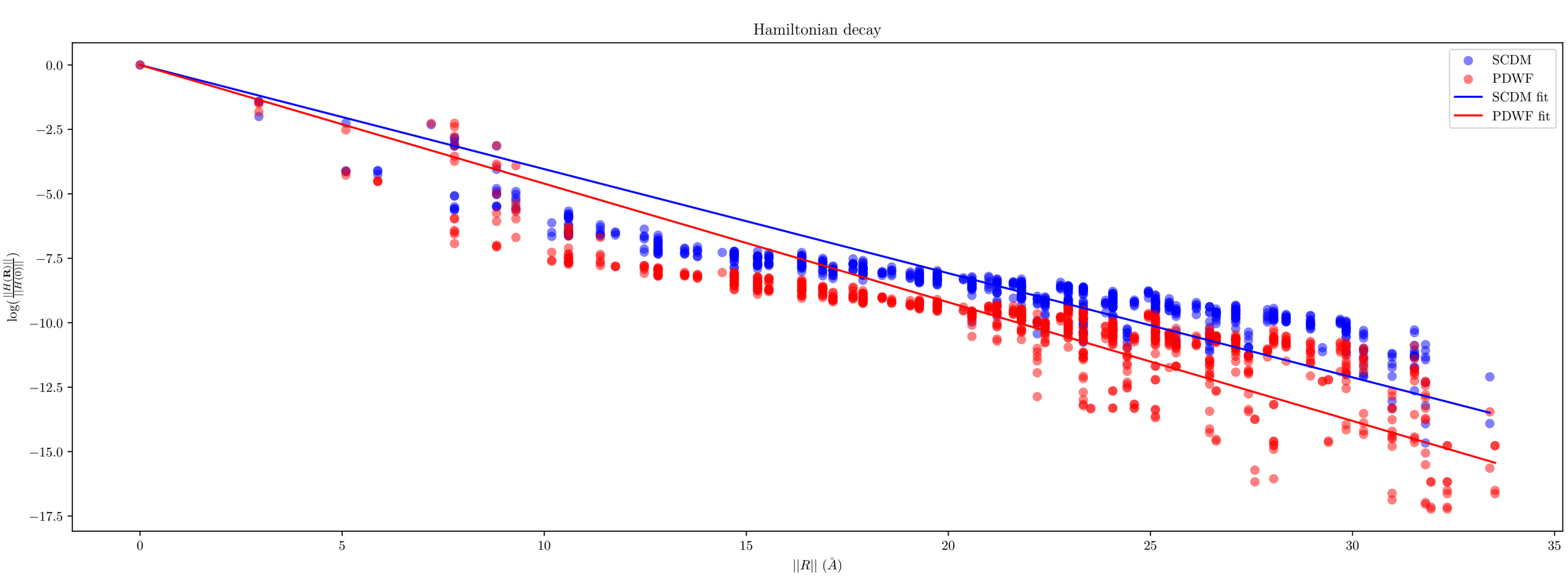
Ni3O3 exclude semicore
PW=def9a65e-4973-4c9e-8ad7-19125966c092
W90=946f1f4a-d654-4491-b9df-023784cafa0b



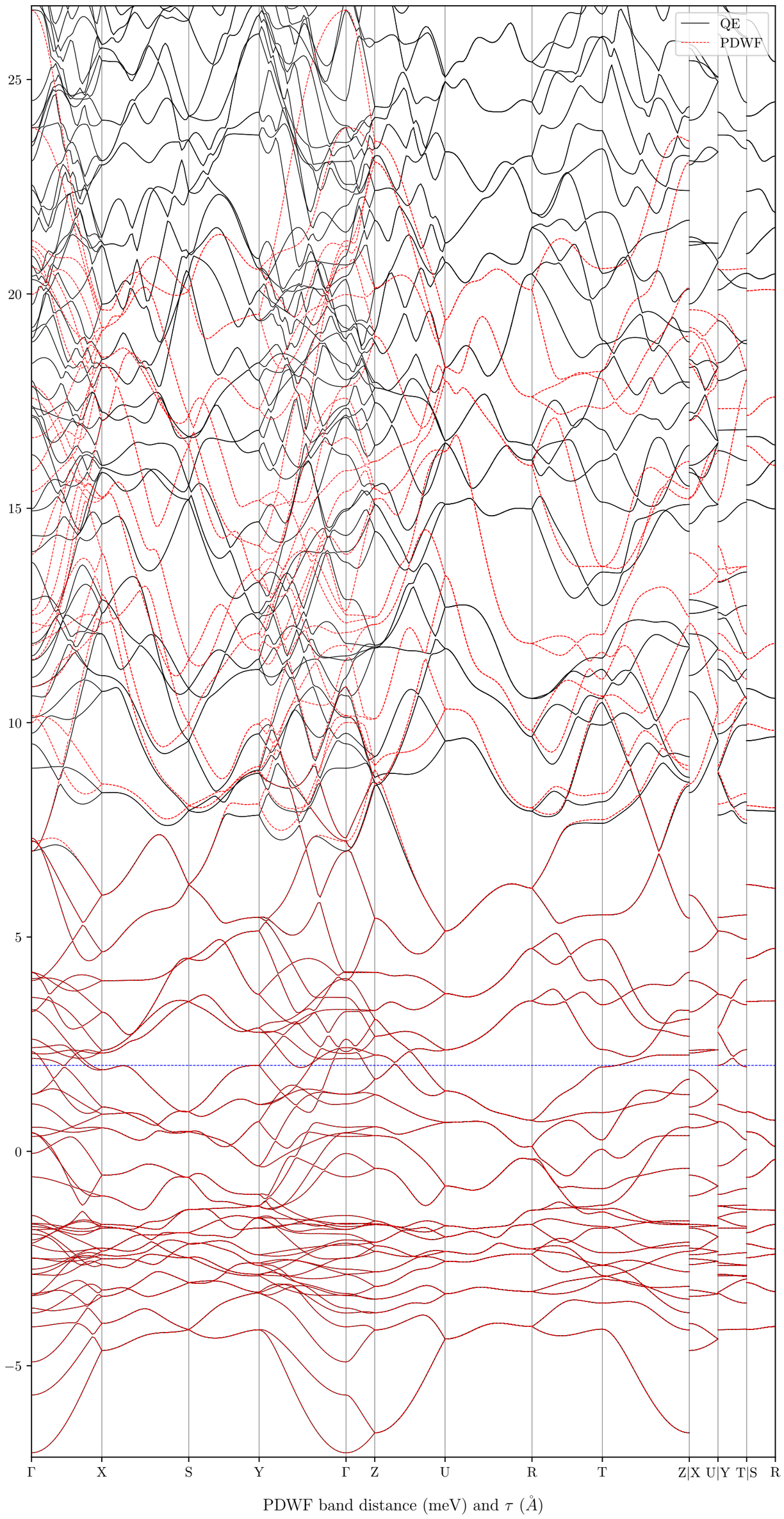

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.9 | 1.9 | 1.9 | 19.8 | 19.8 | 19.8 | 2.475 |

Hamiltonian decay



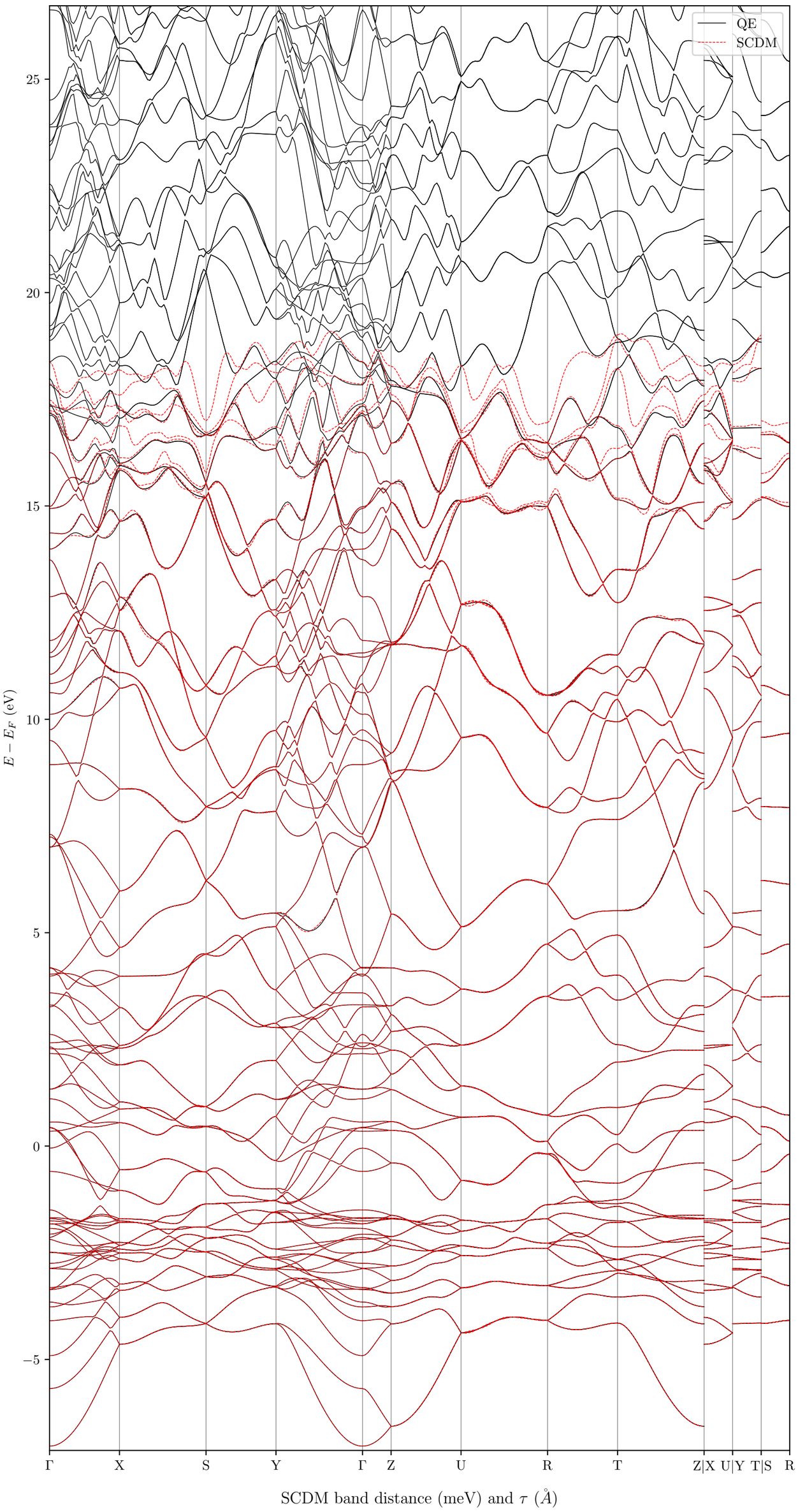
Ni4Zr4 exclude semicore
PW=ad8e8314-cea0-415d-8134-2ec7259e76af
W90=7954992a-1710-4f9d-9772-af727a77a52a




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.4 | 0.5 | 0.6 | 2.7 | 8.2 | 11.0 | 2.256 |

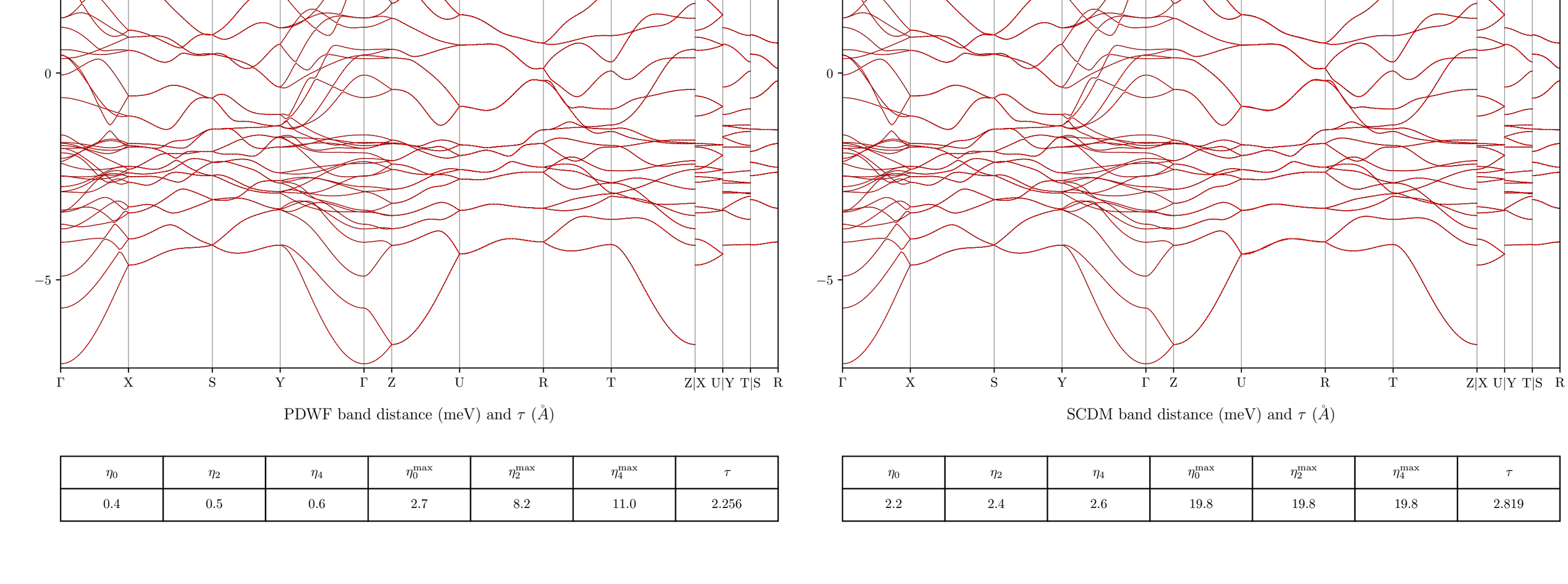
Ni4Zr4 exclude semicore
PW=ad8e8314-cea0-415d-8134-2ec7259e76af
W90=549f0f9b-19da-4bc5-9974-48ba0f627db6

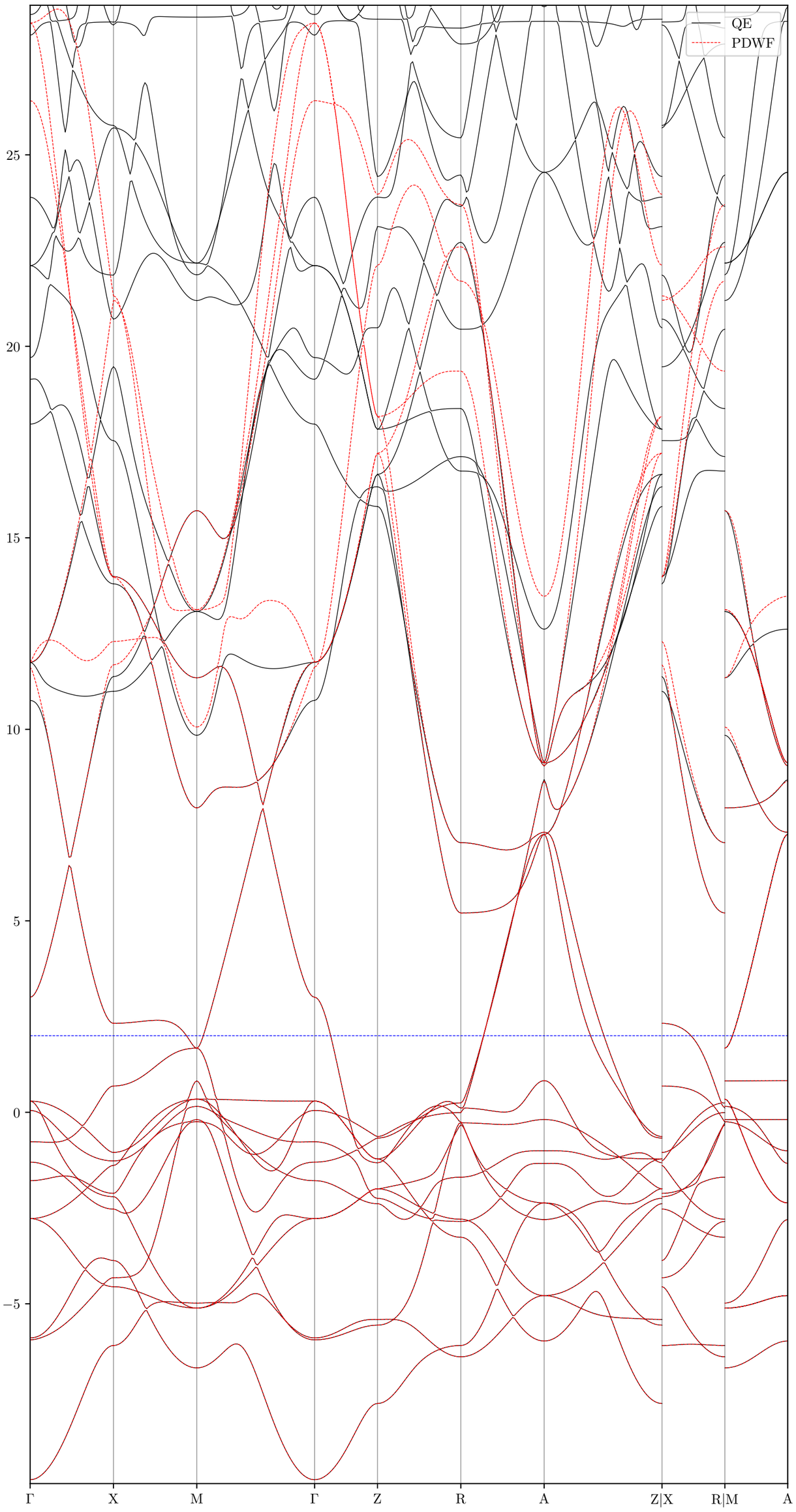



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.2 | 2.4 | 2.6 | 19.8 | 19.8 | 19.8 | 2.819 |

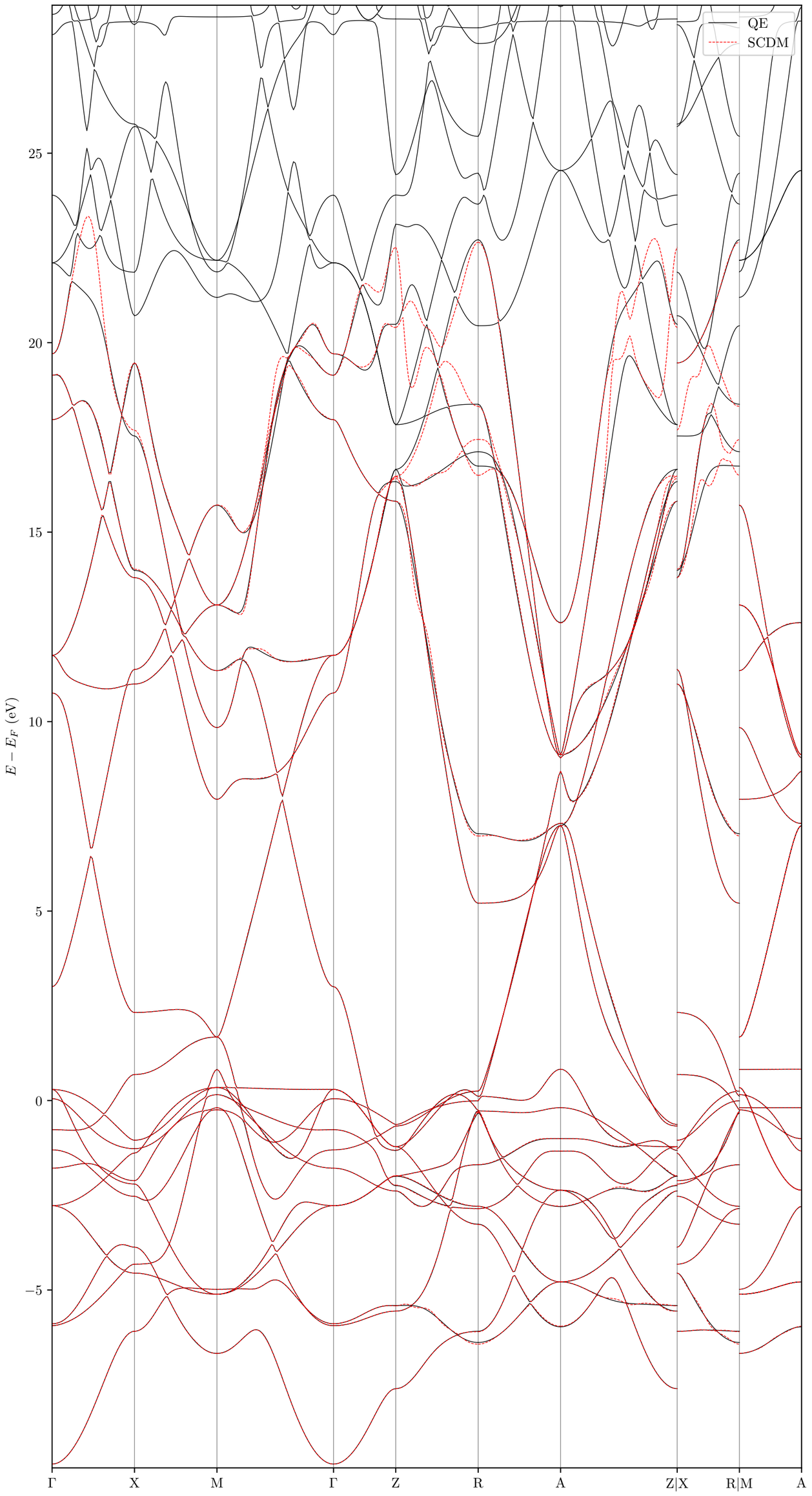
Hamiltonian decay





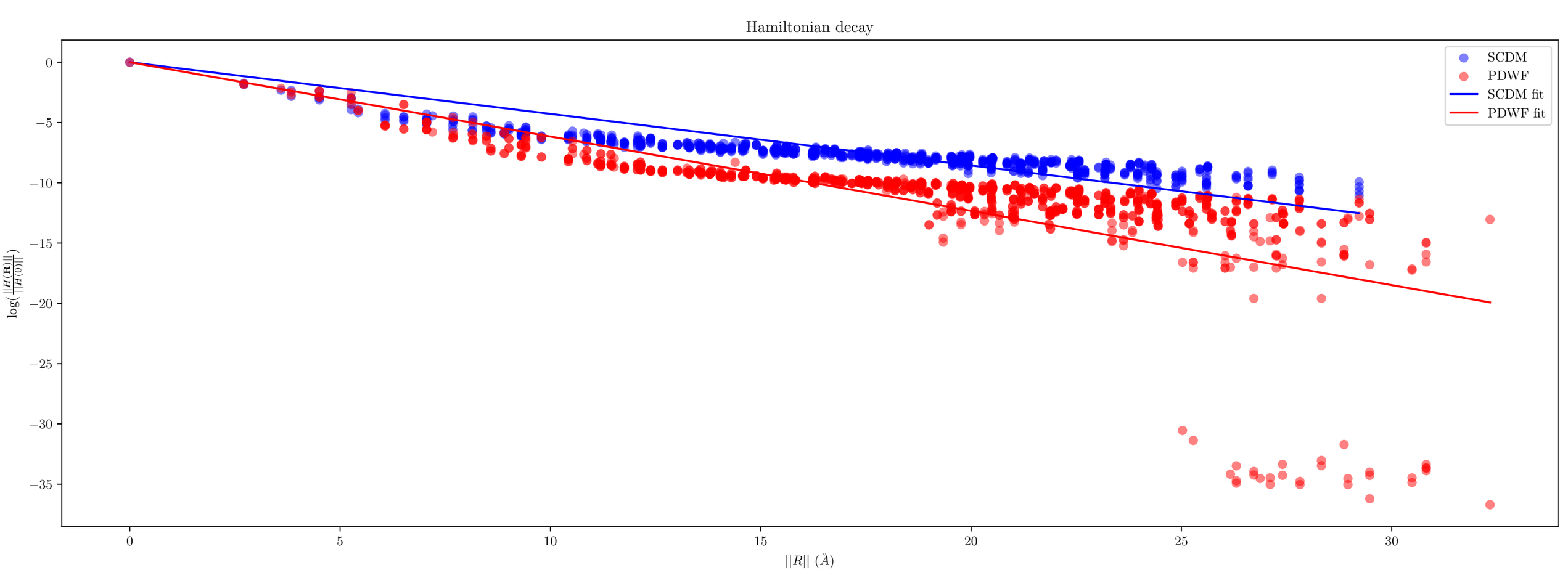

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.9 | 0.9 | 0.9 | 6.6 | 6.6 | 7.9 | 1.623 |

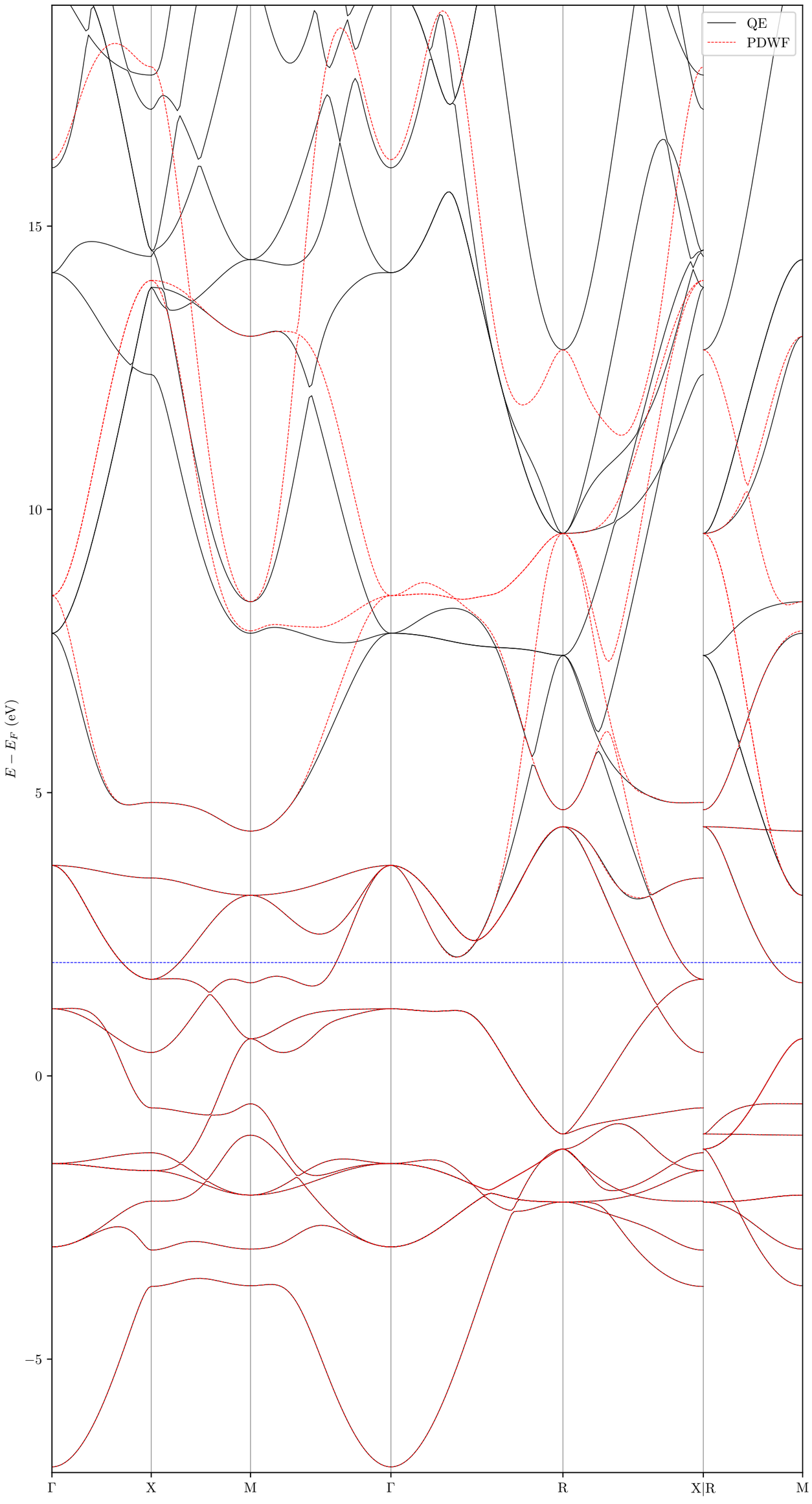



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.5 | 8.1 | 8.3 | 56.6 | 56.6 | 61.0 | 2.336 |



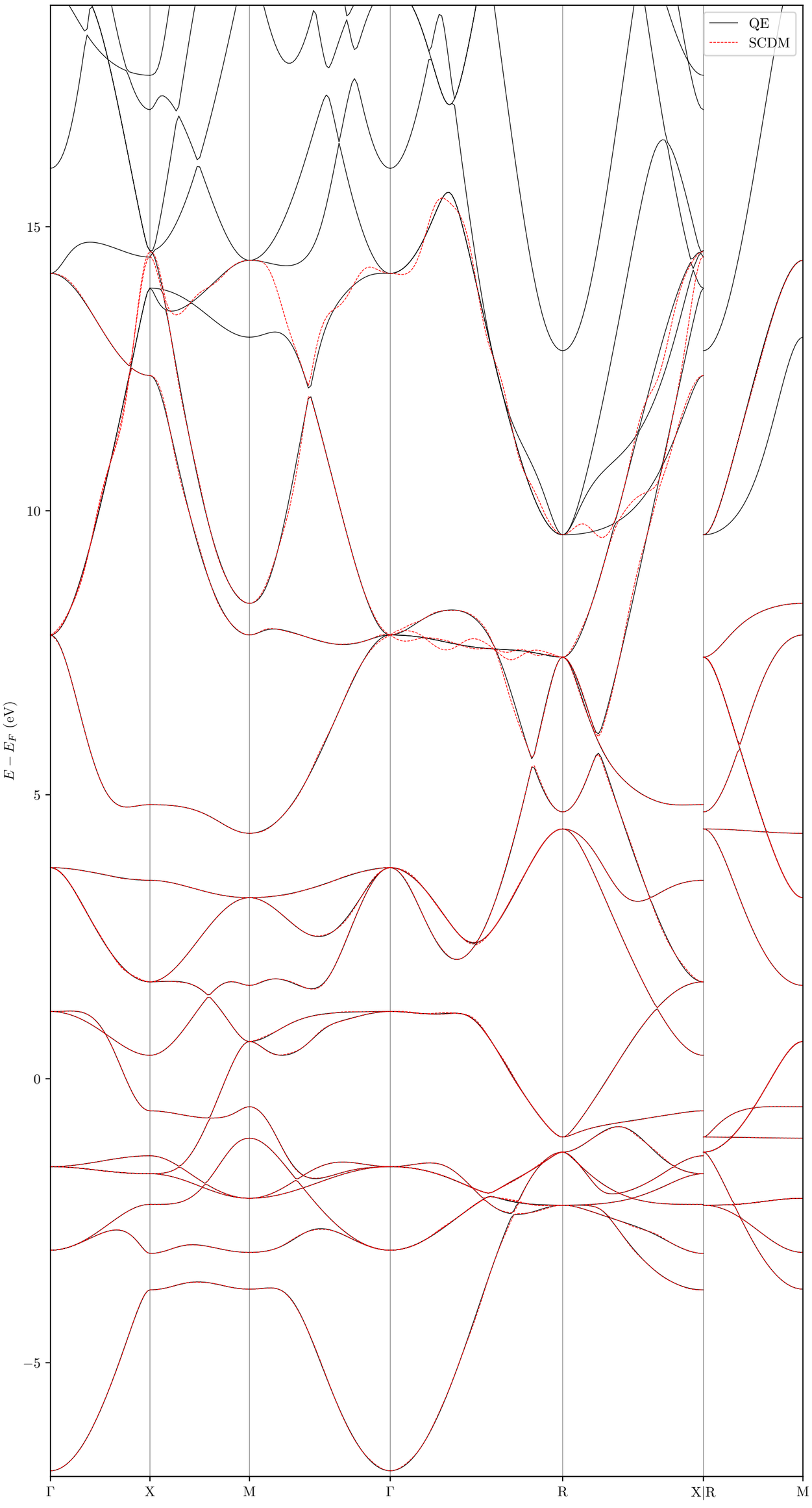
NiSc exclude semicore
PW=87bd431a-d999-4344-83cf-75f636932652
W90=fadb26ea-1d0c-4a4a-b20c-eb63f32654f0




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 0.9 | 9.9 | 7.1 | 7.1 | 175.9 | 1.668 |

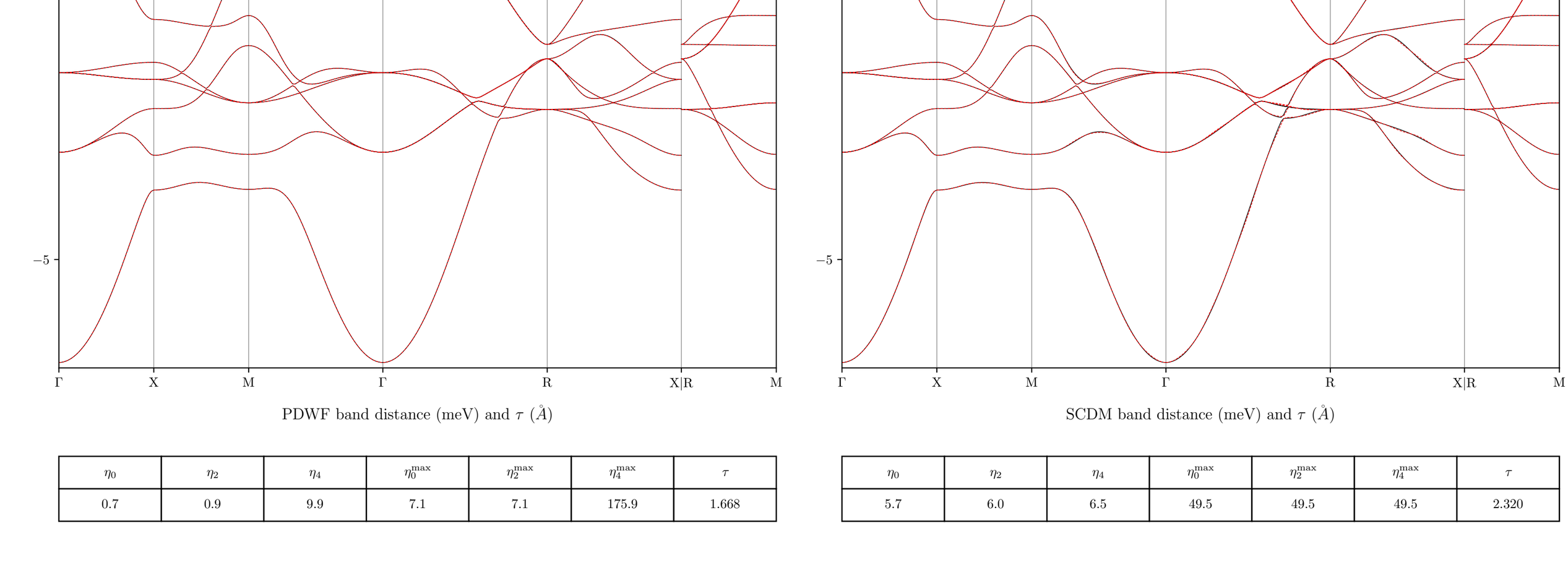
NiSc exclude semicore
PW=87bd431a-d999-4344-83cf-75f636932652
W90=8e6c3164-caef-471d-97bc-09cd121a9dc1



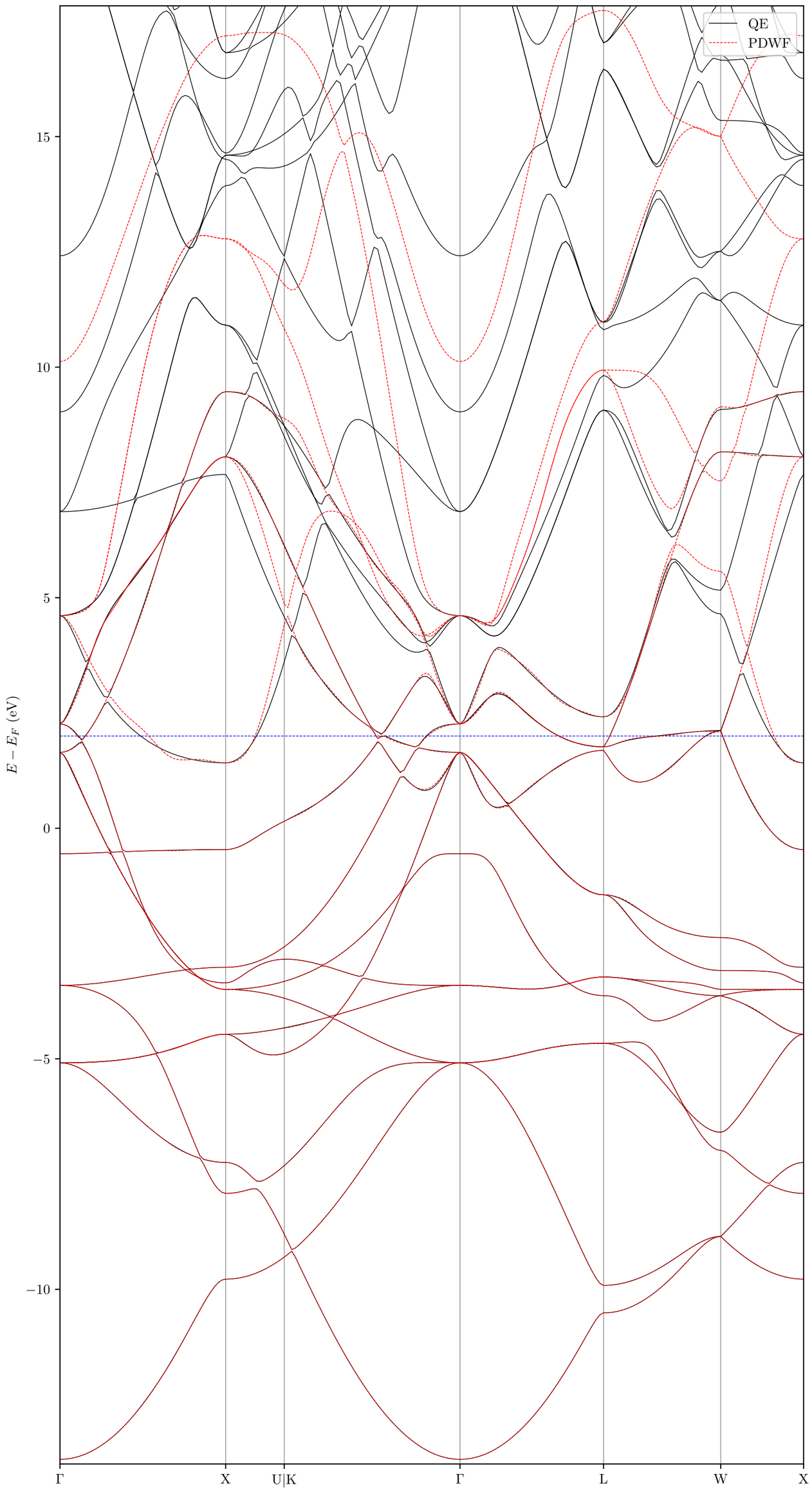

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.7 | 6.0 | 6.5 | 49.5 | 49.5 | 49.5 | 2.320 |

Hamiltonian decay



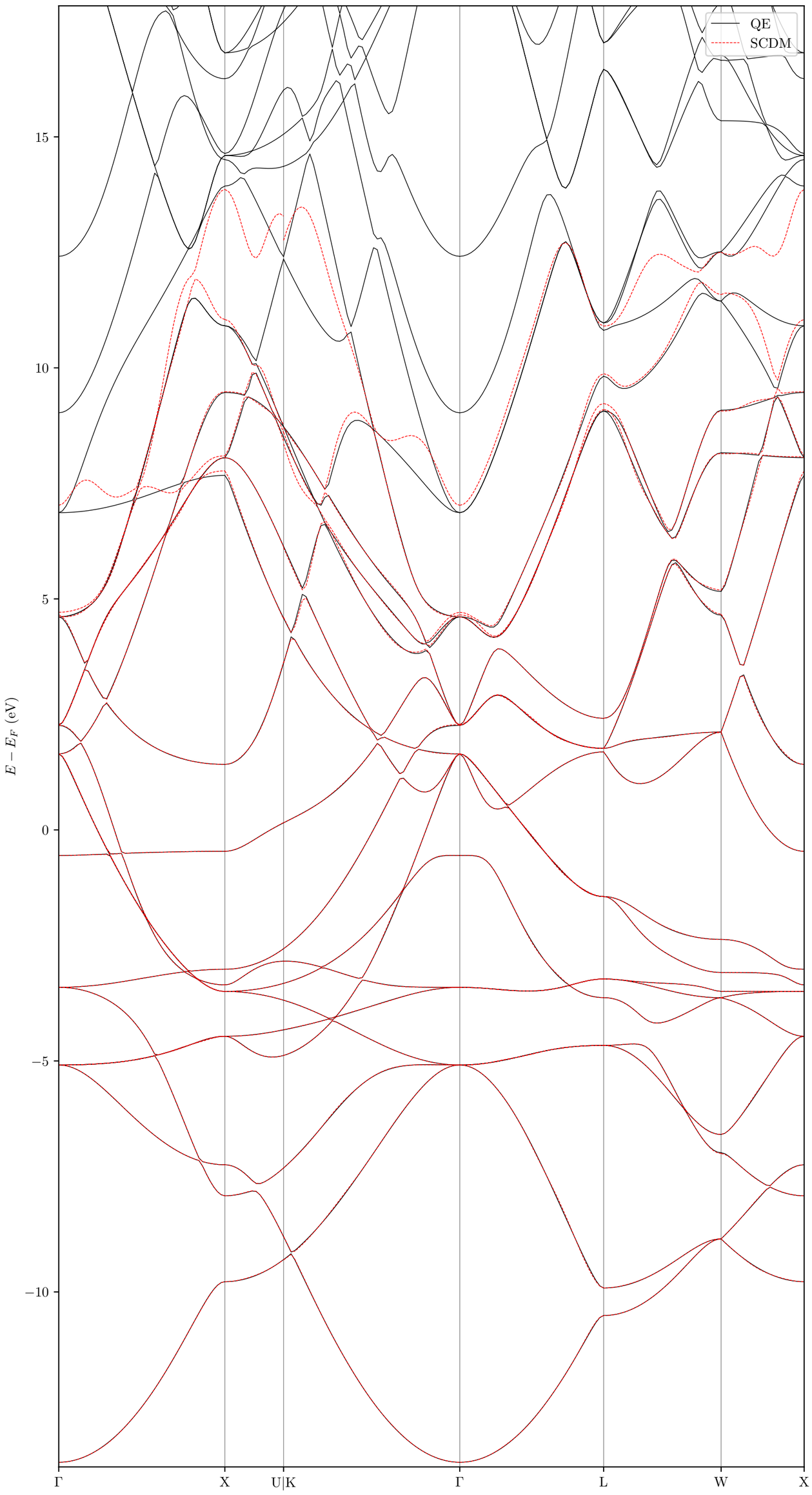
NiSi2 exclude semicore
PW=44b6a71d-1ad5-4e16-a3ef-87c0ef8eb47d
W90=85ebb297-af2e-4e07-acc2-02bdf682e272




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.2 | 9.0 | 43.7 | 15.4 | 91.3 | 636.3 | 2.339 |

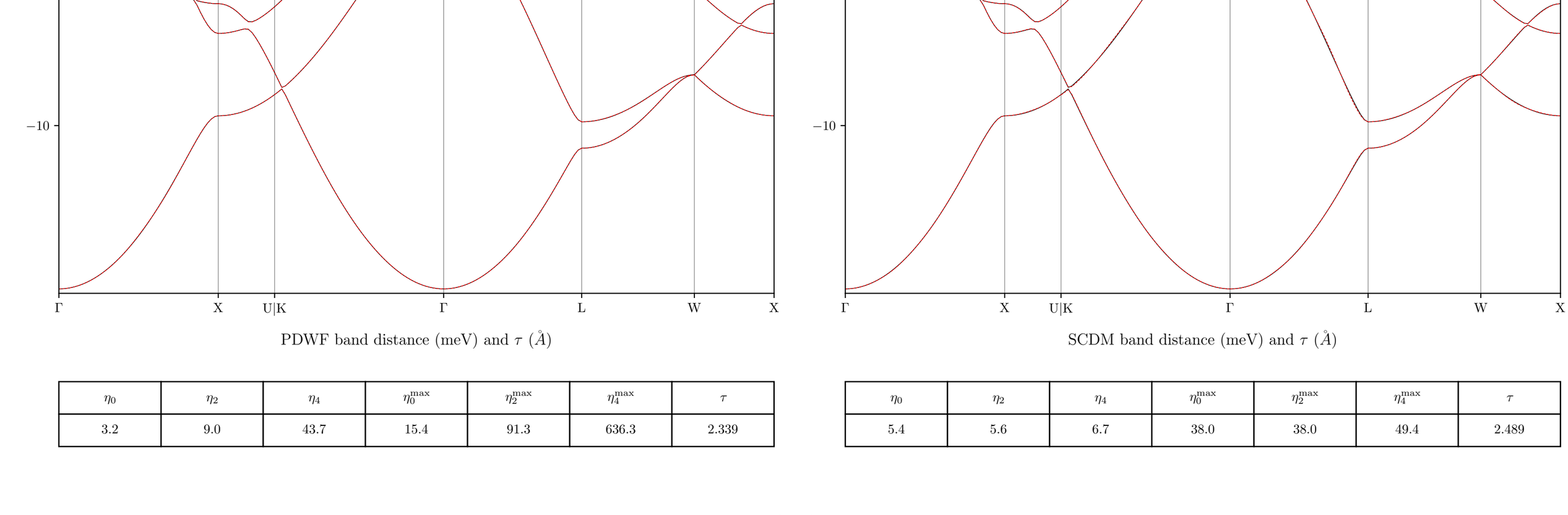
NiSi2 exclude semicore
PW=44b6a71d-1ad5-4e16-a3ef-87c0ef8eb47d
W90=ba5b167d-f590-45f7-9958-769c8728d585



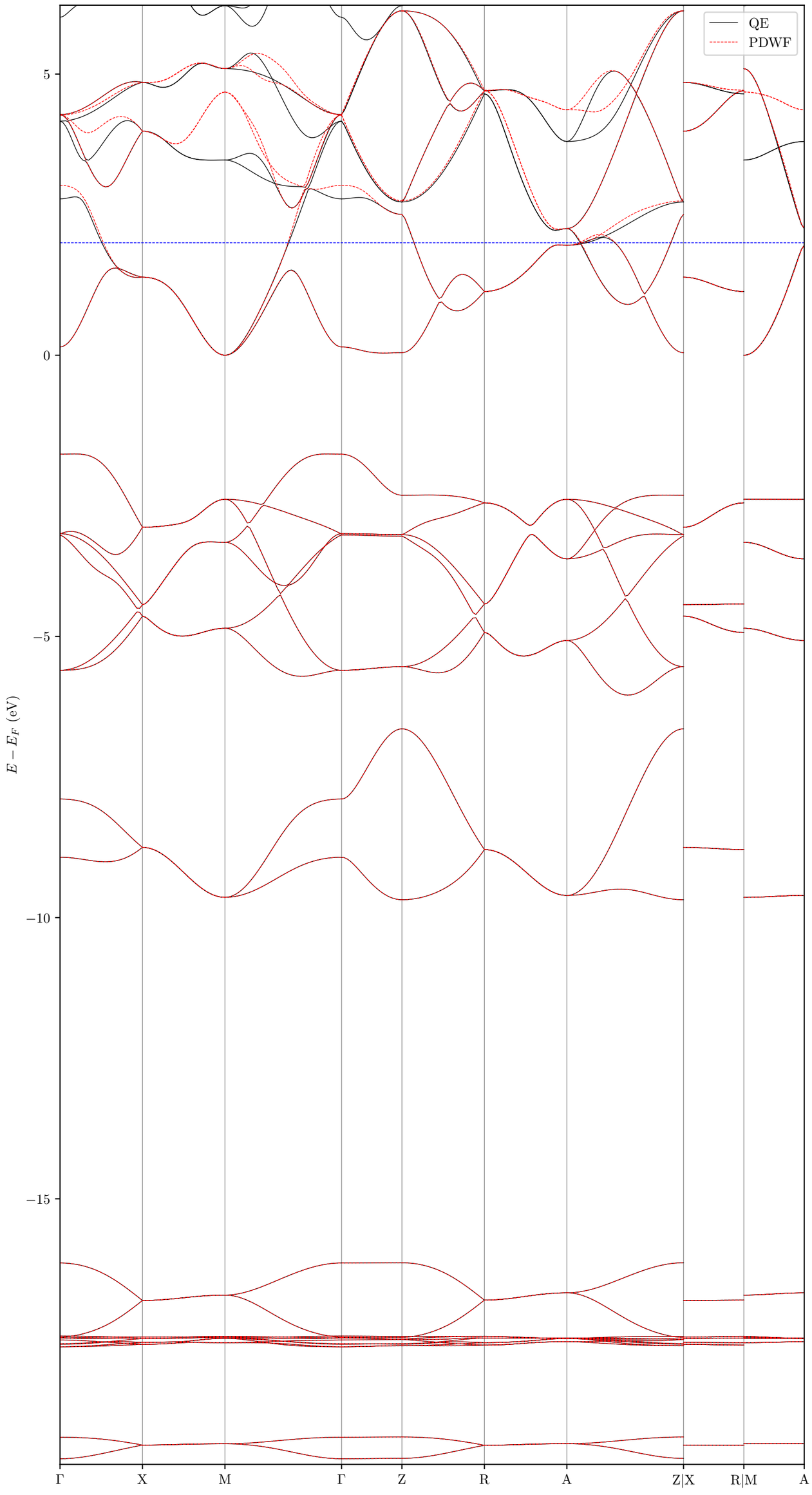

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.4 | 5.6 | 6.7 | 38.0 | 38.0 | 49.4 | 2.489 |

Hamiltonian decay



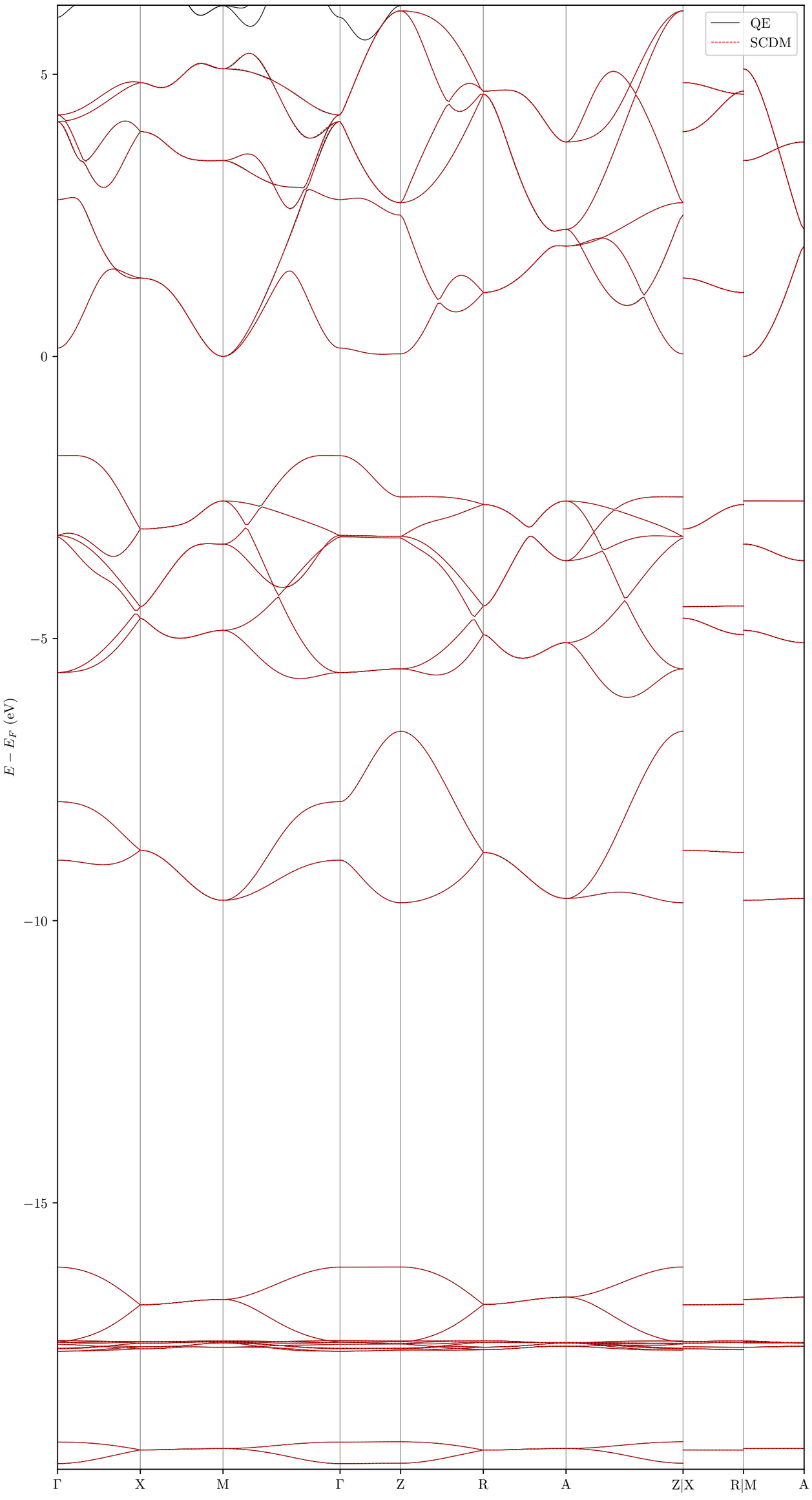
O2Pb2 **INCLUDE** semicore
PW=7a4a74d7-f7dd-413c-9da1-bddc6be7519c
W90=28900b20-59e4-4bbe-8a2a-a547a3a1ee0a




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.8 | 18.8 | 4.6 | 10.1 | 220.5 | 2.189 |

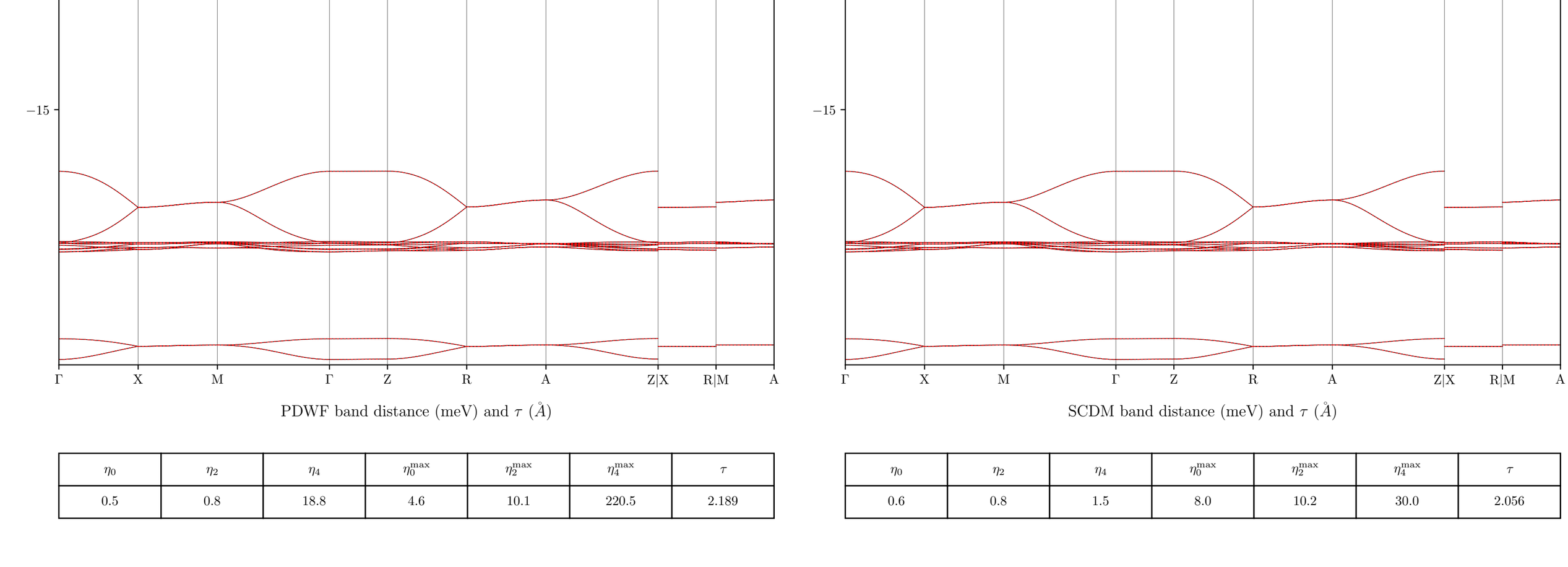
O2Pb2 **INCLUDE** semicore
PW=7a4a74d7-f7dd-413c-9da1-bddc6be7519c
W90=6d75ed9e-b68f-4ef5-8d9f-685f03e41c06

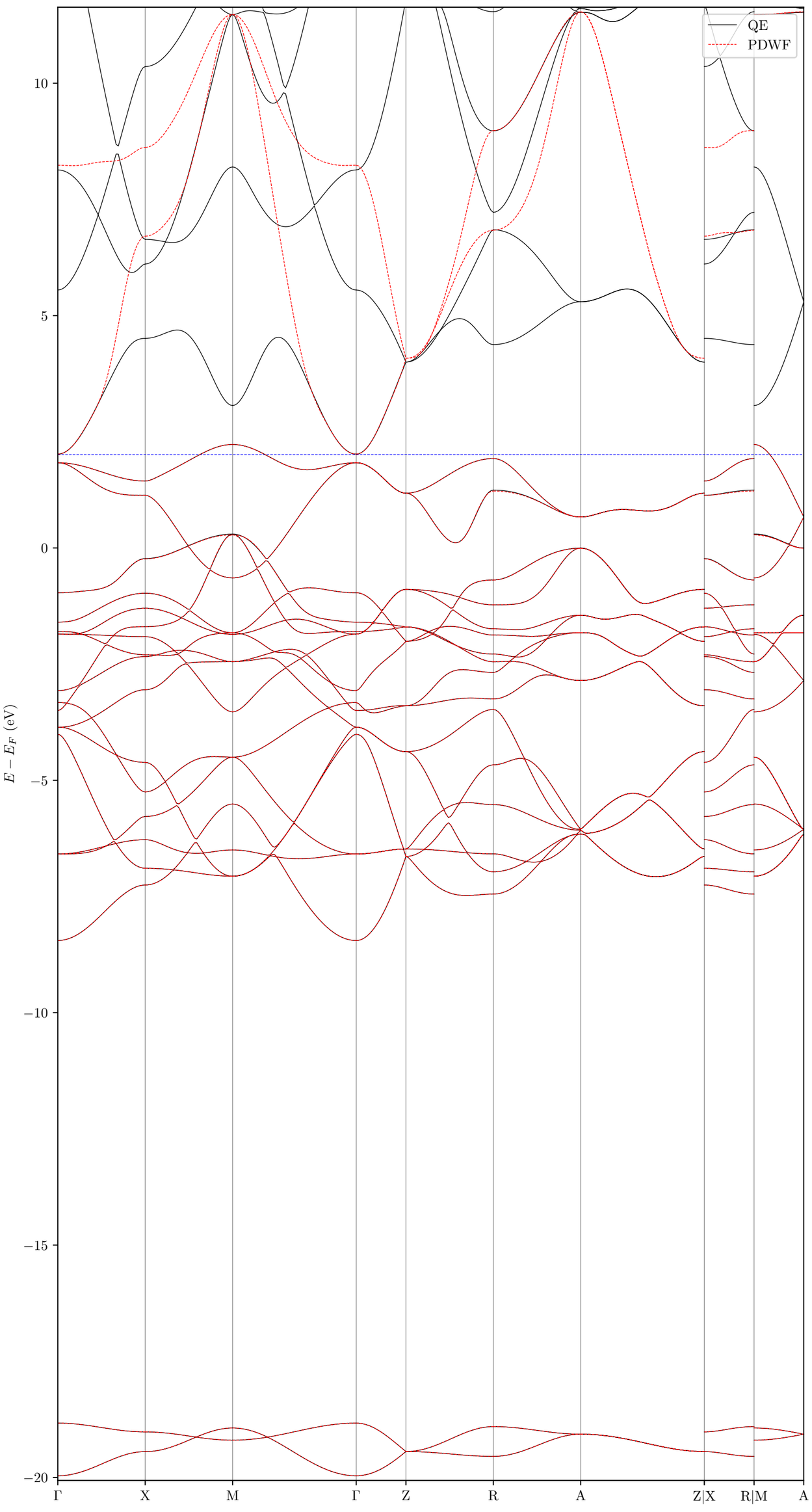



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.8 | 1.5 | 8.0 | 10.2 | 30.0 | 2.056 |

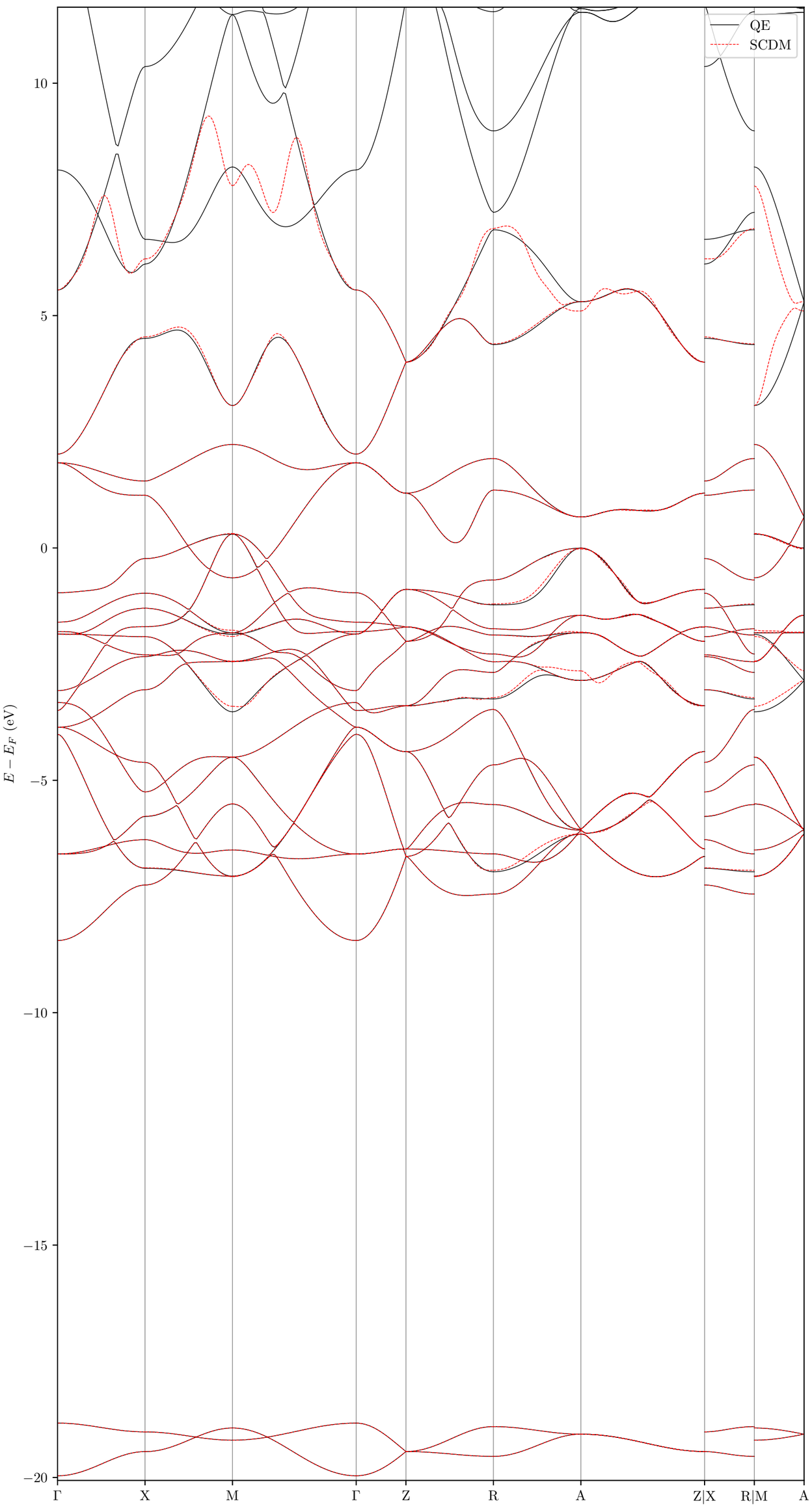
Hamiltonian decay





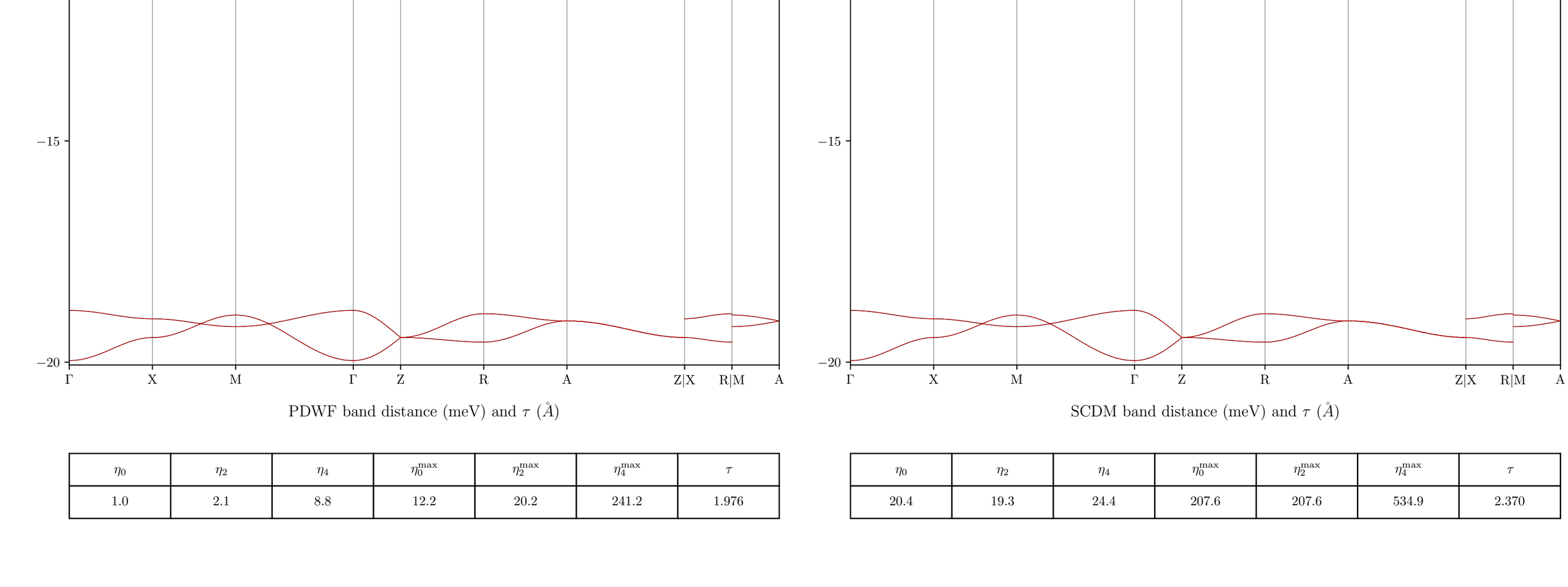

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.0 | 2.1 | 8.8 | 12.2 | 20.2 | 241.2 | 1.976 |

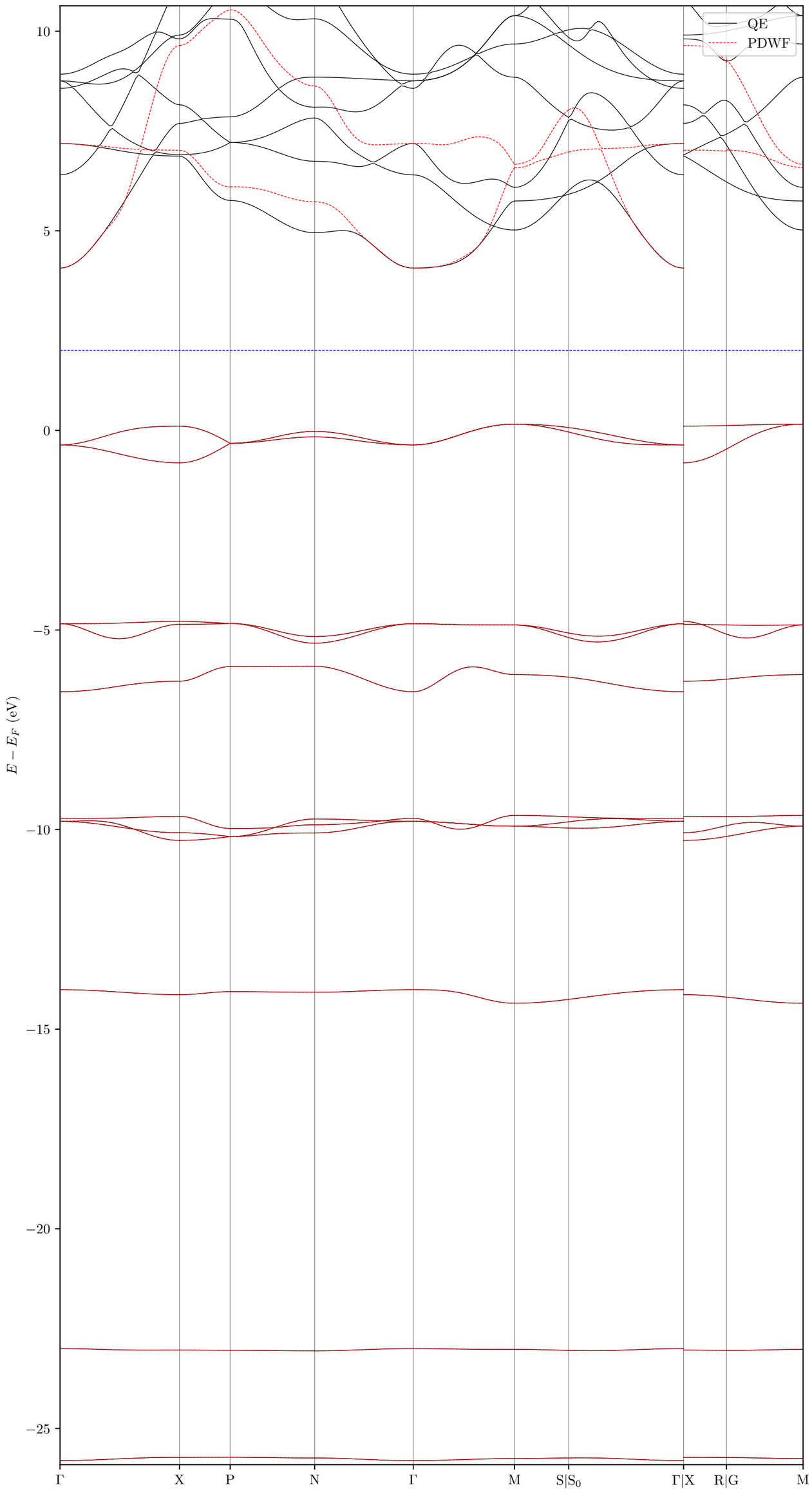



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 20.4 | 19.3 | 24.4 | 207.6 | 207.6 | 534.9 | 2.370 |



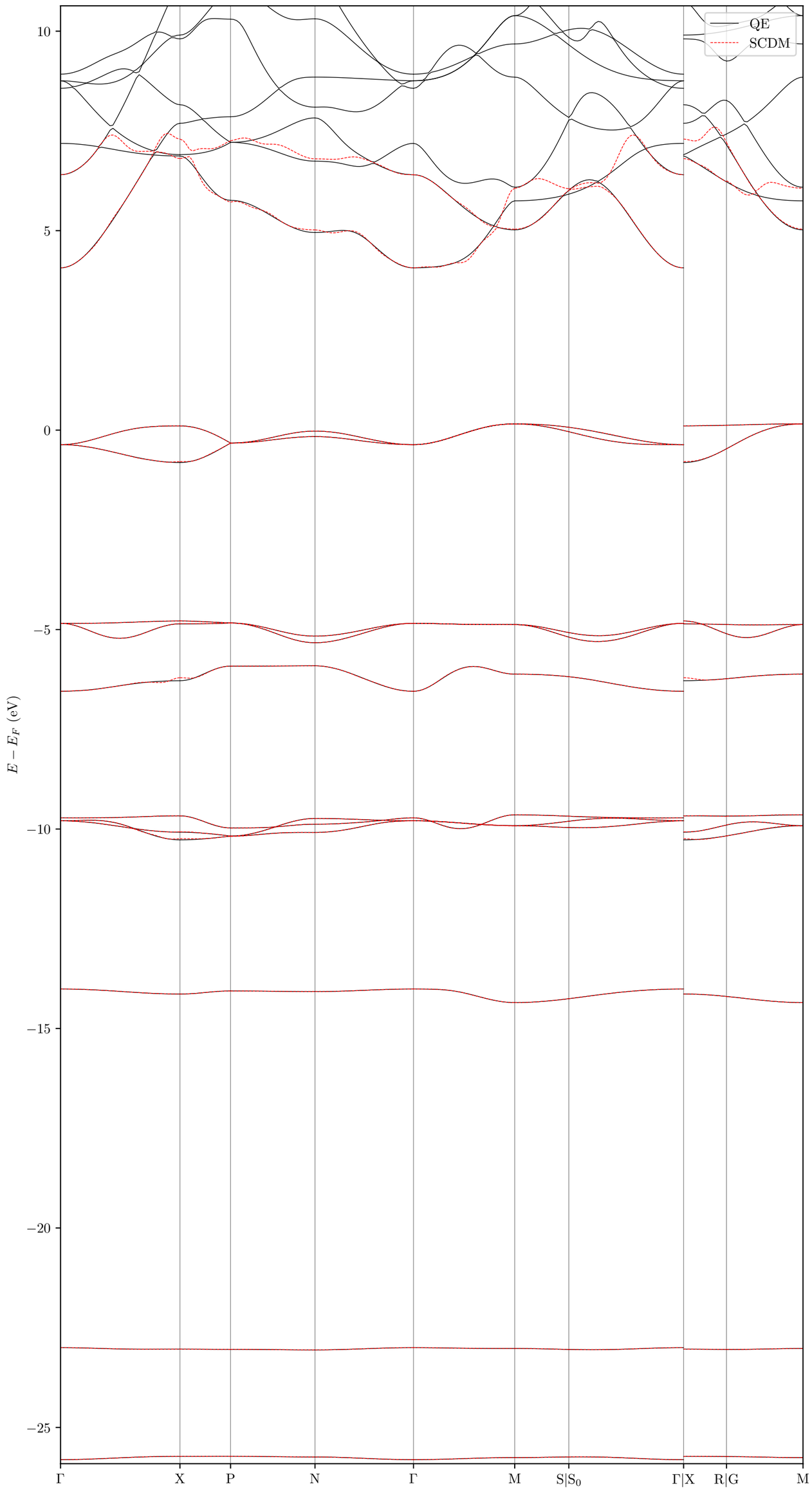
O2Rb **INCLUDE** semicore
PW=f9cdbf71-1b0f-462a-a55d-ecd035676f7c
W90=b9e46f0c-2746-45c4-88d2-7ccb9ca53237




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 0.7 | 0.9 | 3.9 | 3.9 | 3.9 | 2.196 |

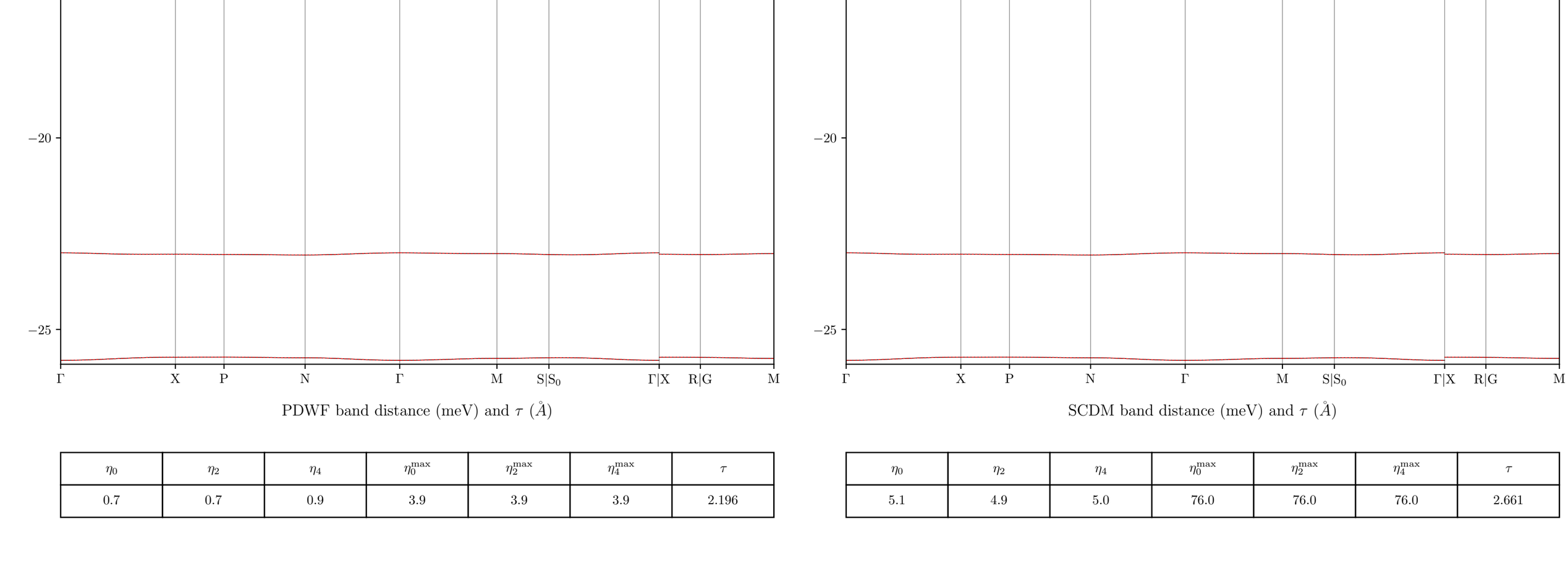
O2Rb **INCLUDE** semicore
PW=f9cdbf71-1b0f-462a-a55d-ecd035676f7c
W90=d6024ccc-3262-444e-ab14-ffecf0c81723



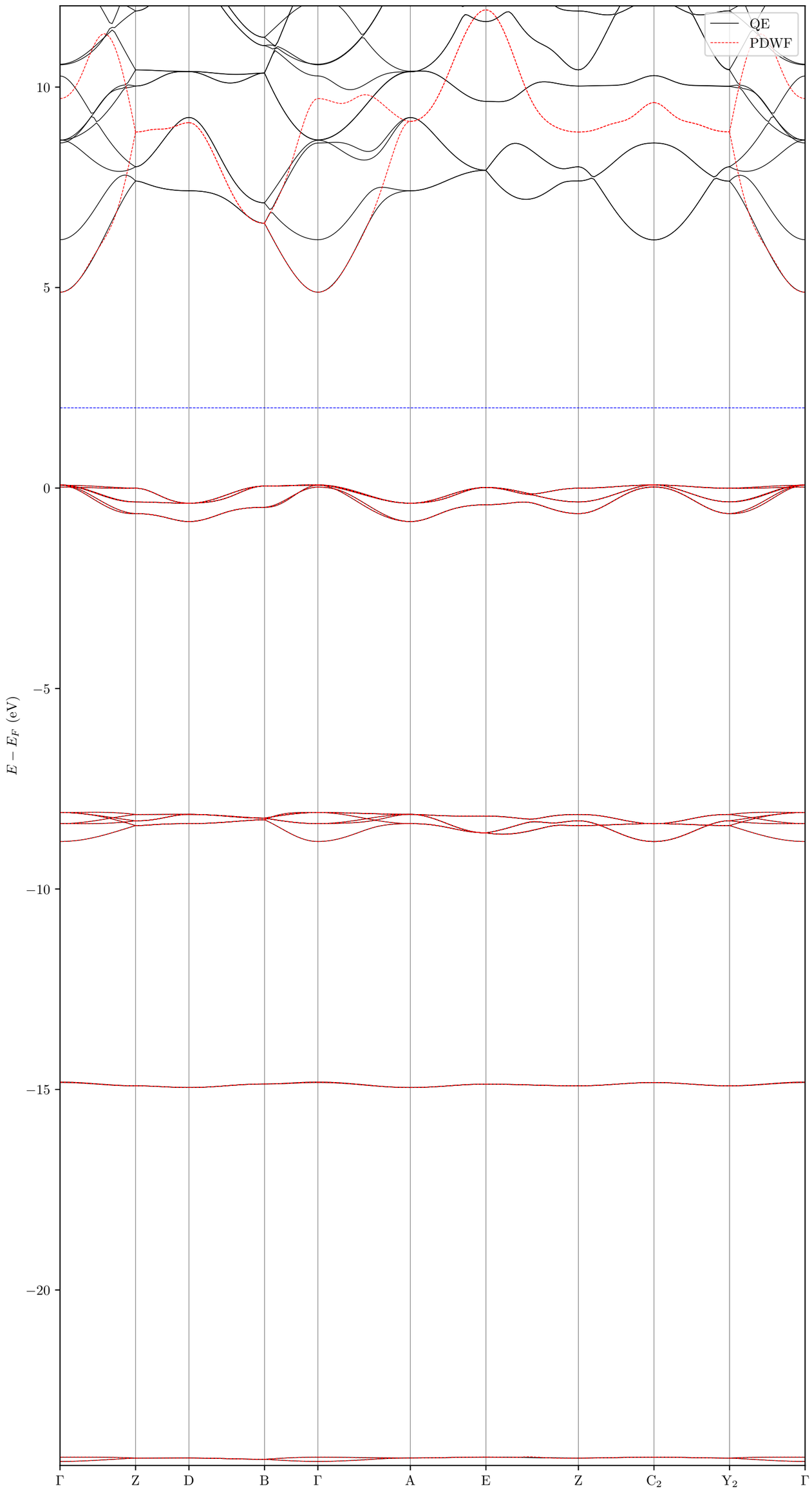

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.1 | 4.9 | 5.0 | 76.0 | 76.0 | 76.0 | 2.661 |

Hamiltonian decay



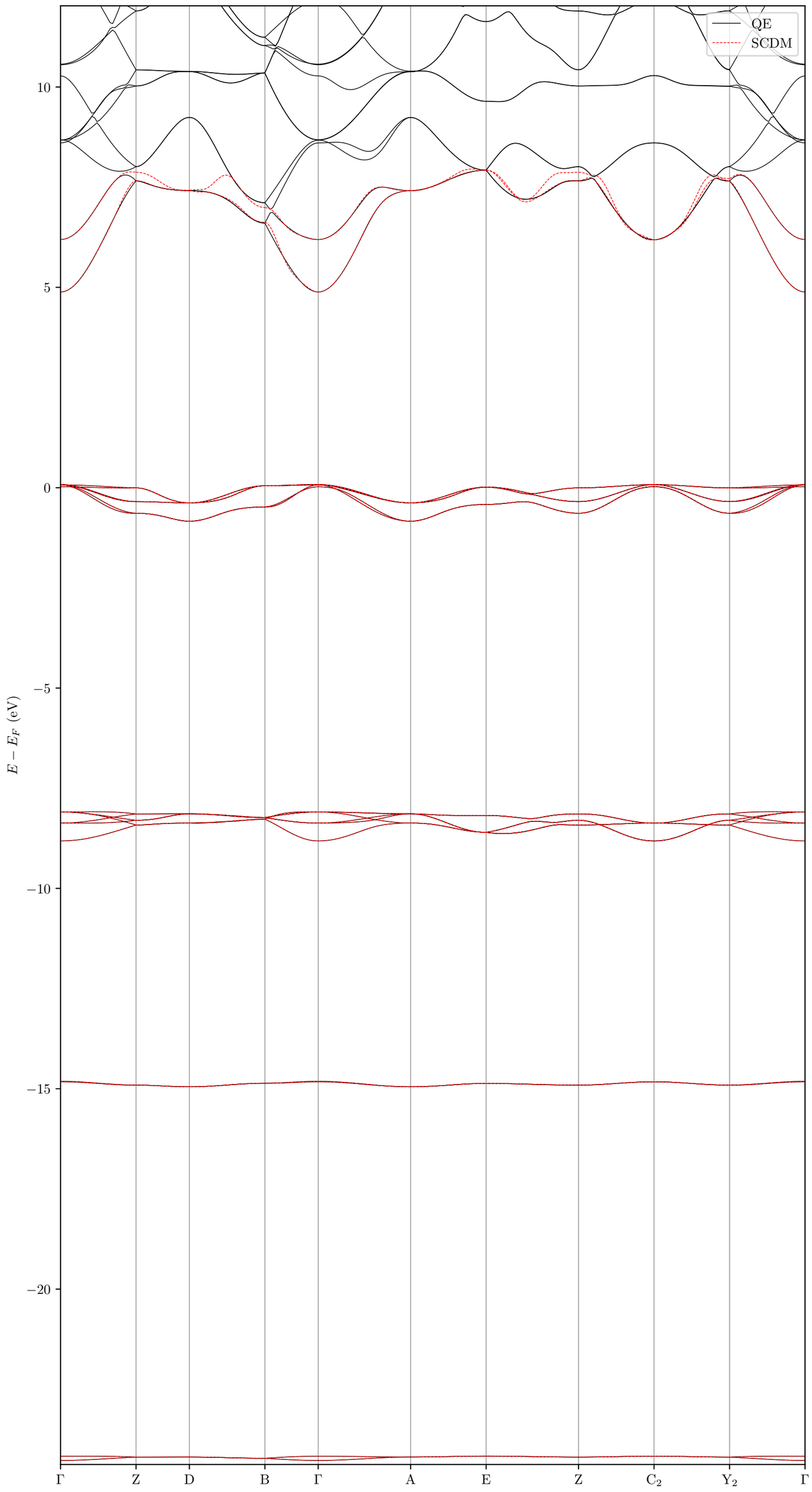
O2Rb2 **INCLUDE** semicore
PW=d7432188-936d-417e-9273-709986f64b5b
W90=1525ee02-8aa6-4f5c-af84-e2998a177843




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.1 | 1.1 | 16.0 | 16.0 | 16.0 | 2.178 |

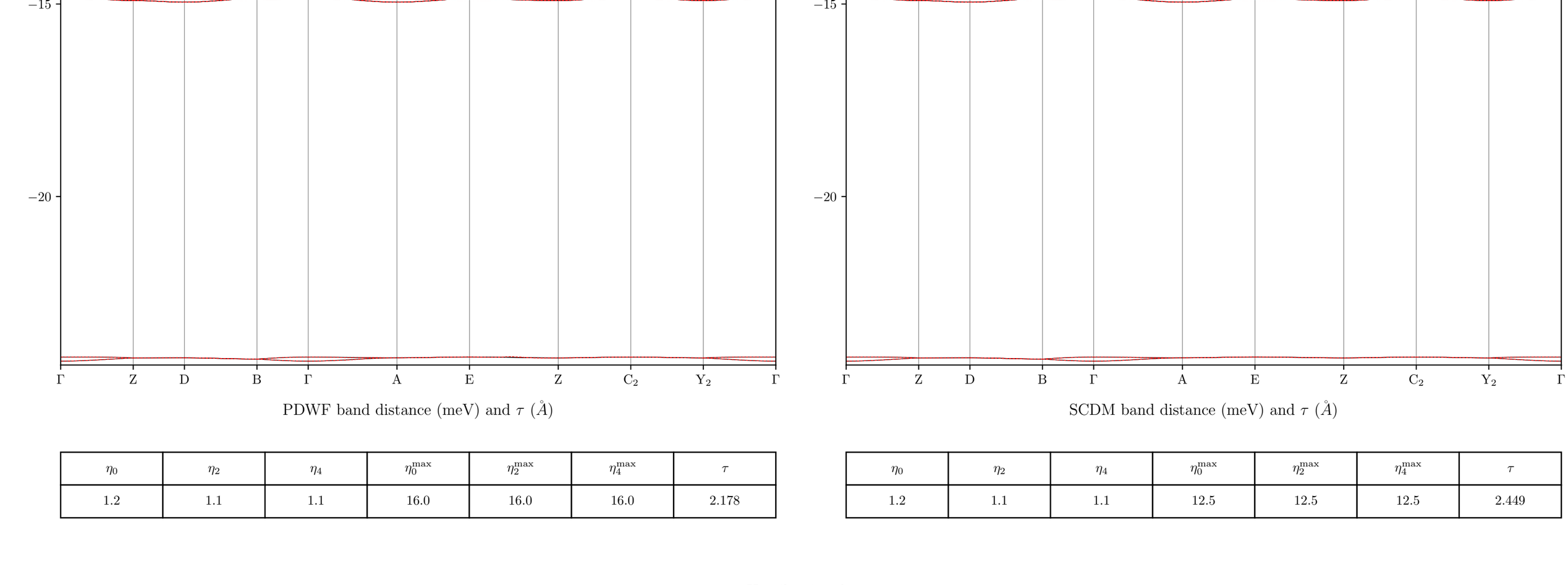
O2Rb2 **INCLUDE** semicore
PW=d7432188-936d-417e-9273-709986f64b5b
W90=ece5d91a-a02e-436b-b5c5-b757f970eb29



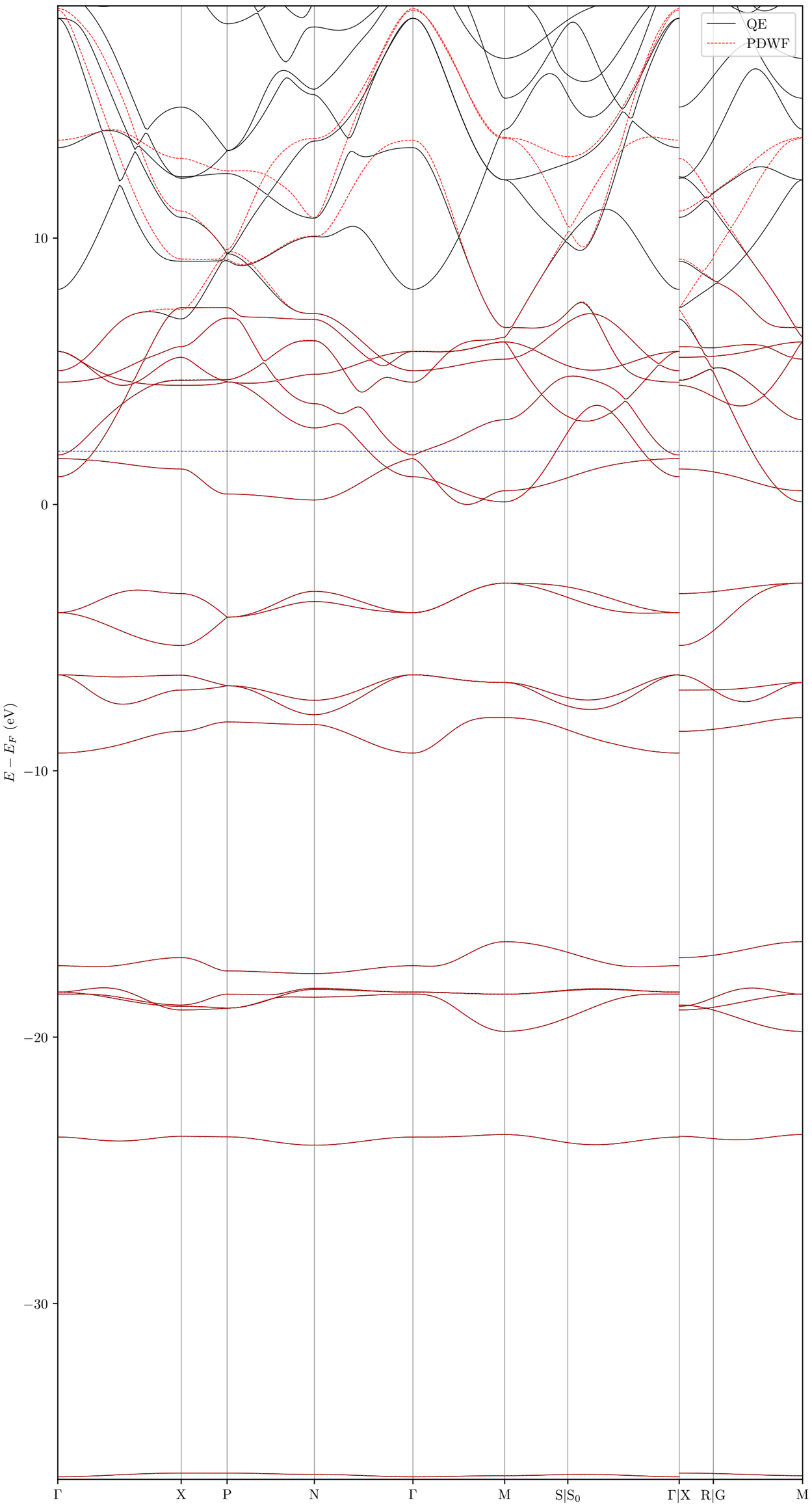

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.1 | 1.1 | 12.5 | 12.5 | 12.5 | 2.449 |

Hamiltonian decay



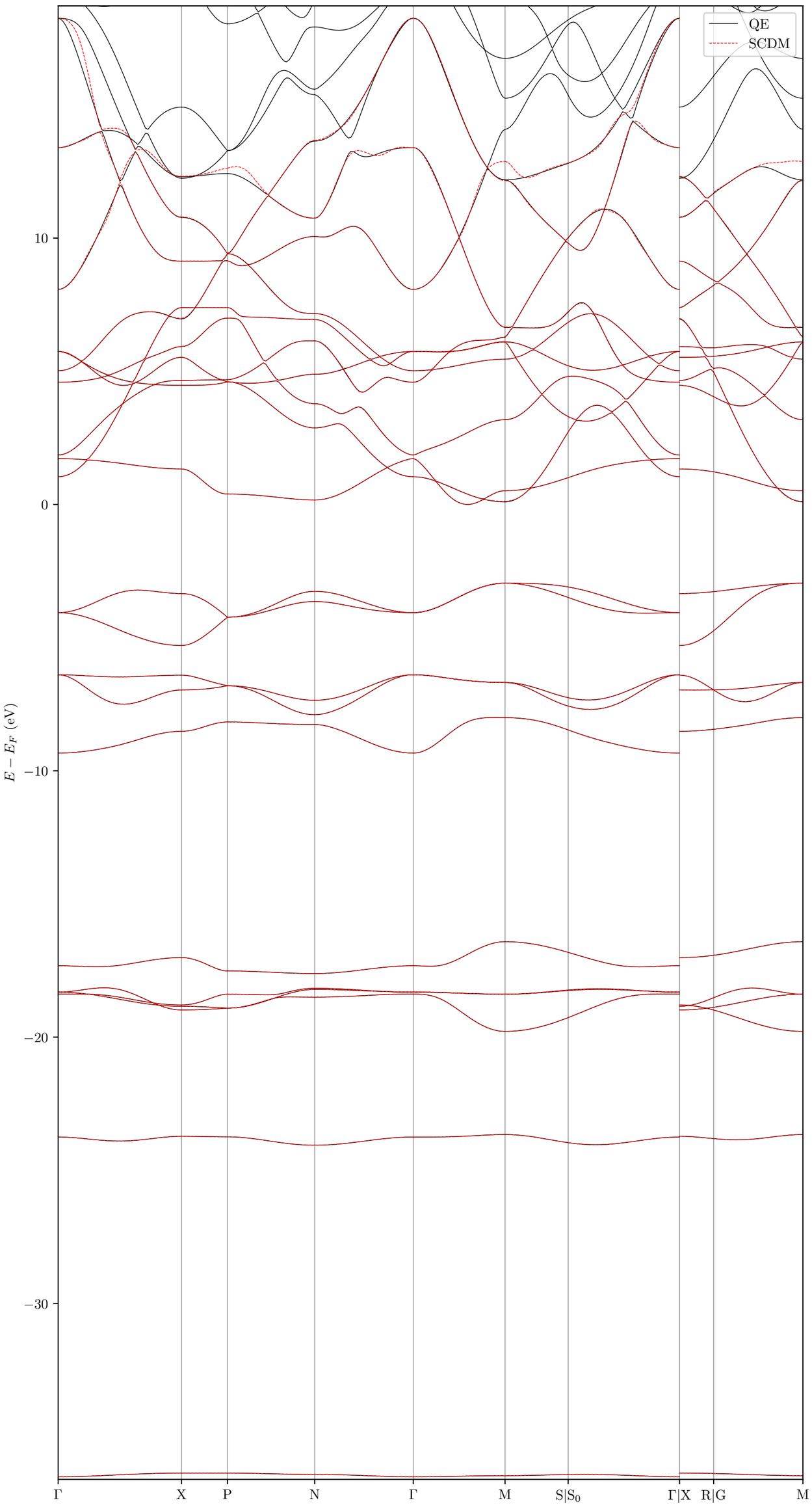
O2Sr **INCLUDE** semicore
PW=23767a8d-8dd3-4522-a646-4e007977a603
W90=db18bb6f-97a9-416d-8495-bafa8c561447




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 0.5 | 0.6 | 2.5 | 7.6 | 7.6 | 2.175 |

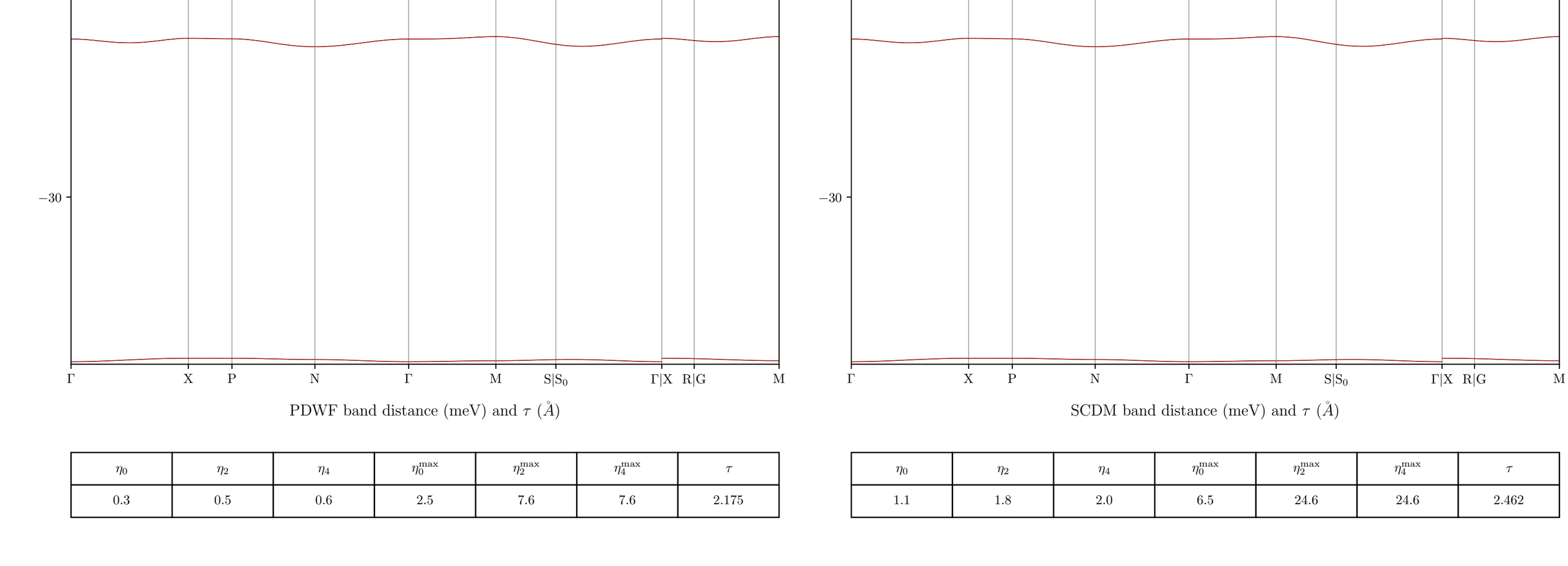
O2Sr **INCLUDE** semicore
PW=23767a8d-8dd3-4522-a646-4e007977a603
W90=415251d8-c67b-4902-bcfd-036d8ea57206

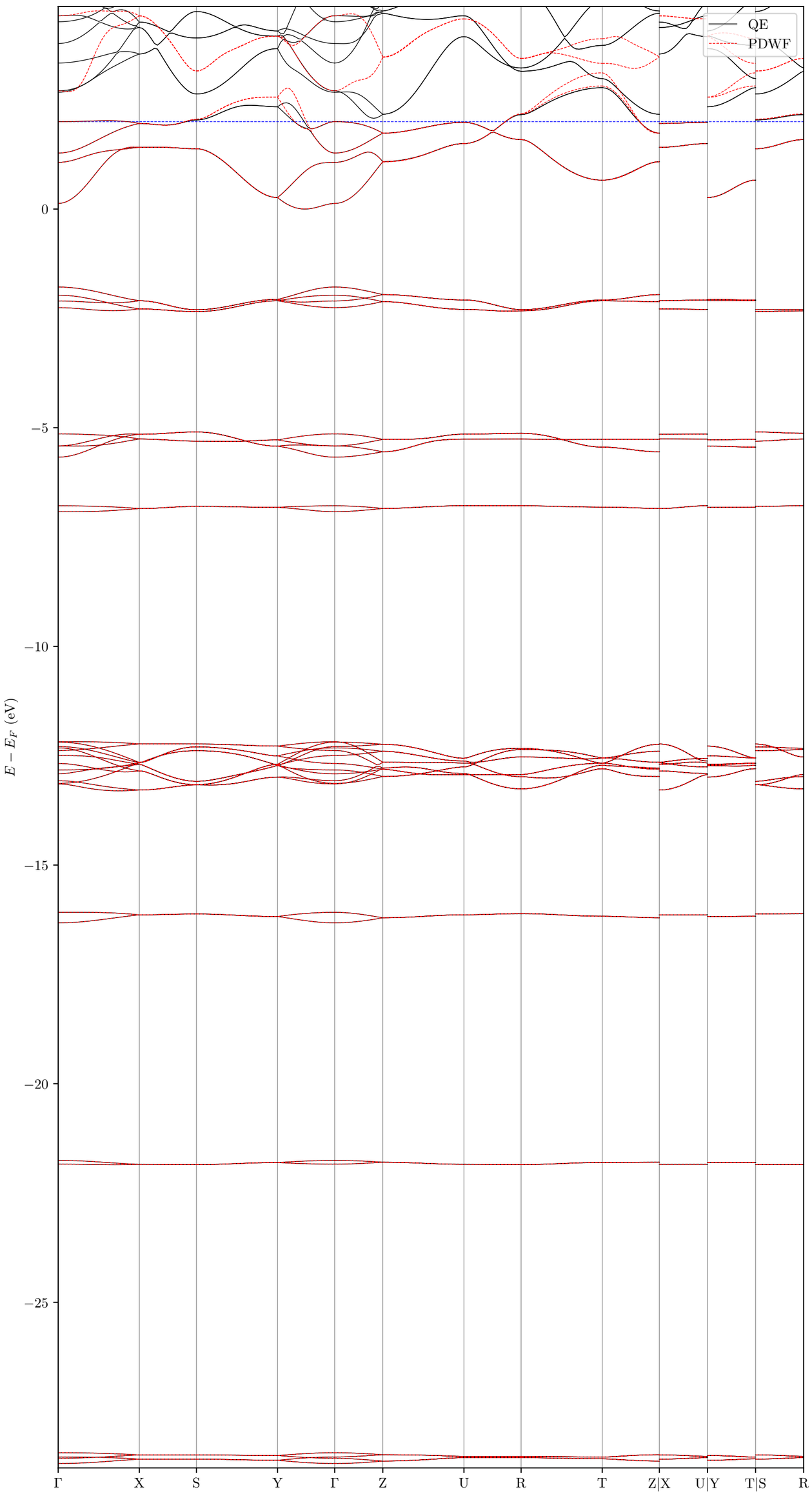



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.8 | 2.0 | 6.5 | 24.6 | 24.6 | 2.462 |

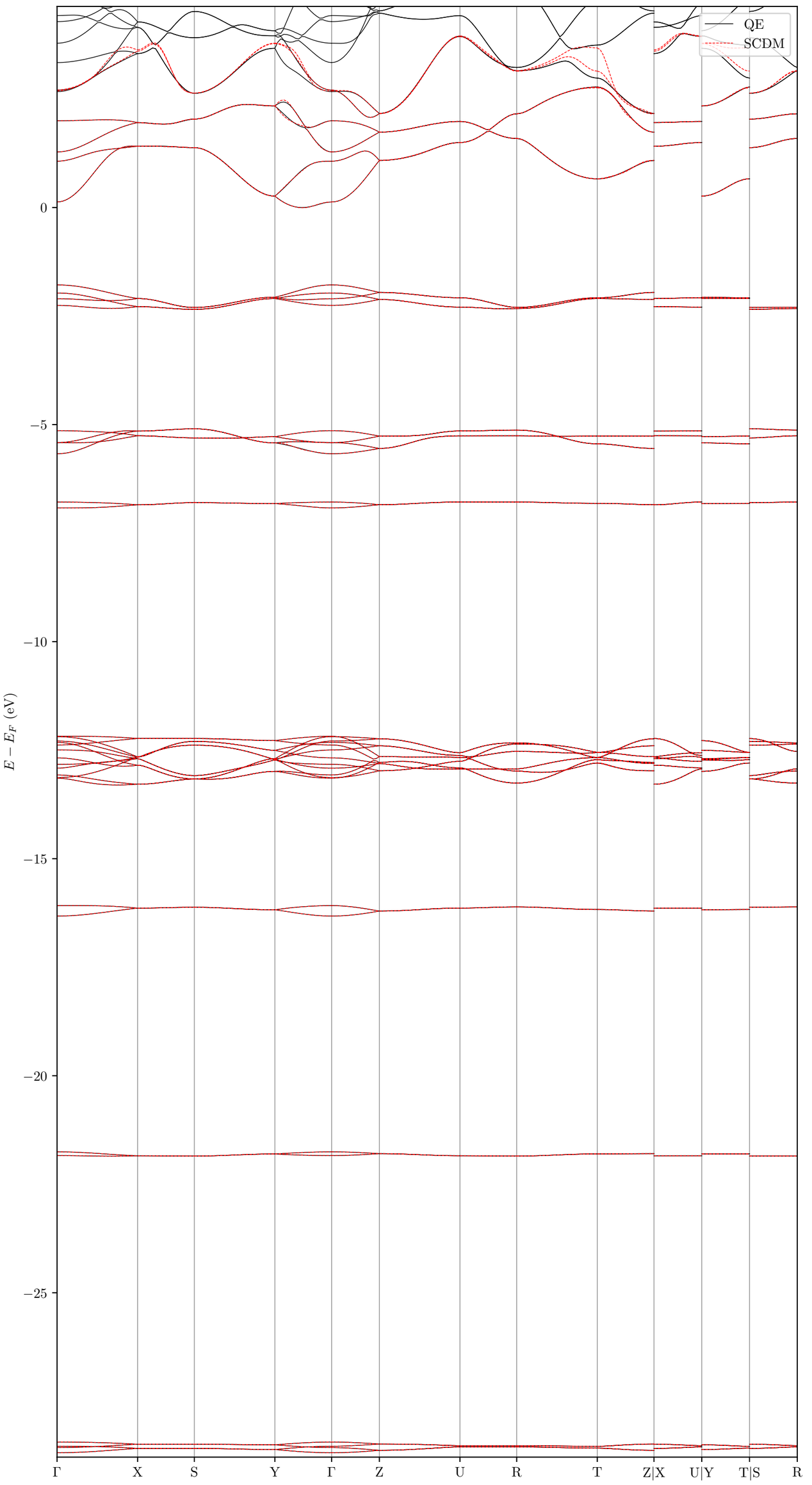
Hamiltonian decay





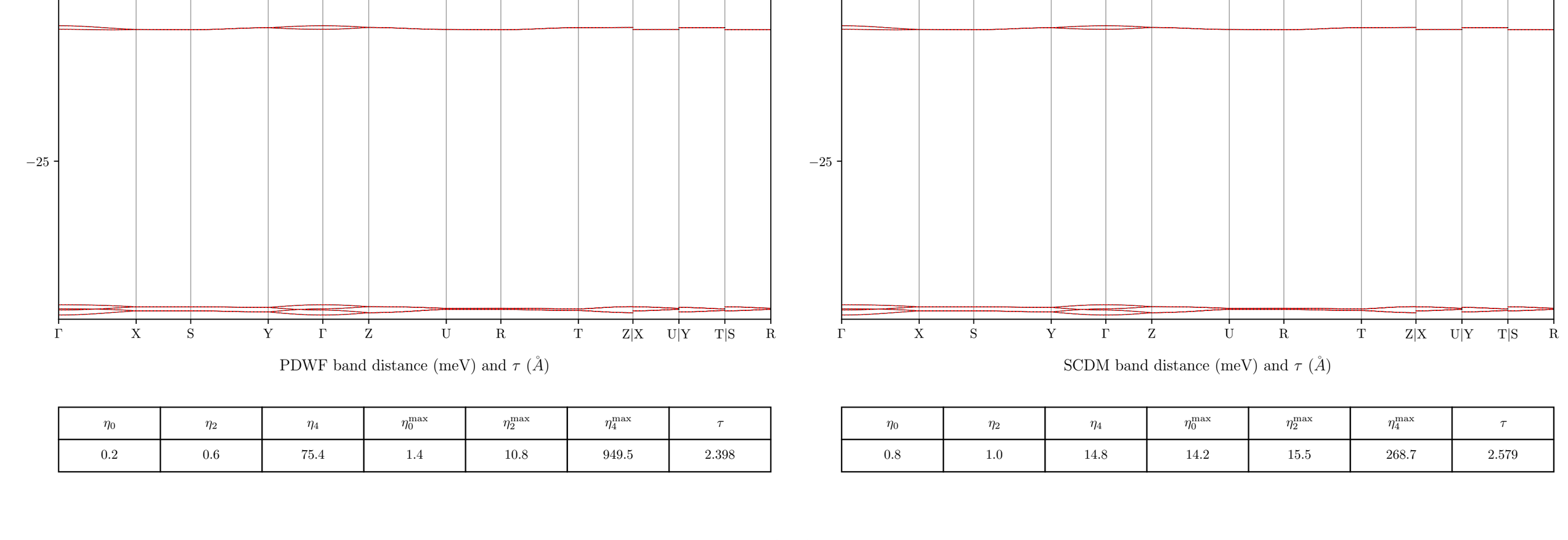

PDWF band distance (meV) and $\tau$ ($\AA$)

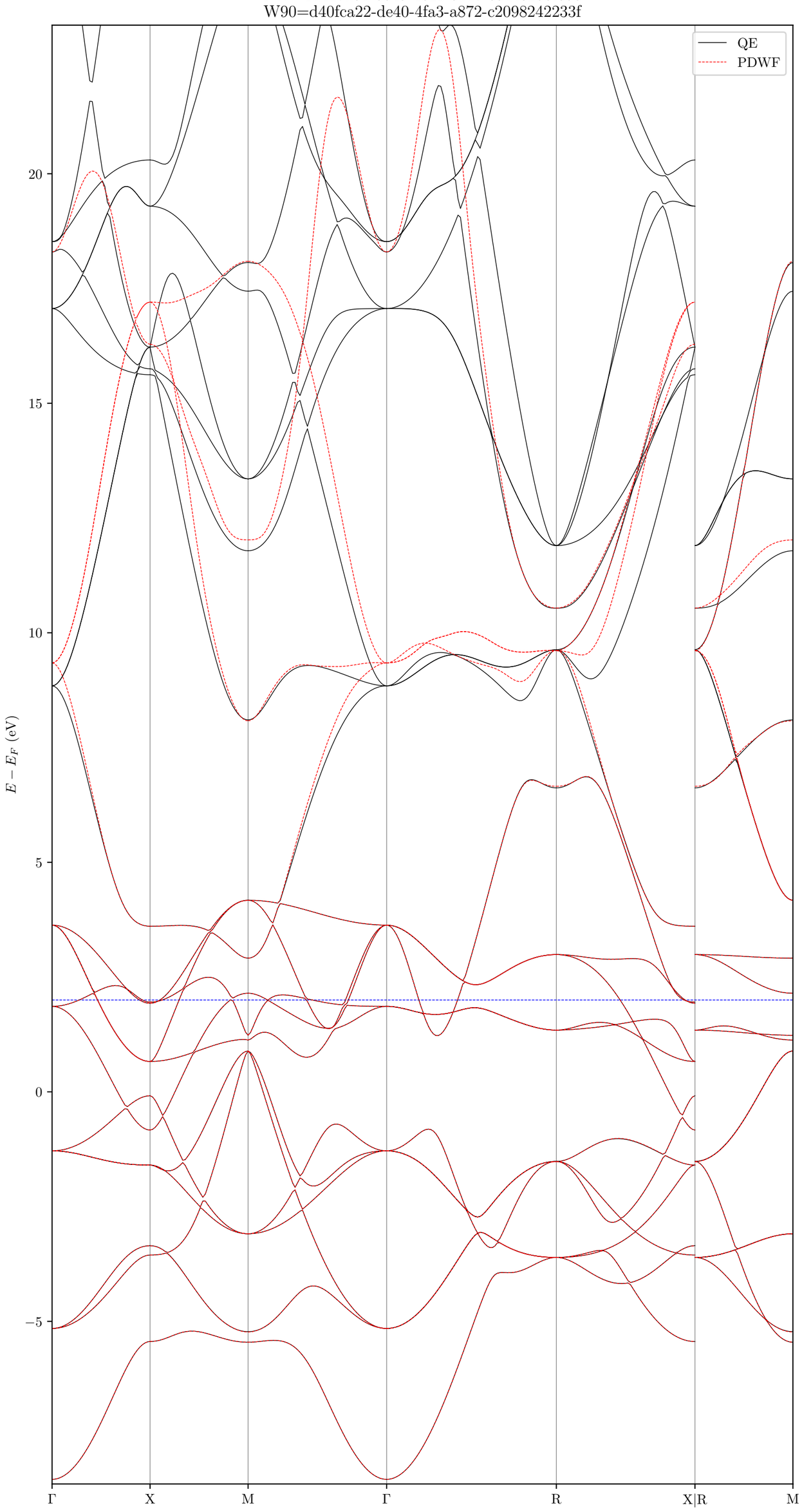
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.2 | 0.6 | 75.4 | 1.4 | 10.8 | 949.5 | 2.398 |




SCDM band distance (meV) and $\tau$ ($\AA$)

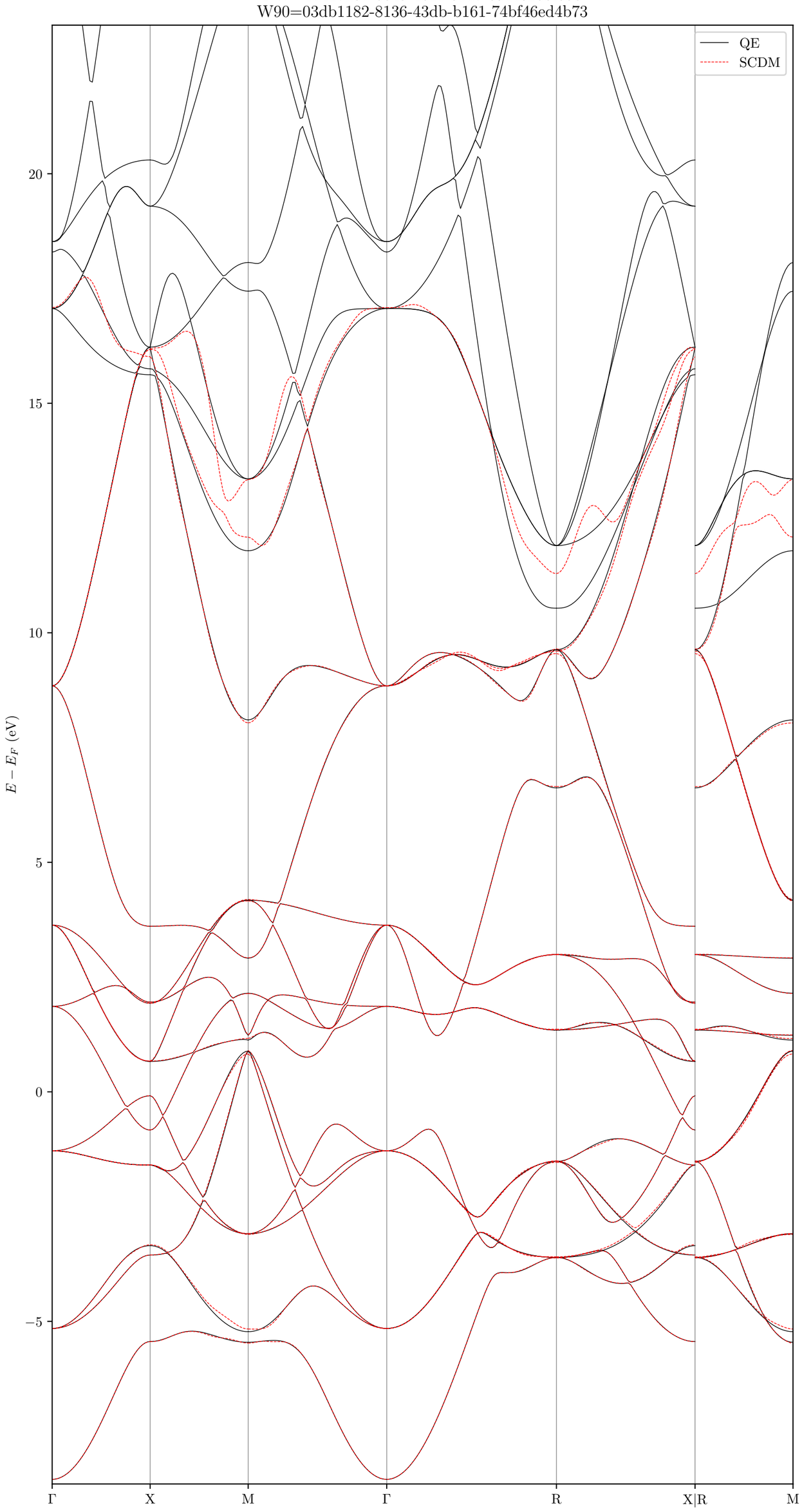
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.8 | 1.0 | 14.8 | 14.2 | 15.5 | 268.7 | 2.579 |





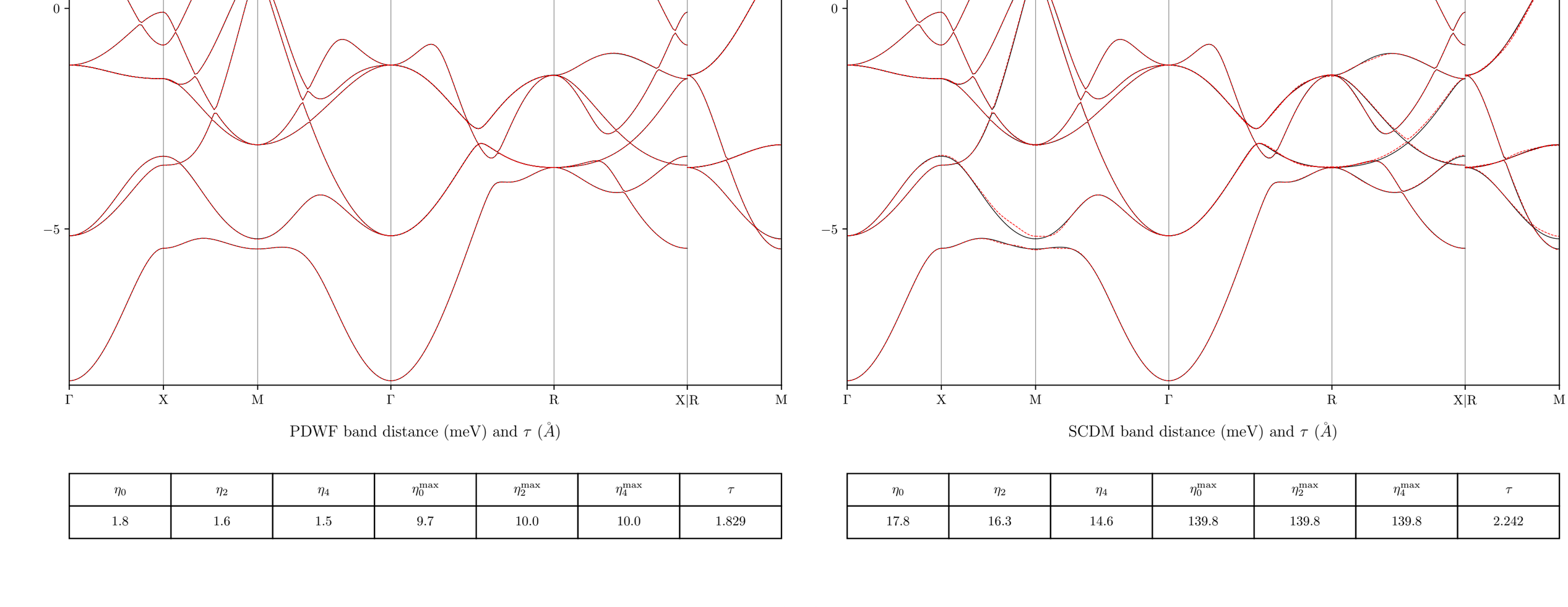

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.8 | 1.6 | 1.5 | 9.7 | 10.0 | 10.0 | 1.829 |

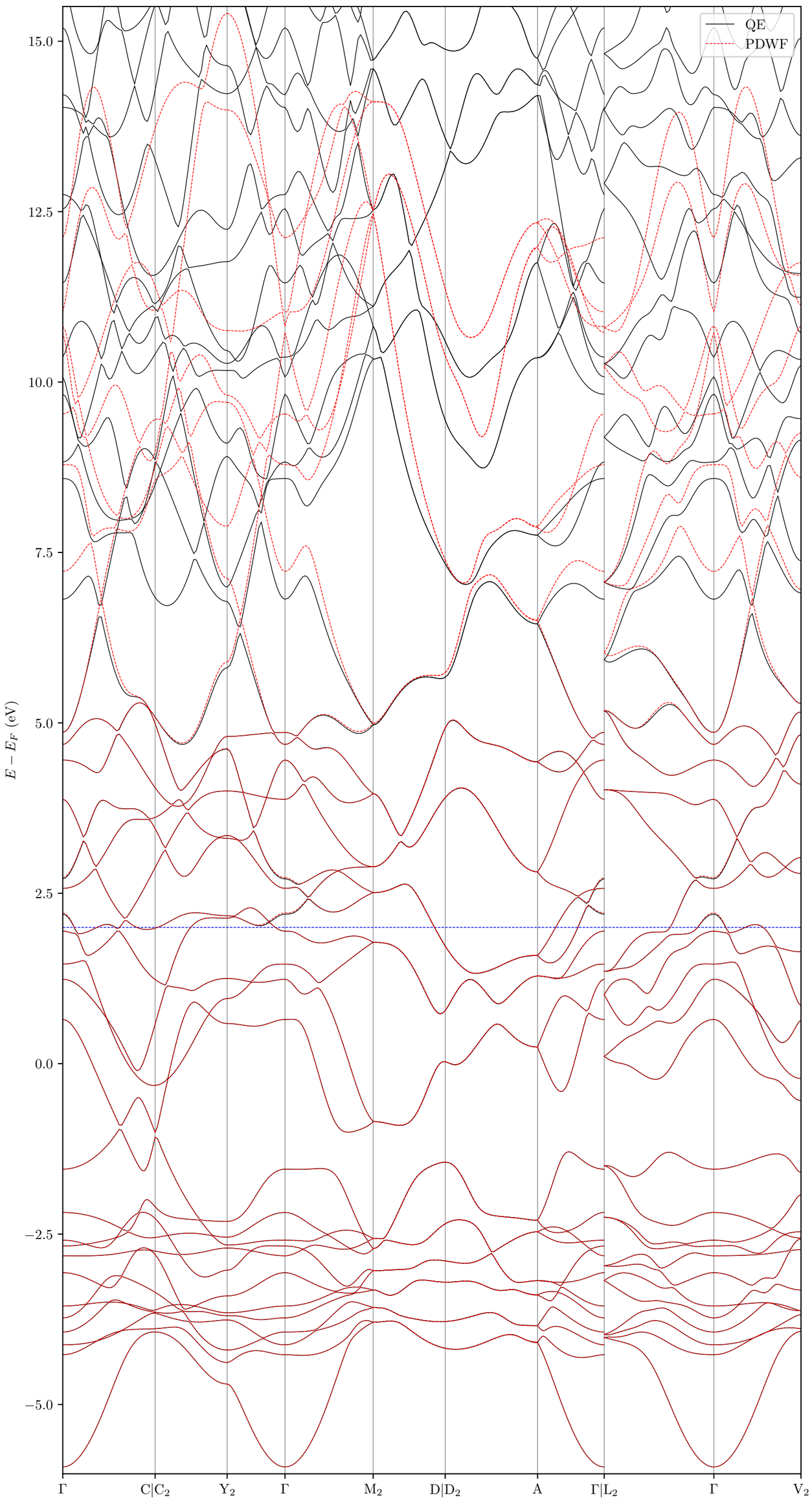



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 17.8 | 16.3 | 14.6 | 139.8 | 139.8 | 139.8 | 2.242 |



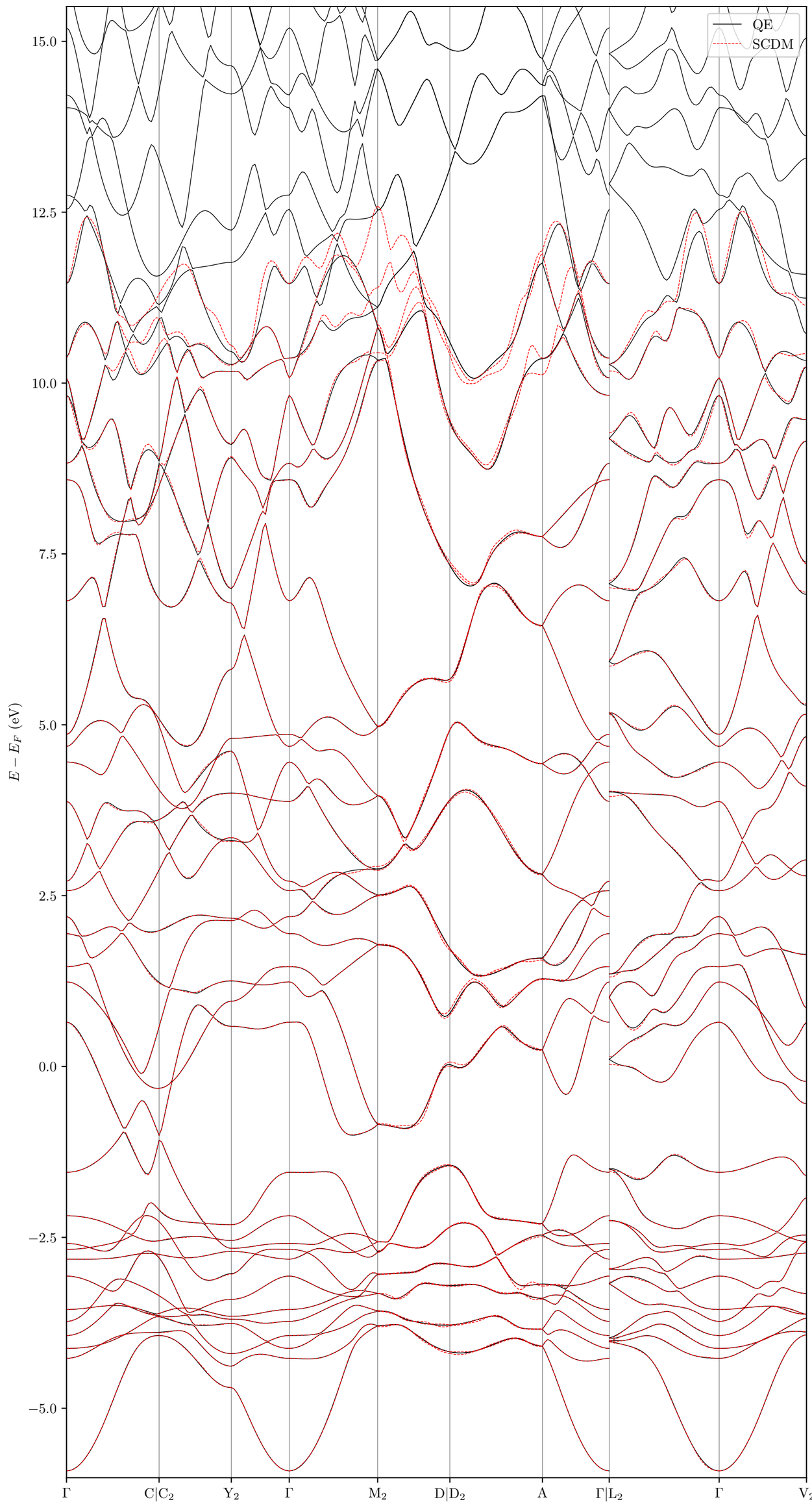
Pd2Y2 exclude semicore
PW=712b7fa0-bd0c-463e-883a-f797c87cf2da
W90=508e3899-4634-4572-b736-ea5f60bfdfbe




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 1.2 | 2.3 | 6.8 | 8.7 | 19.9 | 2.333 |

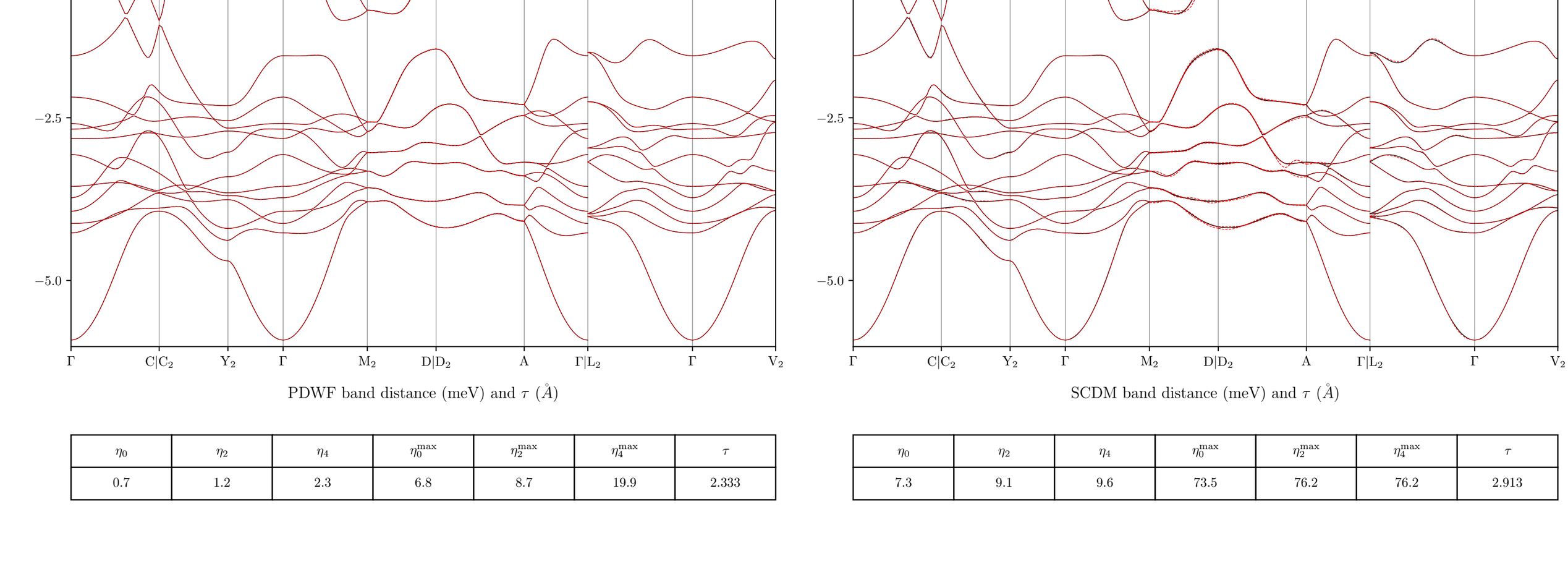
Pd2Y2 exclude semicore
PW=712b7fa0-bd0c-463e-883a-f797c87cf2da
W90=6ba9804c-5faa-4d7c-8f37-f2308635f8e3

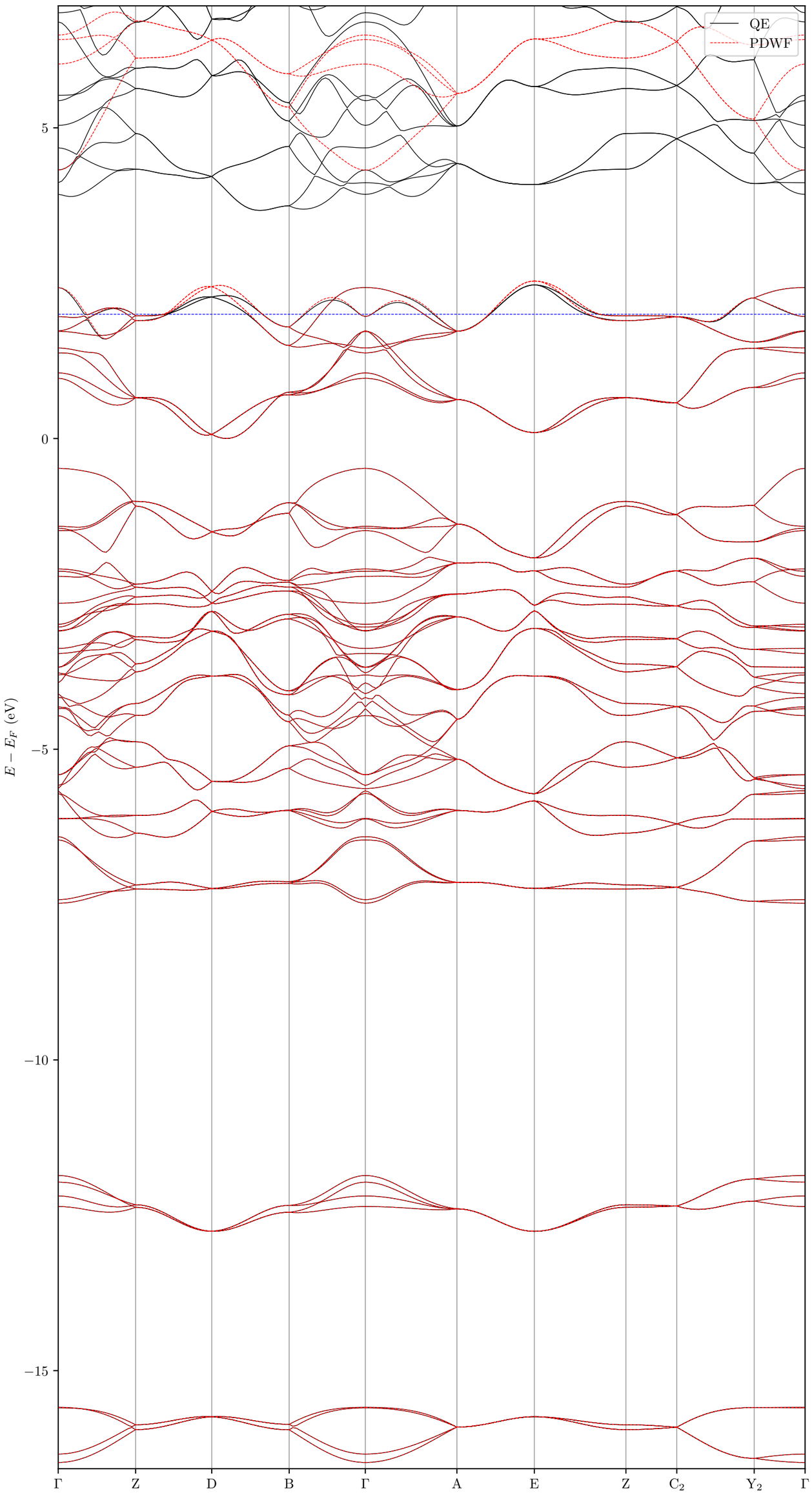



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.3 | 9.1 | 9.6 | 73.5 | 76.2 | 76.2 | 2.913 |

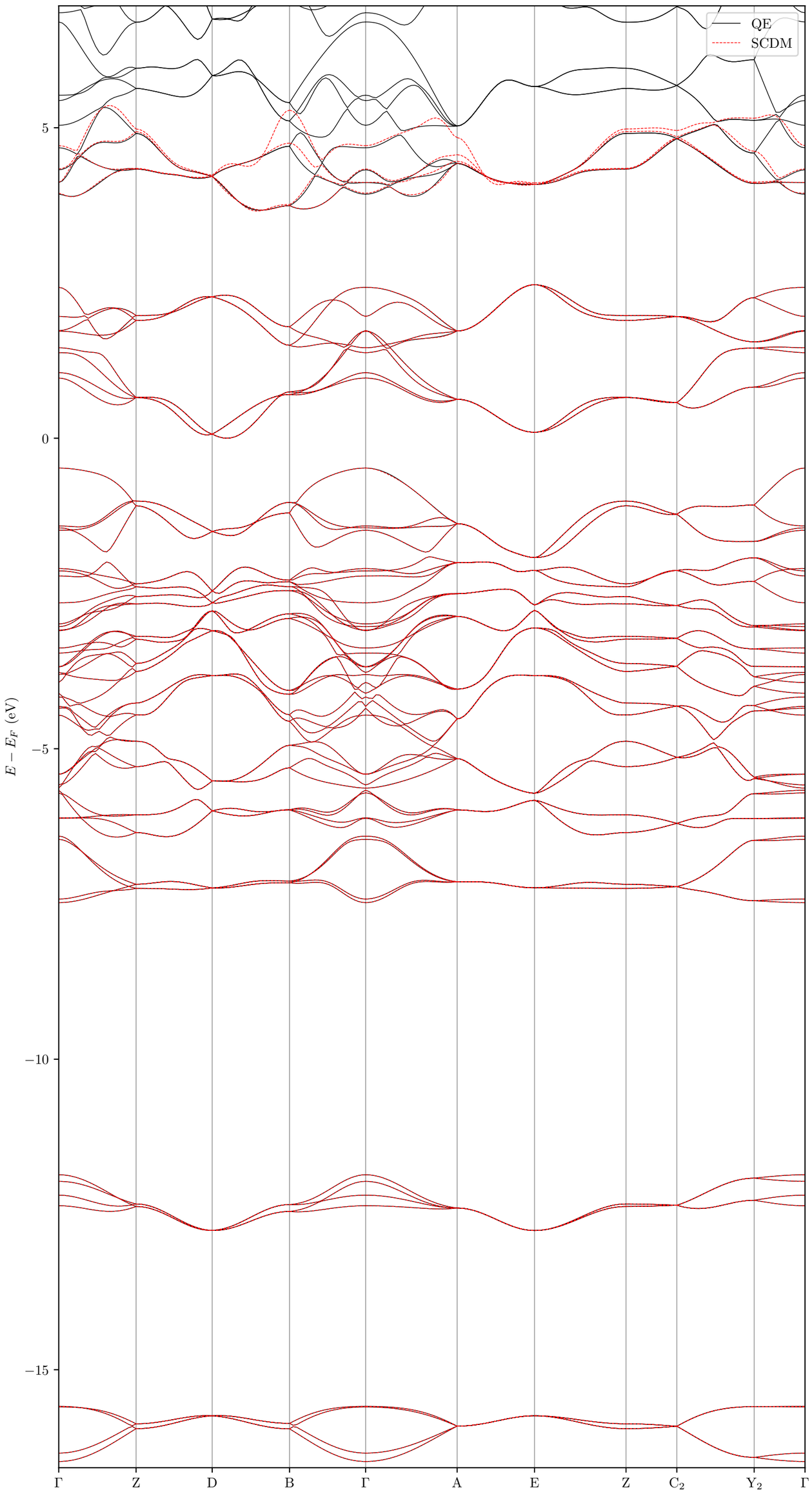
Hamiltonian decay





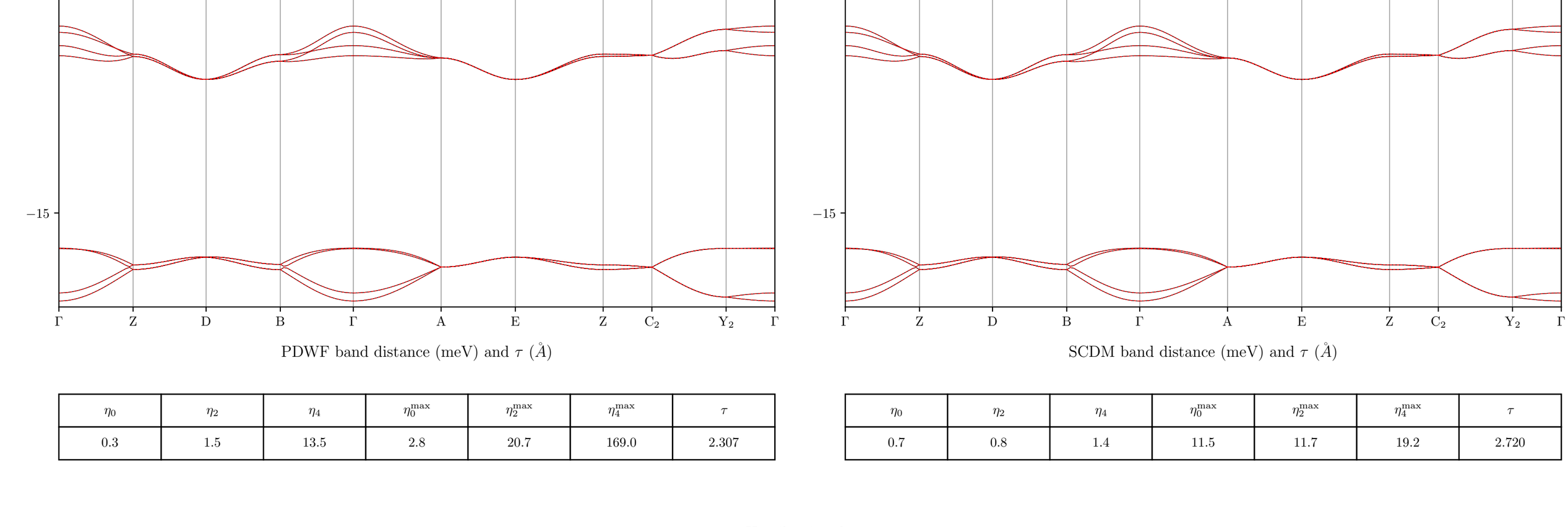

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.3 | 1.5 | 13.5 | 2.8 | 20.7 | 169.0 | 2.307 |

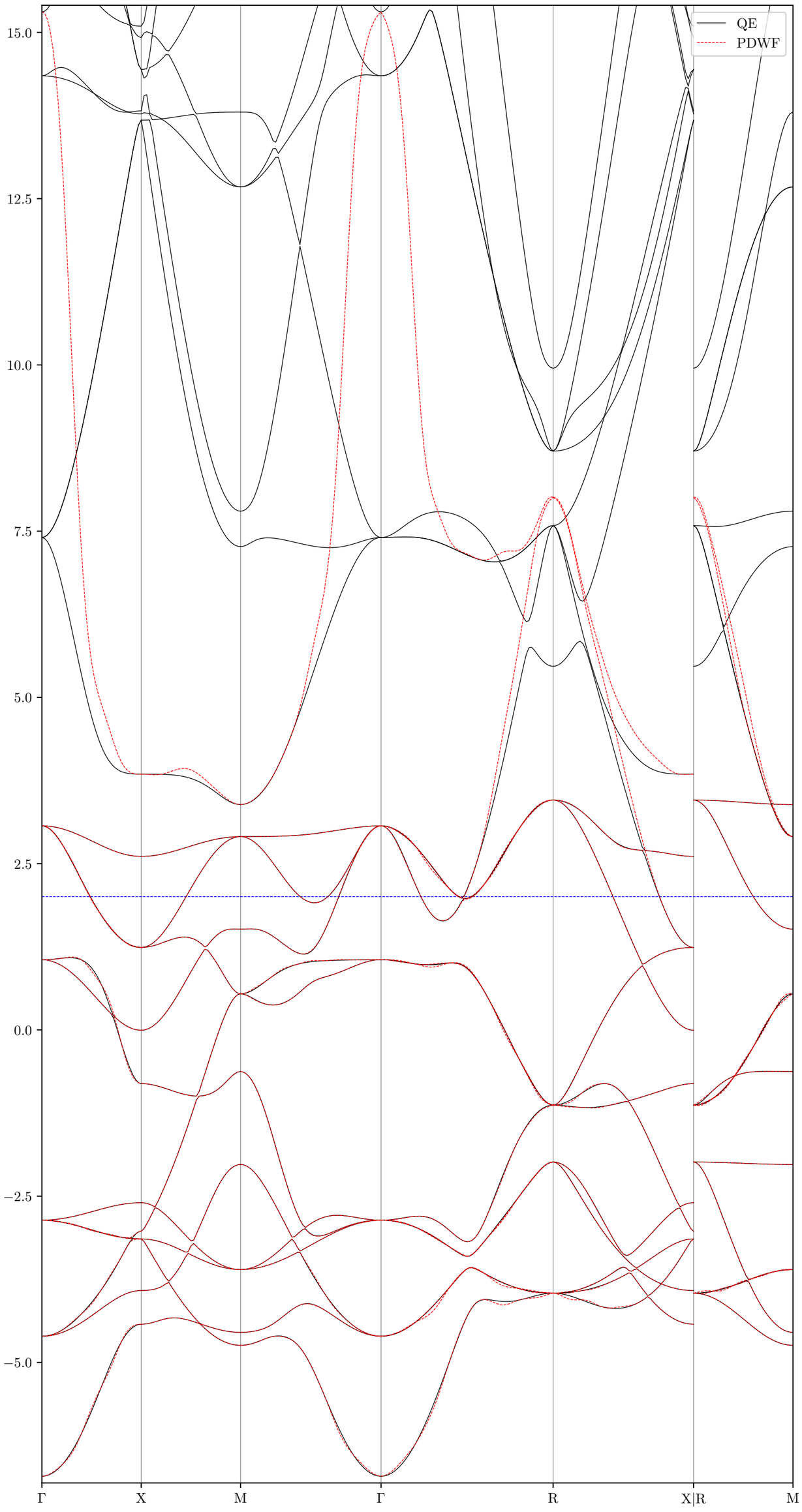



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 0.8 | 1.4 | 11.5 | 11.7 | 19.2 | 2.720 |



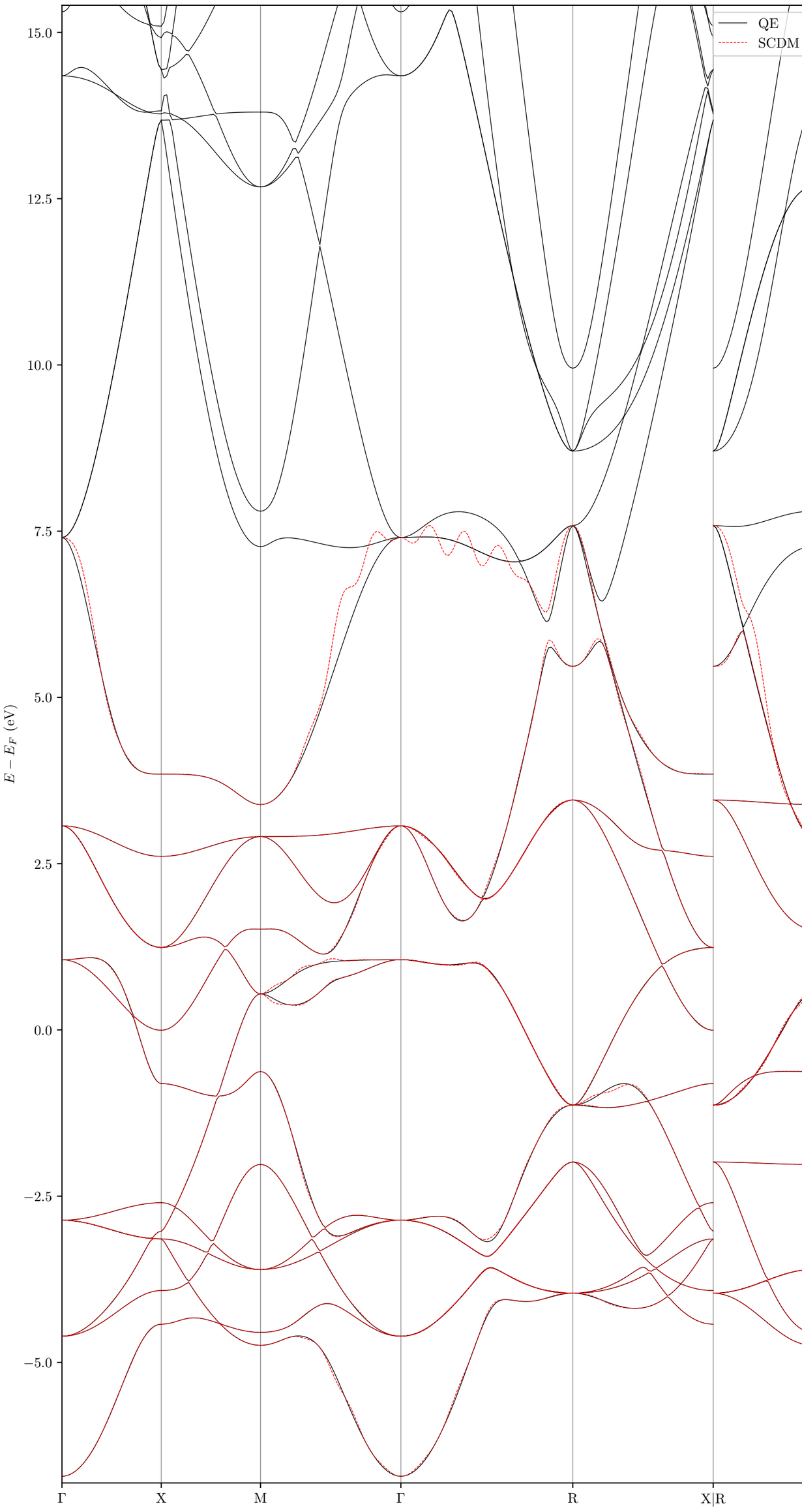
PdSc exclude semicore
PW=537dbaef-eb03-4524-ba31-d34fa5d94704
W90=bf12dffb-cc45-4b03-8e85-d99afc9247e2




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 10.8 | 10.6 | 21.4 | 75.7 | 75.7 | 244.3 | 2.411 |

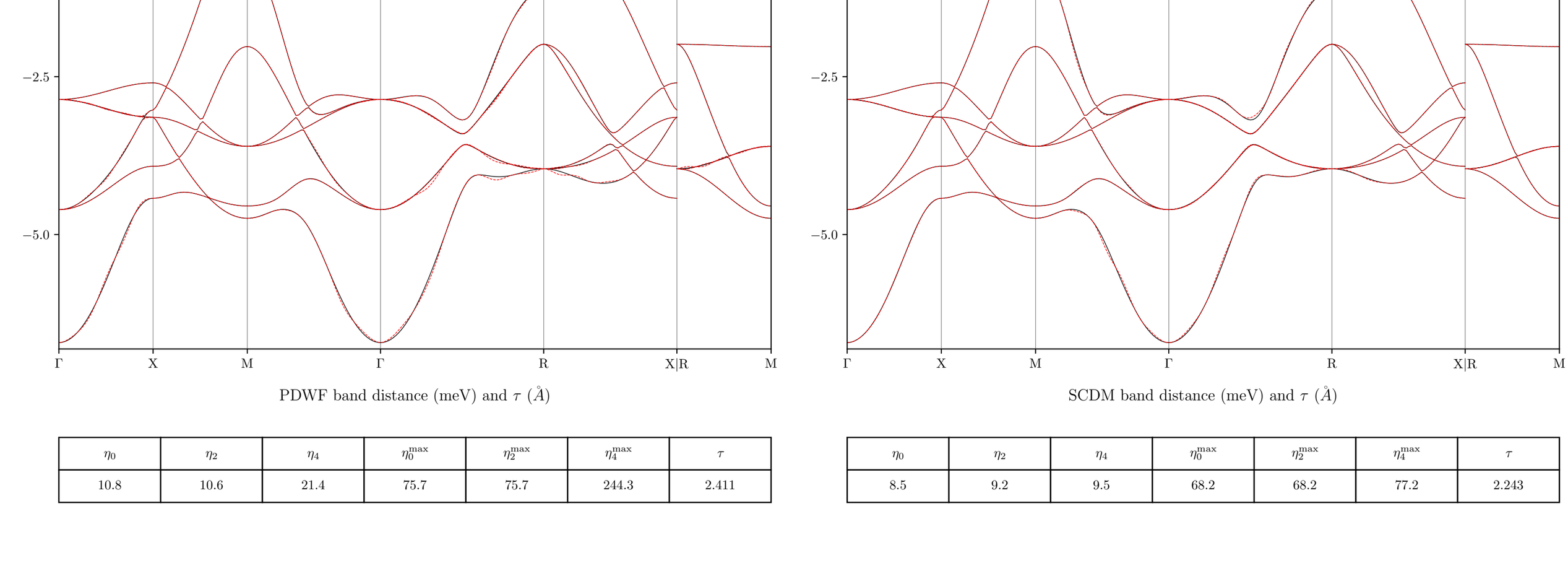
PdSc exclude semicore
PW=537dbaef-eb03-4524-ba31-d34fa5d94704
W90=0827ffa0-629a-43b0-a0be-05fe96d57458



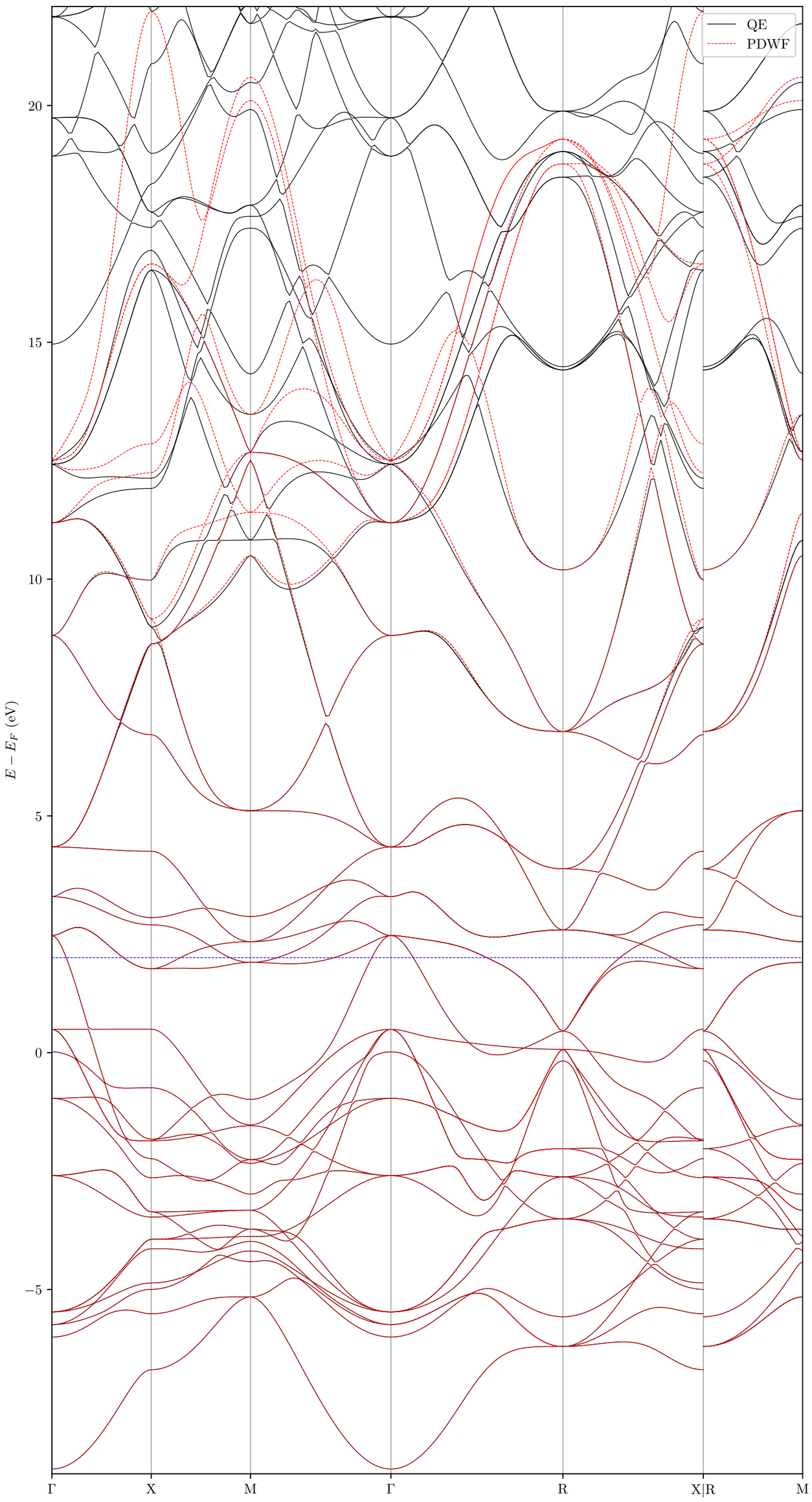

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.5 | 9.2 | 9.5 | 68.2 | 68.2 | 77.2 | 2.243 |

Hamiltonian decay



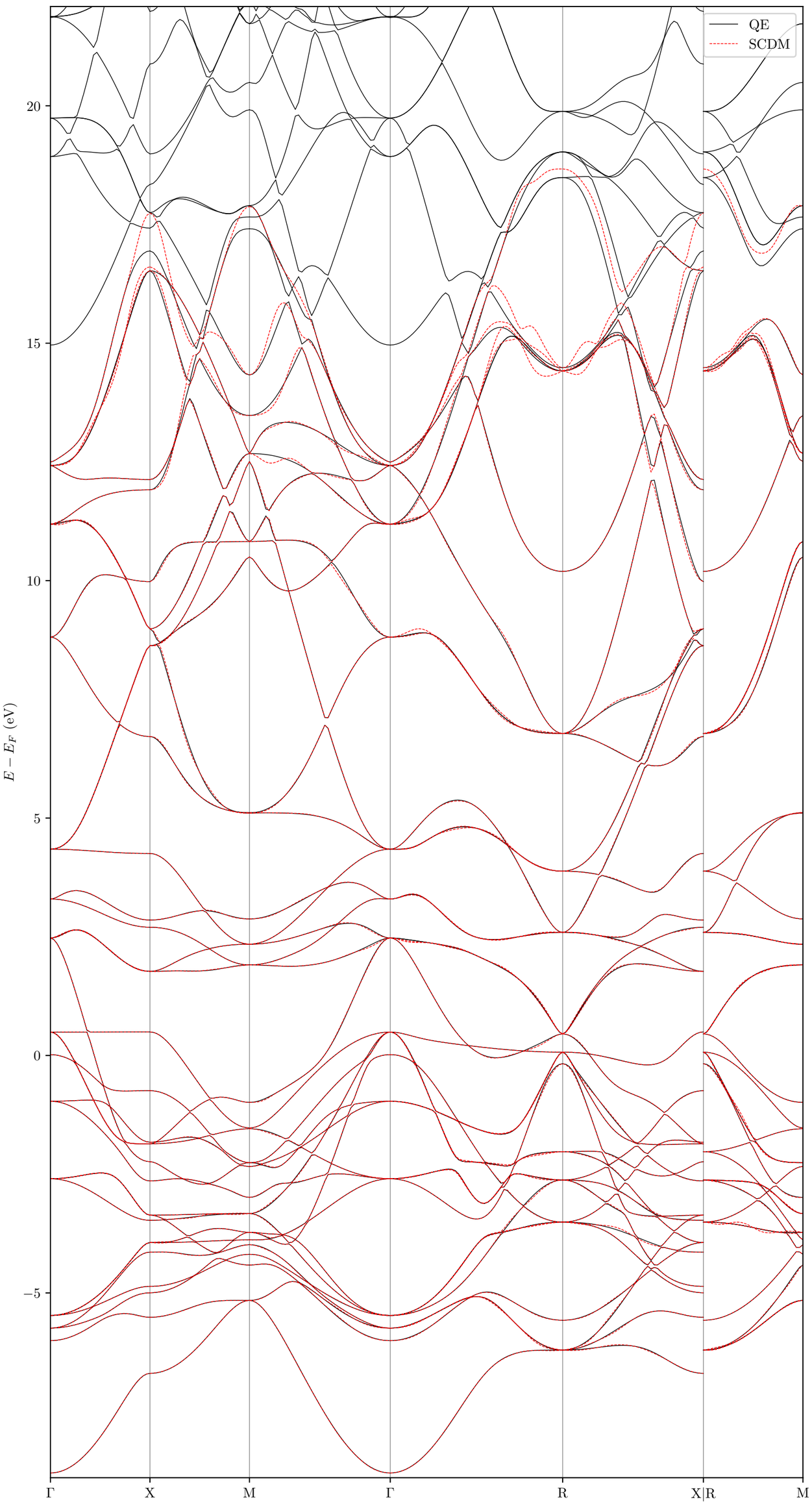
Pt3Sc exclude semicore
PW=93ba436d-3192-466d-b3e6-61171256b843
W90=252903d9-c96a-437a-aa58-aede11b83b47




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 0.7 | 4.3 | 4.3 | 4.3 | 1.739 |

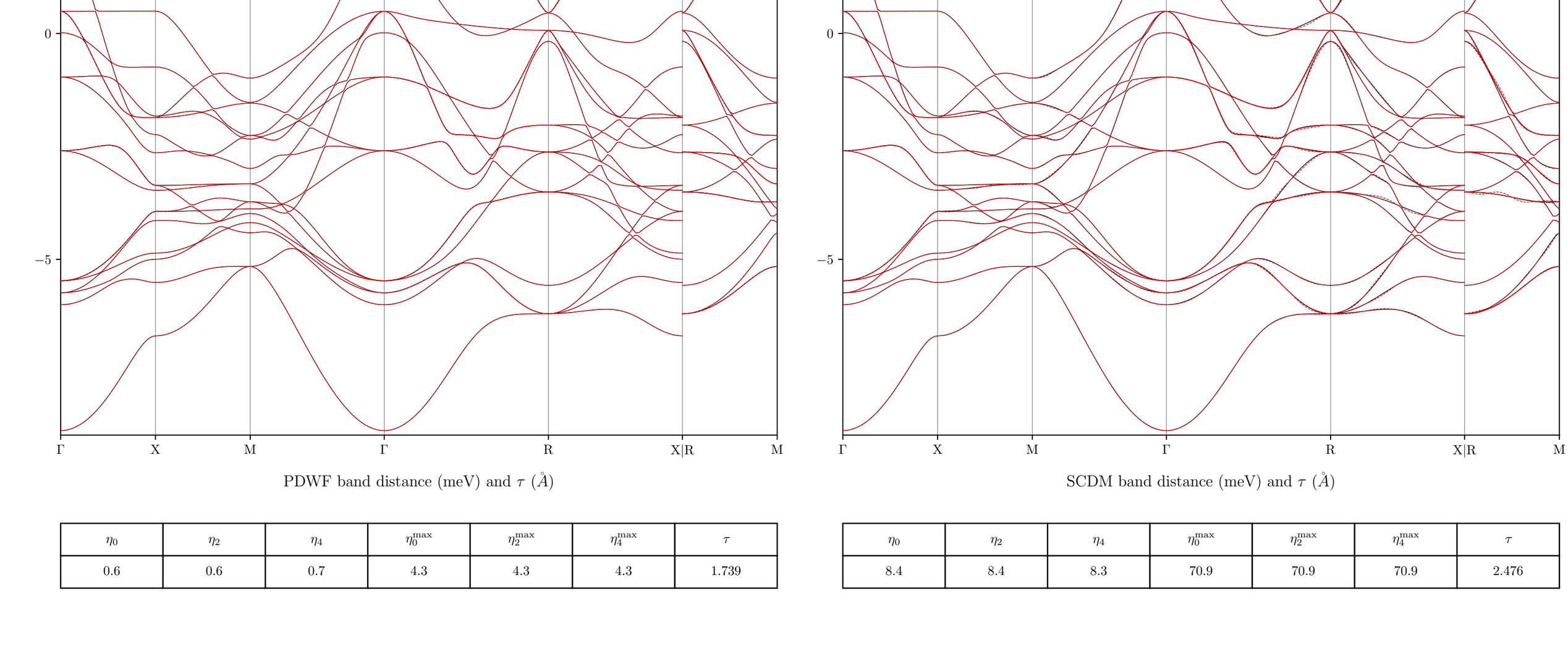
Pt3Sc exclude semicore
PW=93ba436d-3192-466d-b3e6-61171256b843
W90=2384e854-0b4e-4ce2-a310-635124b851f7



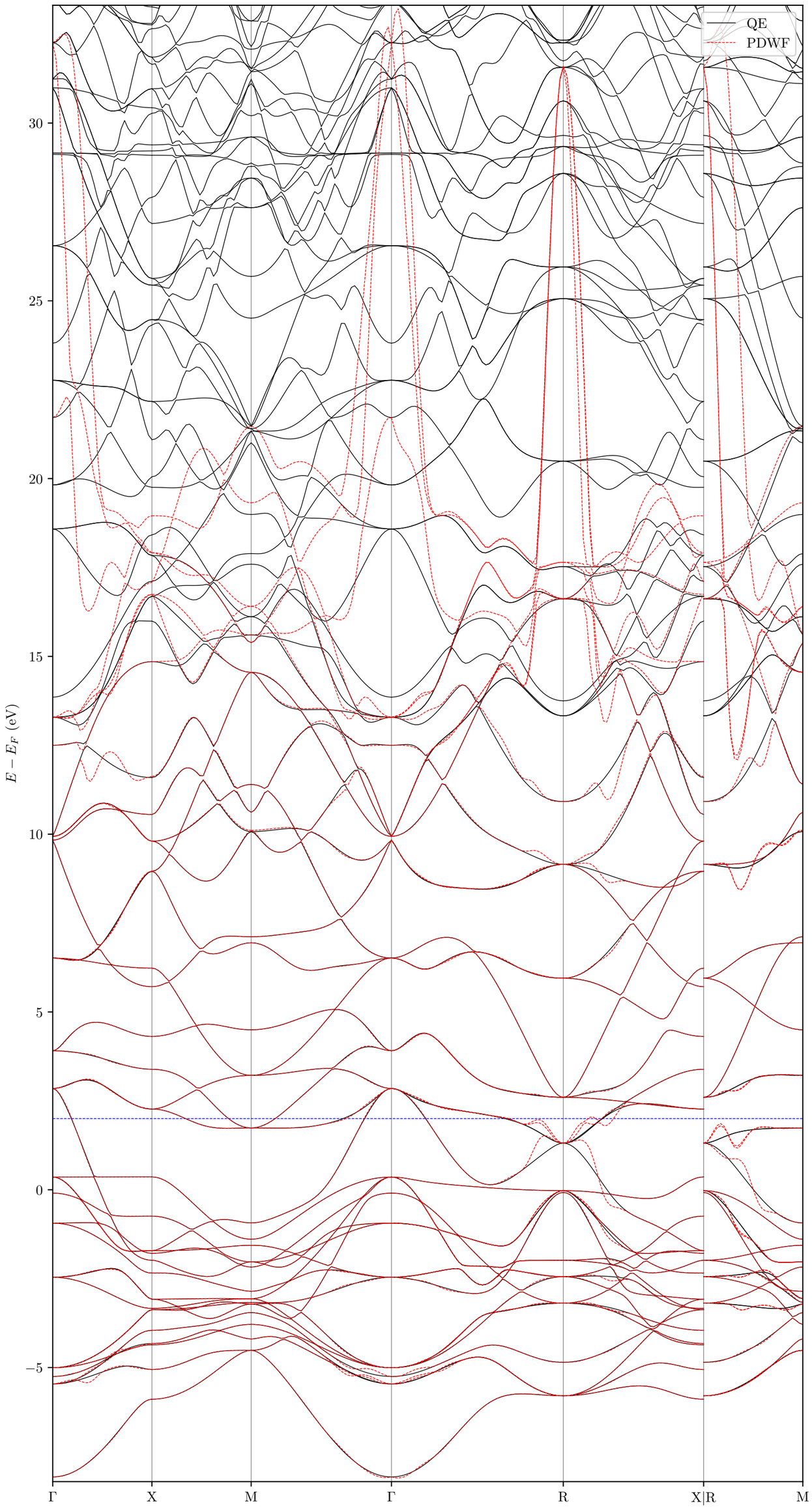

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.4 | 8.4 | 8.3 | 70.9 | 70.9 | 70.9 | 2.476 |

Hamiltonian decay



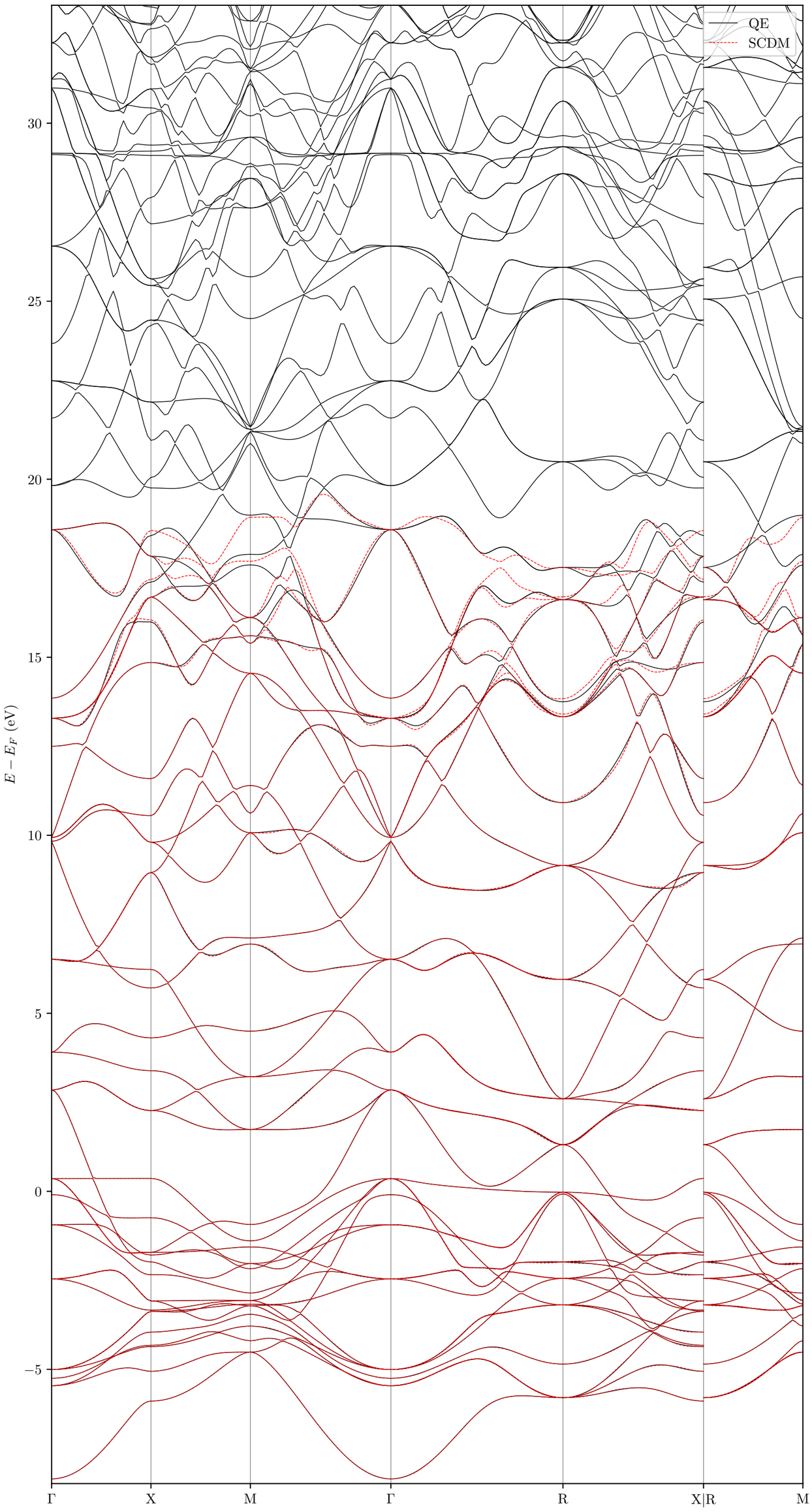
Pt3Y exclude semicore
PW=f22d8788-f913-402d-a789-c93d8e7ae2e6
W90=38df72cf-dbd0-492e-b99b-aa7f24eb38d4




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 23.2 | 45.6 | 43.9 | 271.6 | 503.3 | 505.2 | 1.987 |

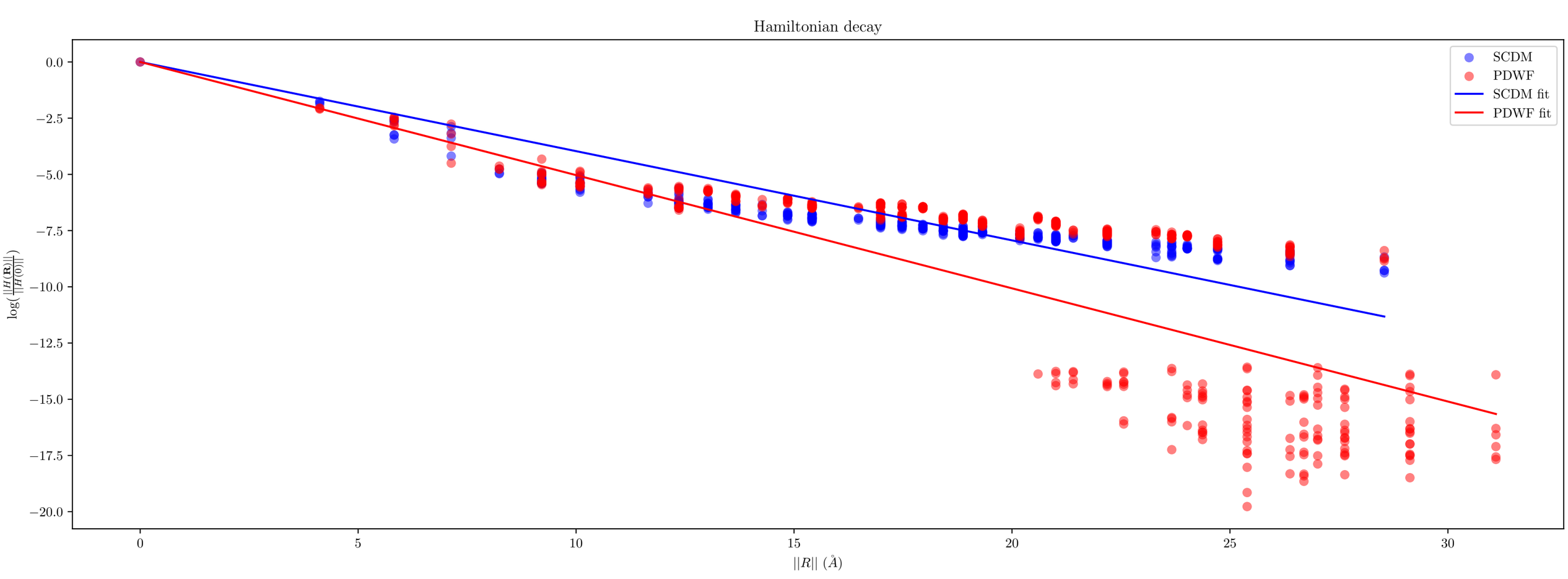
Pt3Y exclude semicore
PW=f22d8788-f913-402d-a789-c93d8e7ae2e6
W90=780c7715-4041-46b9-b4fd-f15cffa60222



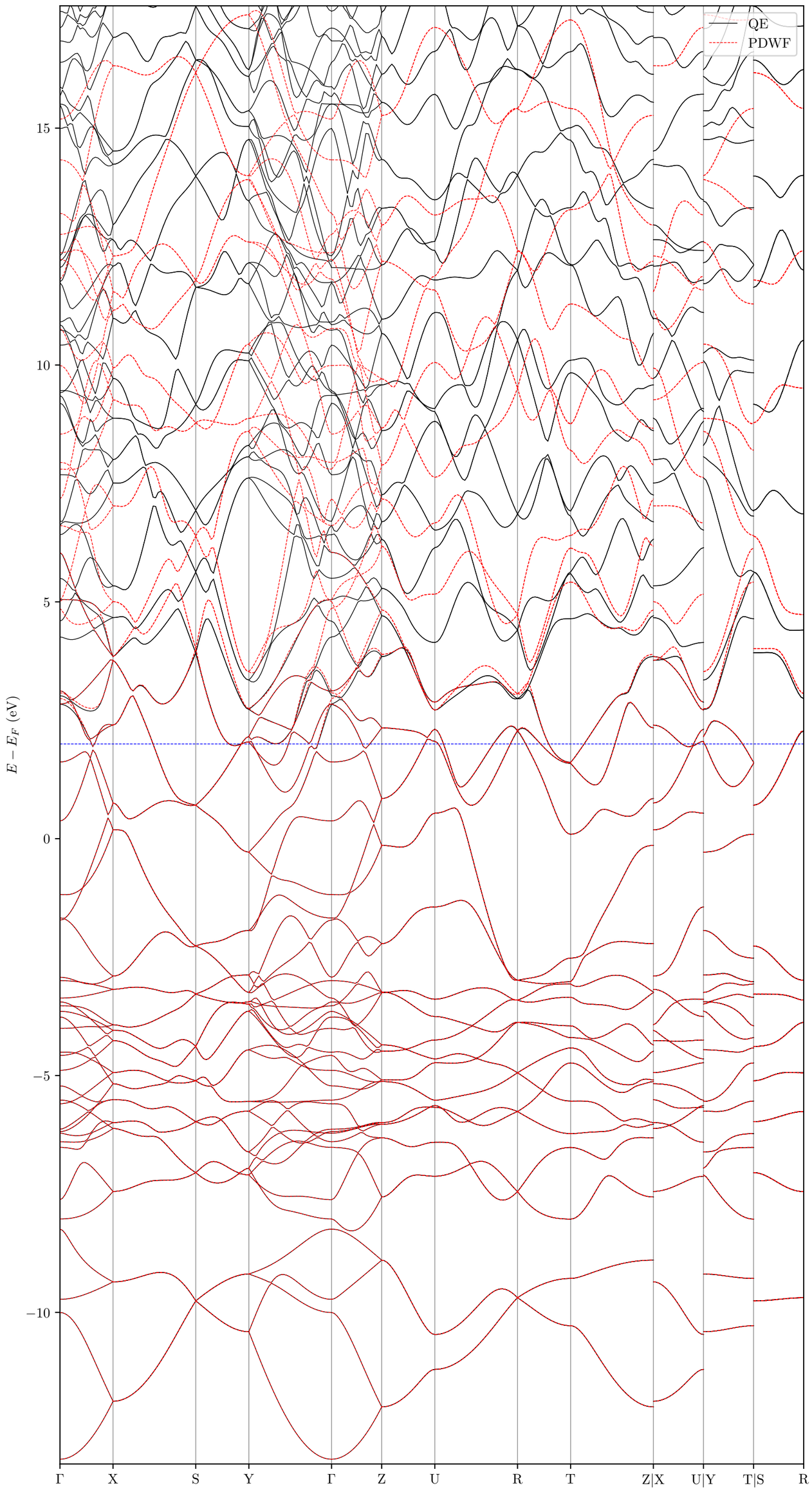

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.0 | 5.0 | 5.3 | 26.5 | 31.3 | 32.7 | 2.521 |

Hamiltonian decay



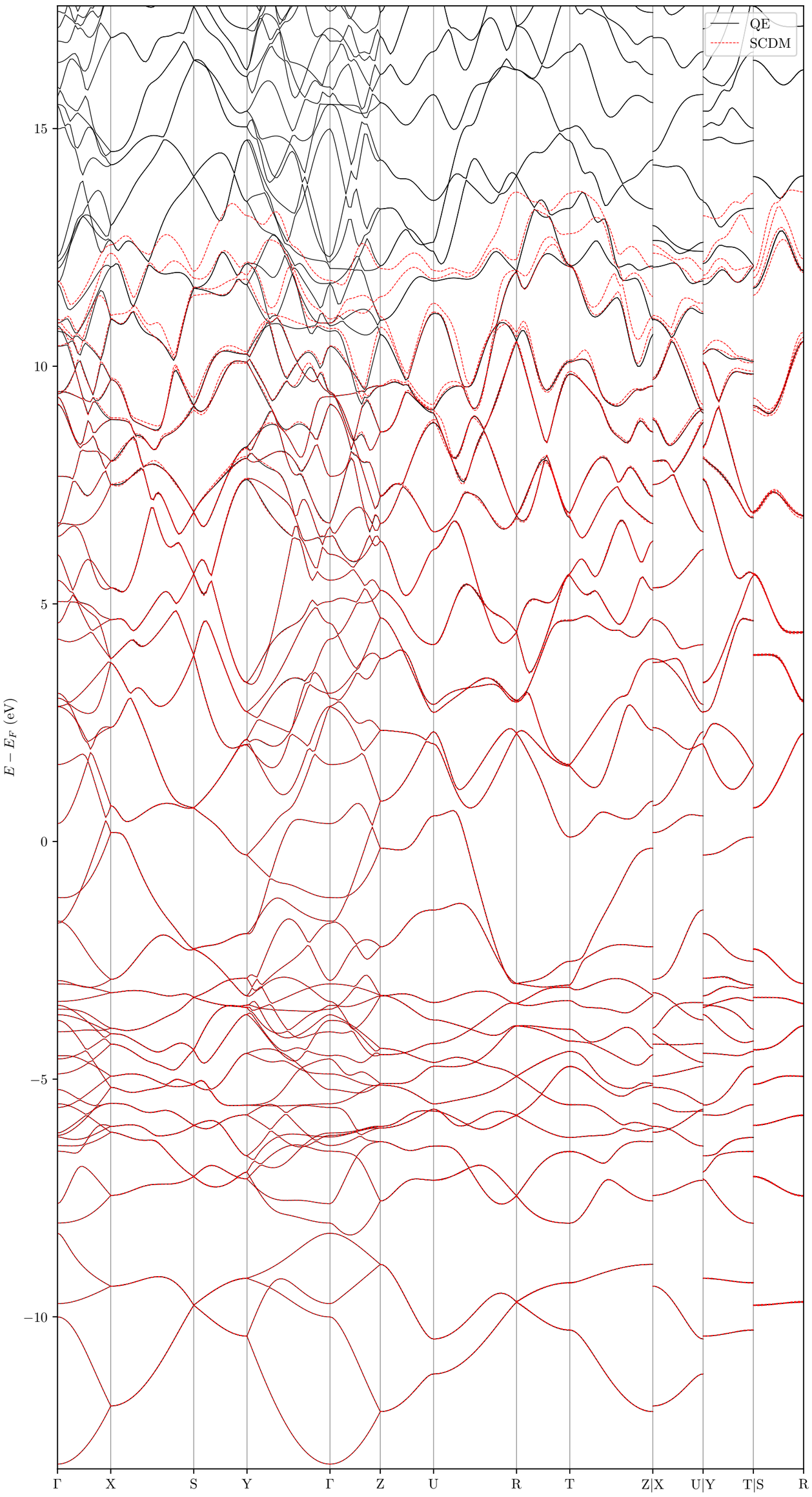
Pt4Si4 exclude semicore
PW=a9f64a79-0d30-45eb-b6b0-32204b50b9f6
W90=c8499275-1495-4216-a620-2c48b15d903f




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.4 | 25.7 | 8.6 | 11.2 | 256.9 | 2.322 |

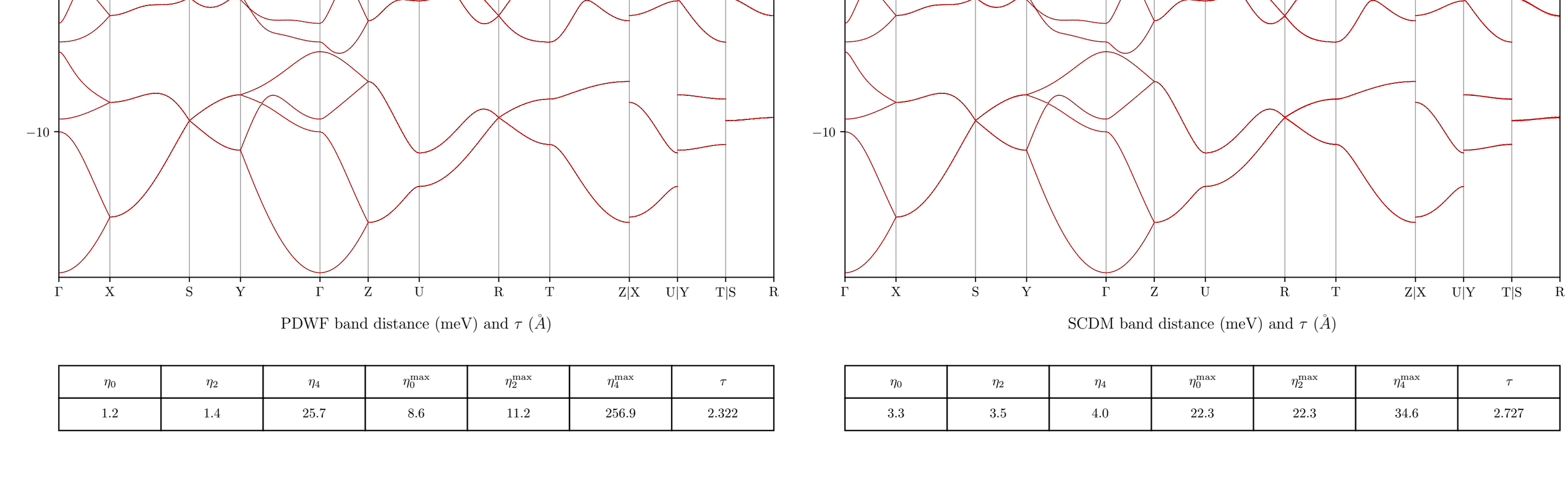
Pt4Si4 exclude semicore
PW=a9f64a79-0d30-45eb-b6b0-32204b50b9f6
W90=bb75d671-c3f2-42b6-a7d2-0e52e0a61503



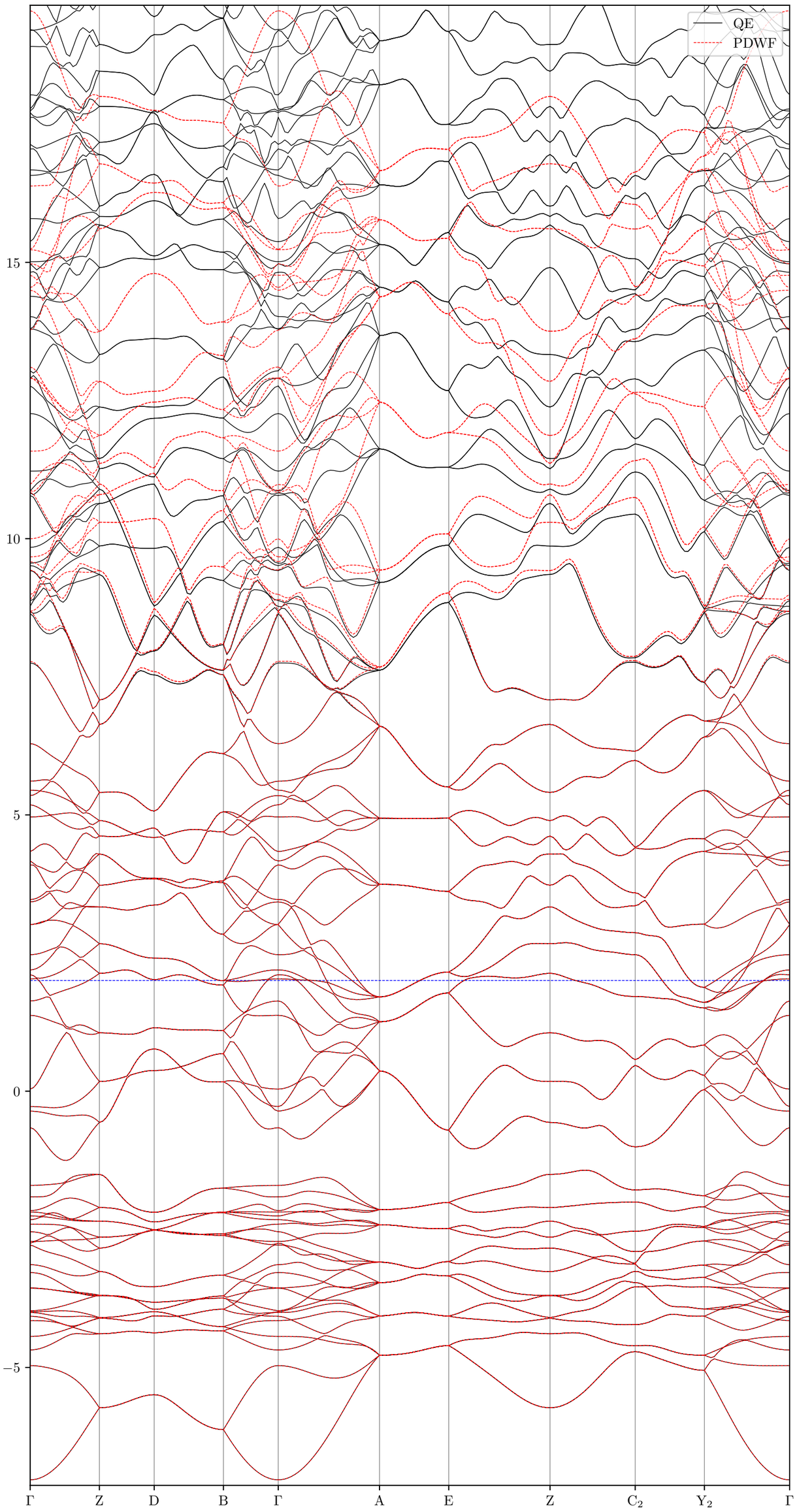

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.3 | 3.5 | 4.0 | 22.3 | 22.3 | 34.6 | 2.727 |

Hamiltonian decay



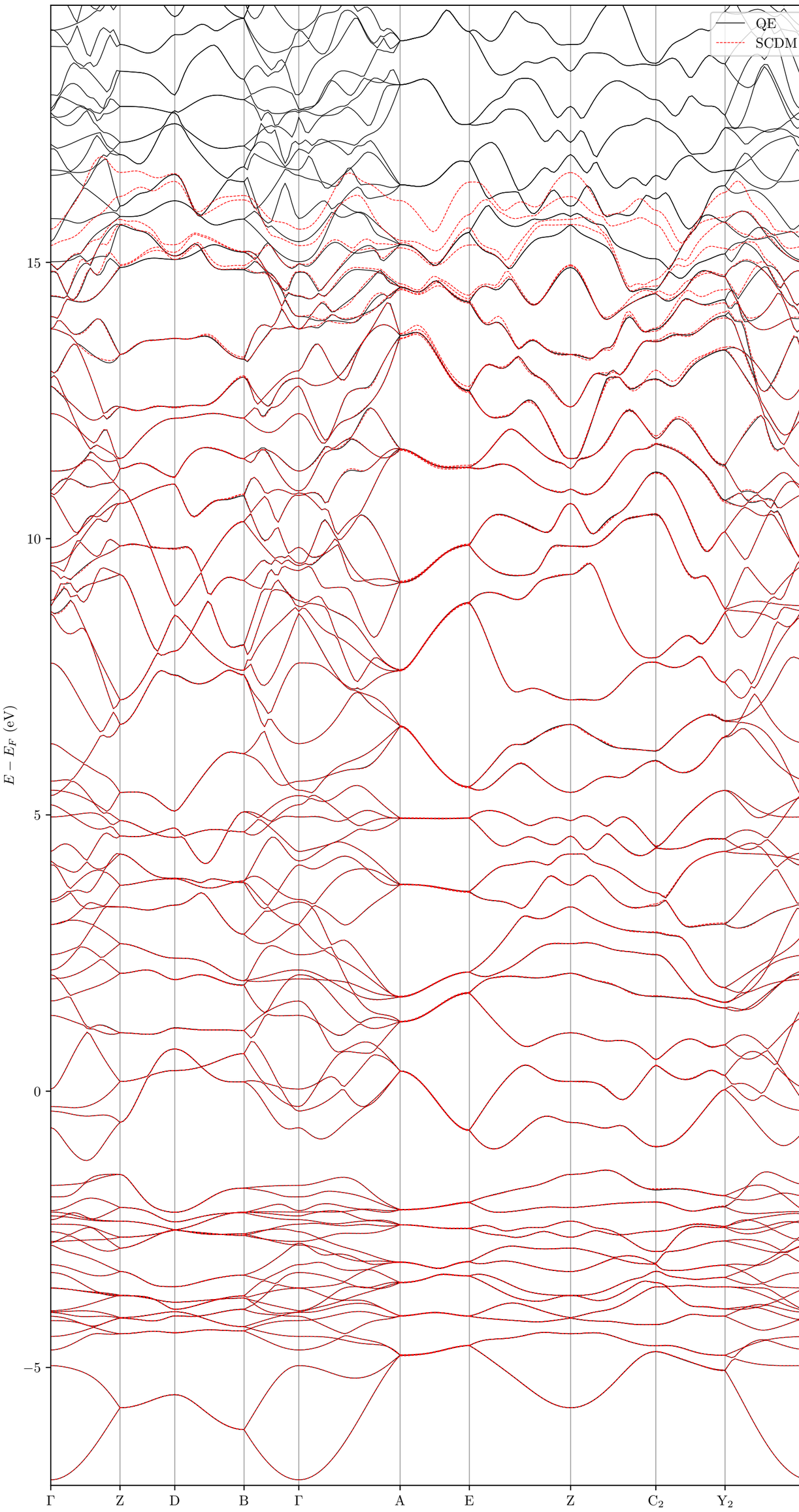
Pt4Y4 exclude semicore
PW=b2196137-c41b-4f8e-8ecf-b8b23816ad1c
W90=bb04ed0a-be66-4392-a698-3d633062303f




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.5 | 0.7 | 0.7 | 3.7 | 5.5 | 5.5 | 2.247 |

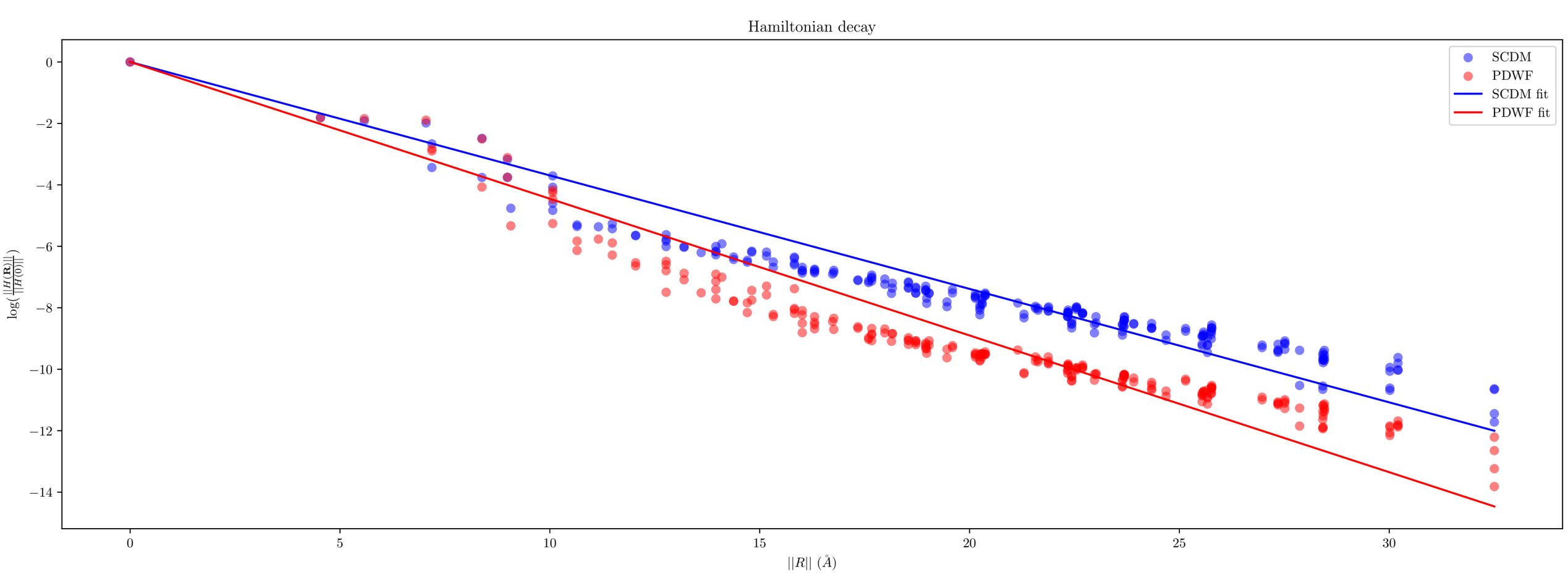
Pt4Y4 exclude semicore
PW=b2196137-c41b-4f8e-8ecf-b8b23816ad1c
W90=c2dbe092-3cc9-4dee-90ae-d2239e18546e



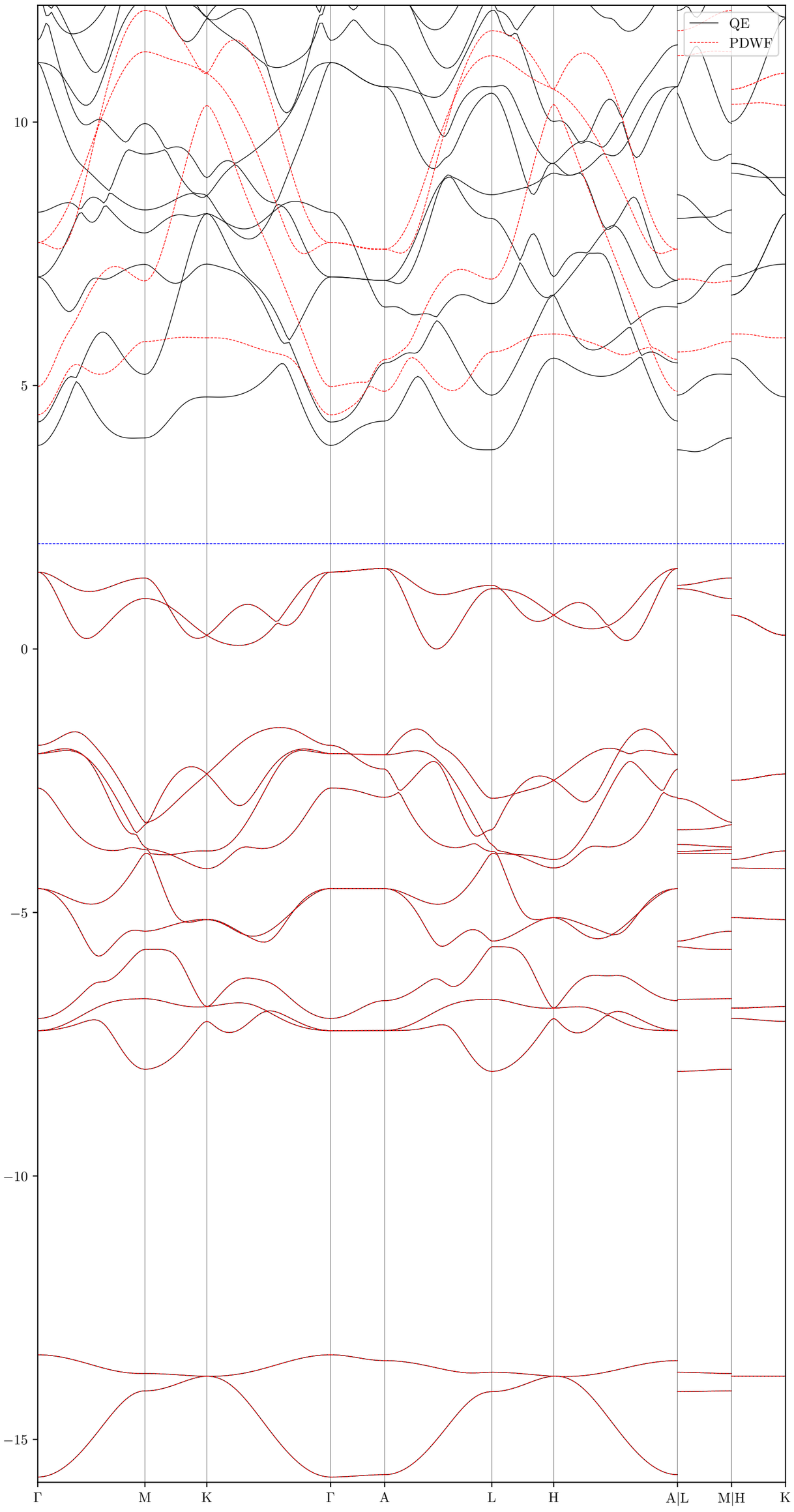

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.8 | 3.2 | 3.5 | 20.7 | 20.7 | 32.3 | 2.708 |

Hamiltonian decay



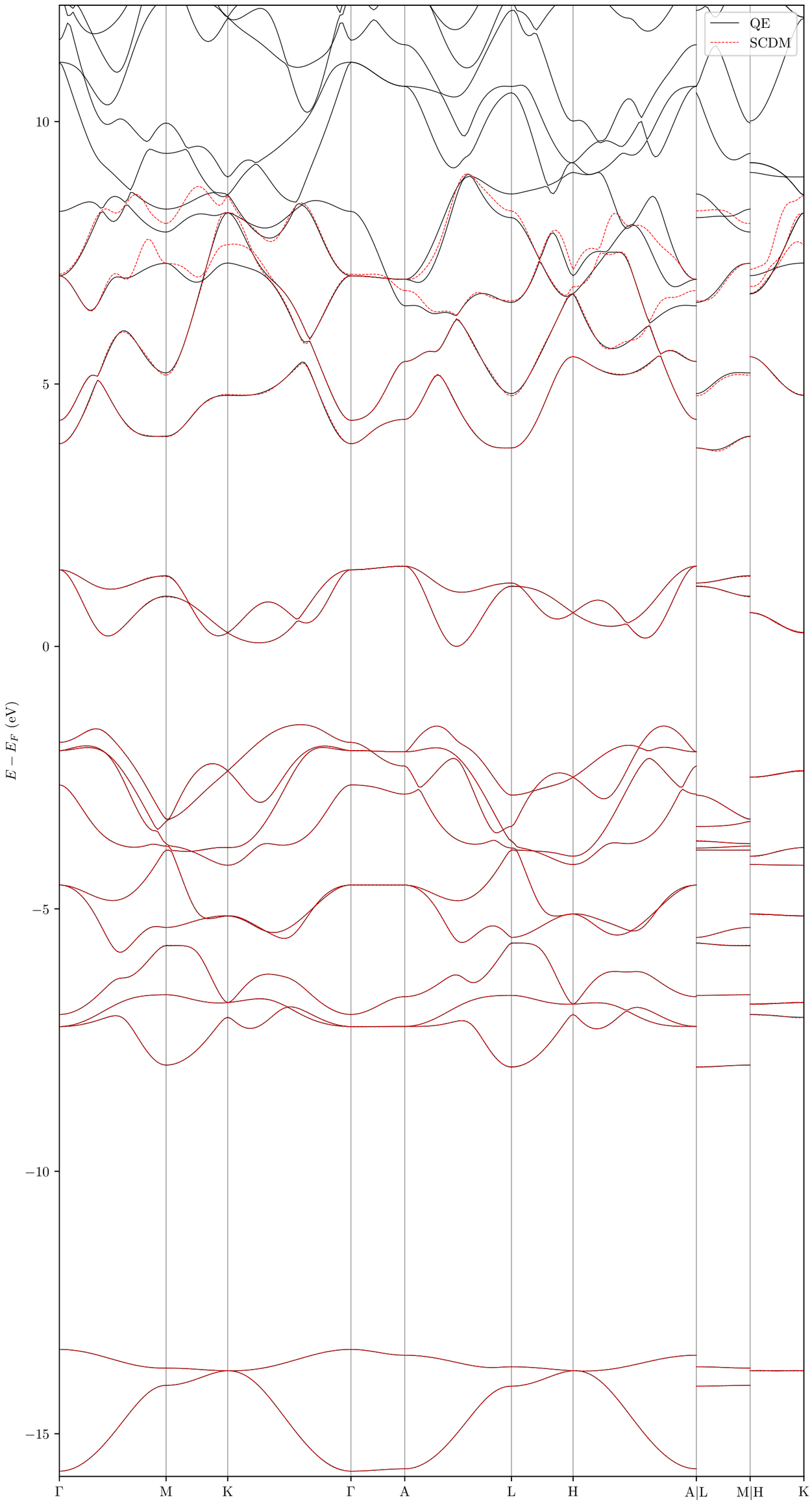
PtS2 exclude semicore
PW=52a69bb3-adcb-4ed6-85ed-9c4646724933
W90=59dcd9f2-9424-4fc9-a067-4d50d8dc7cce




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.6 | 0.8 | 4.6 | 4.6 | 4.6 | 2.184 |

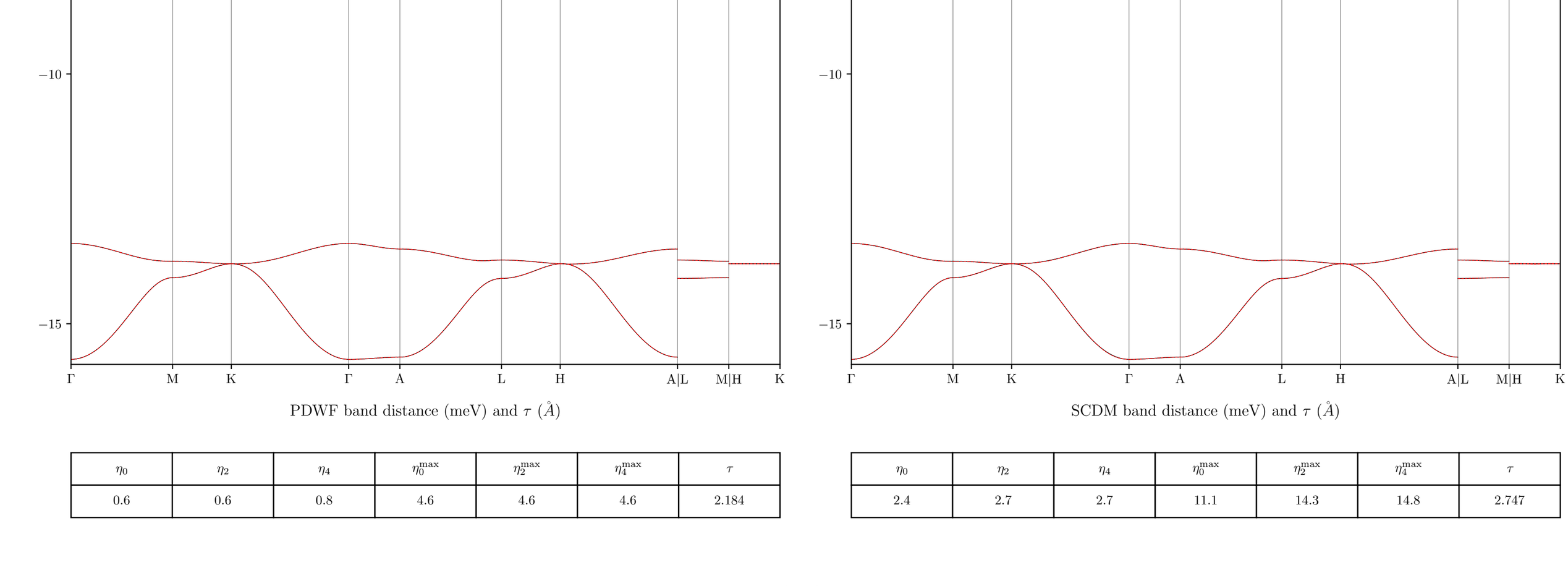
PtS2 exclude semicore
PW=52a69bb3-adcb-4ed6-85ed-9c4646724933
W90=e06e6c41-80dc-40fd-bf9b-2c7d10fd3286



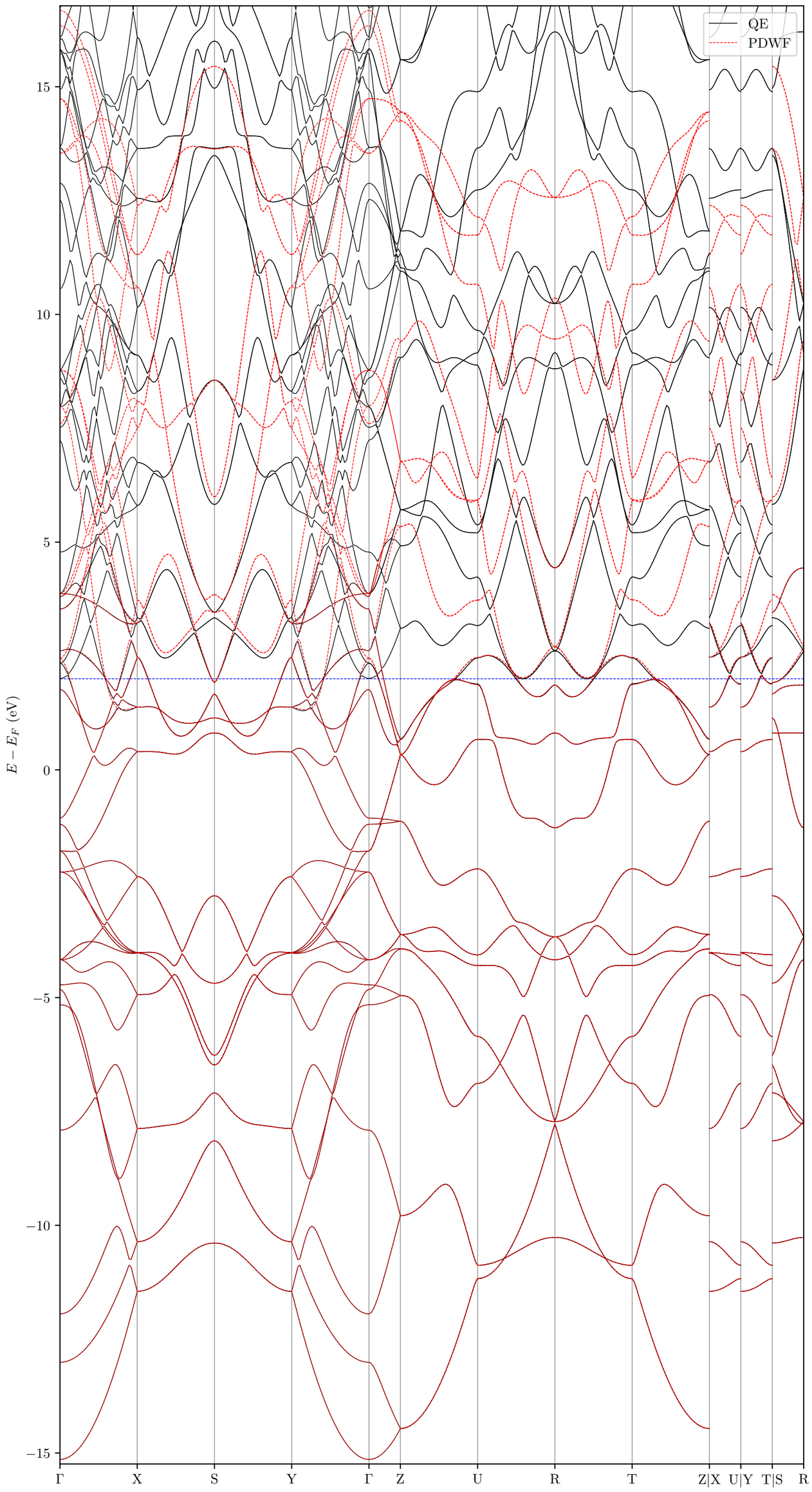

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.4 | 2.7 | 2.7 | 11.1 | 14.3 | 14.8 | 2.747 |

Hamiltonian decay



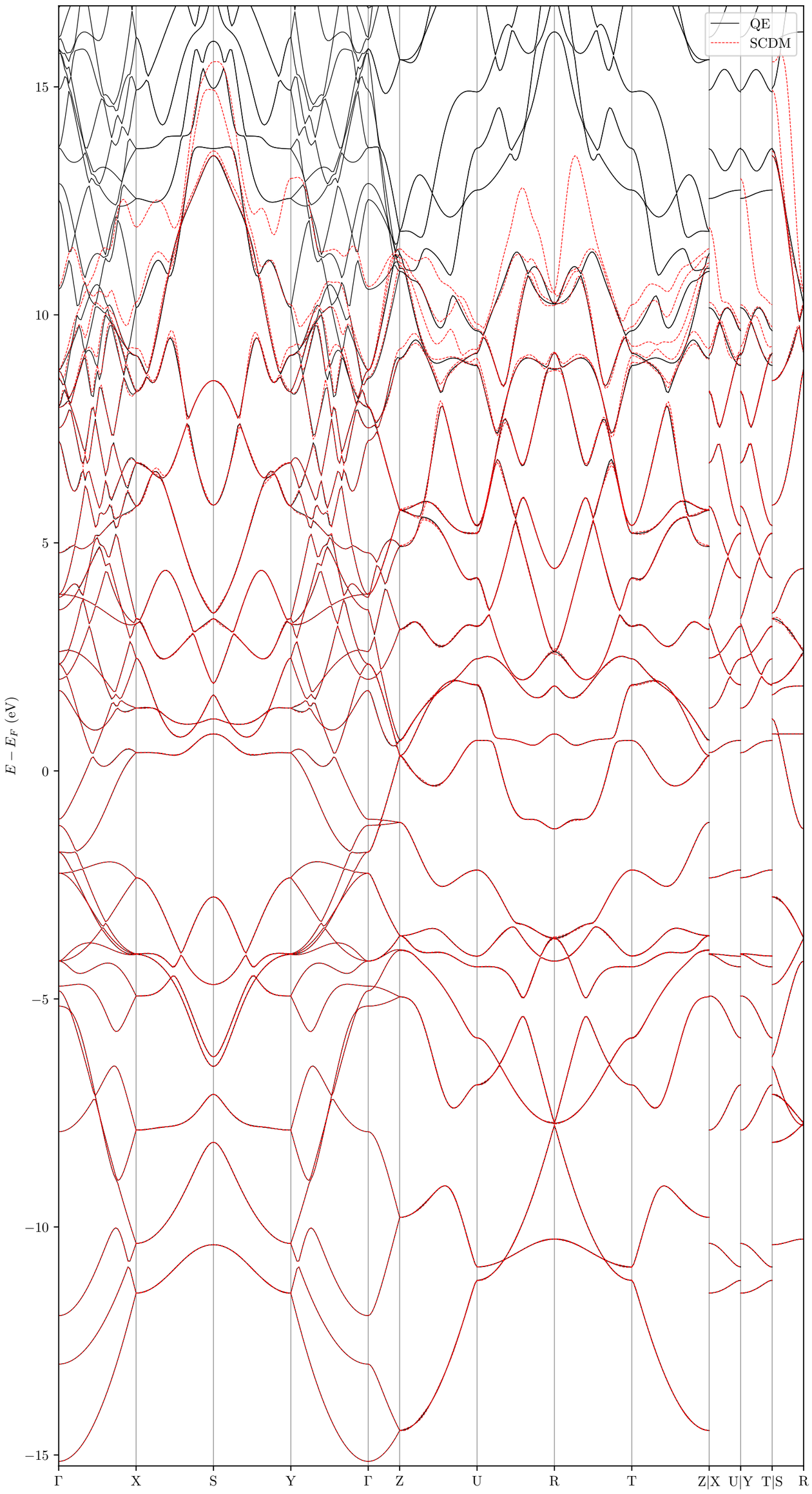
Re2Si4 exclude semicore
PW=58136a25-9238-4dcd-b503-28ddf6728452
W90=6769cb6f-5e92-4888-86c8-94c5ec636494




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.5 | 6.9 | 122.1 | 17.0 | 86.2 | 1405.3 | 2.391 |

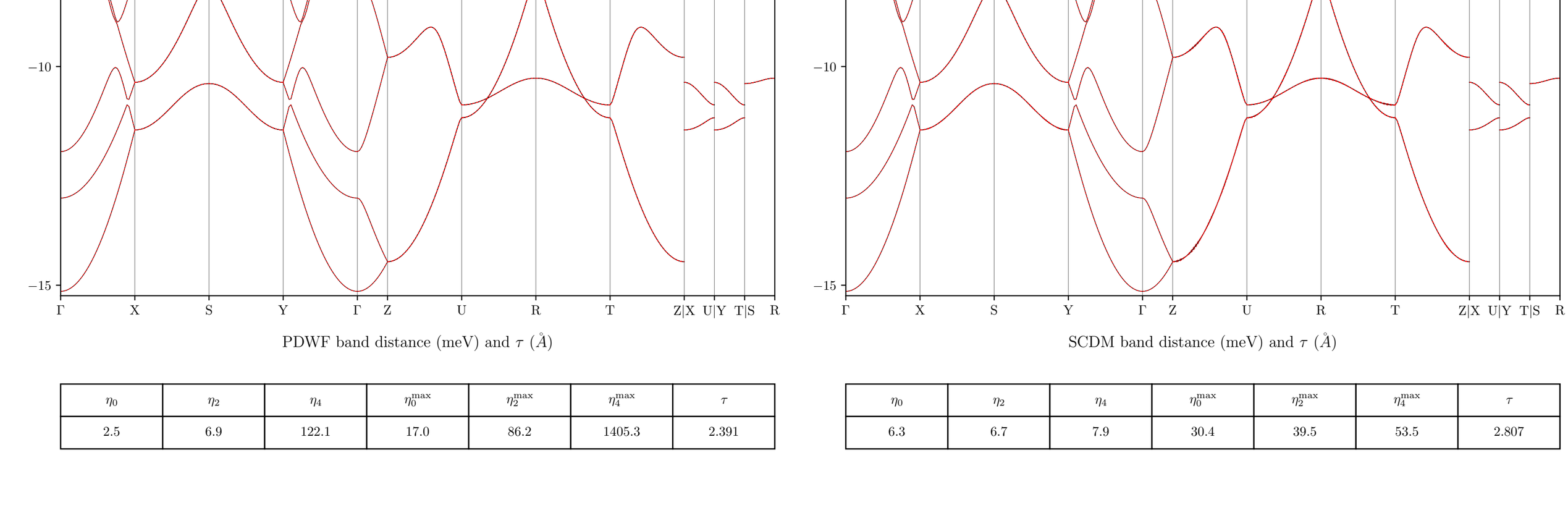
Re2Si4 exclude semicore
PW=58136a25-9238-4dcd-b503-28ddf6728452
W90=7b2f049e-7b41-4dda-8d56-a3128d870ac9



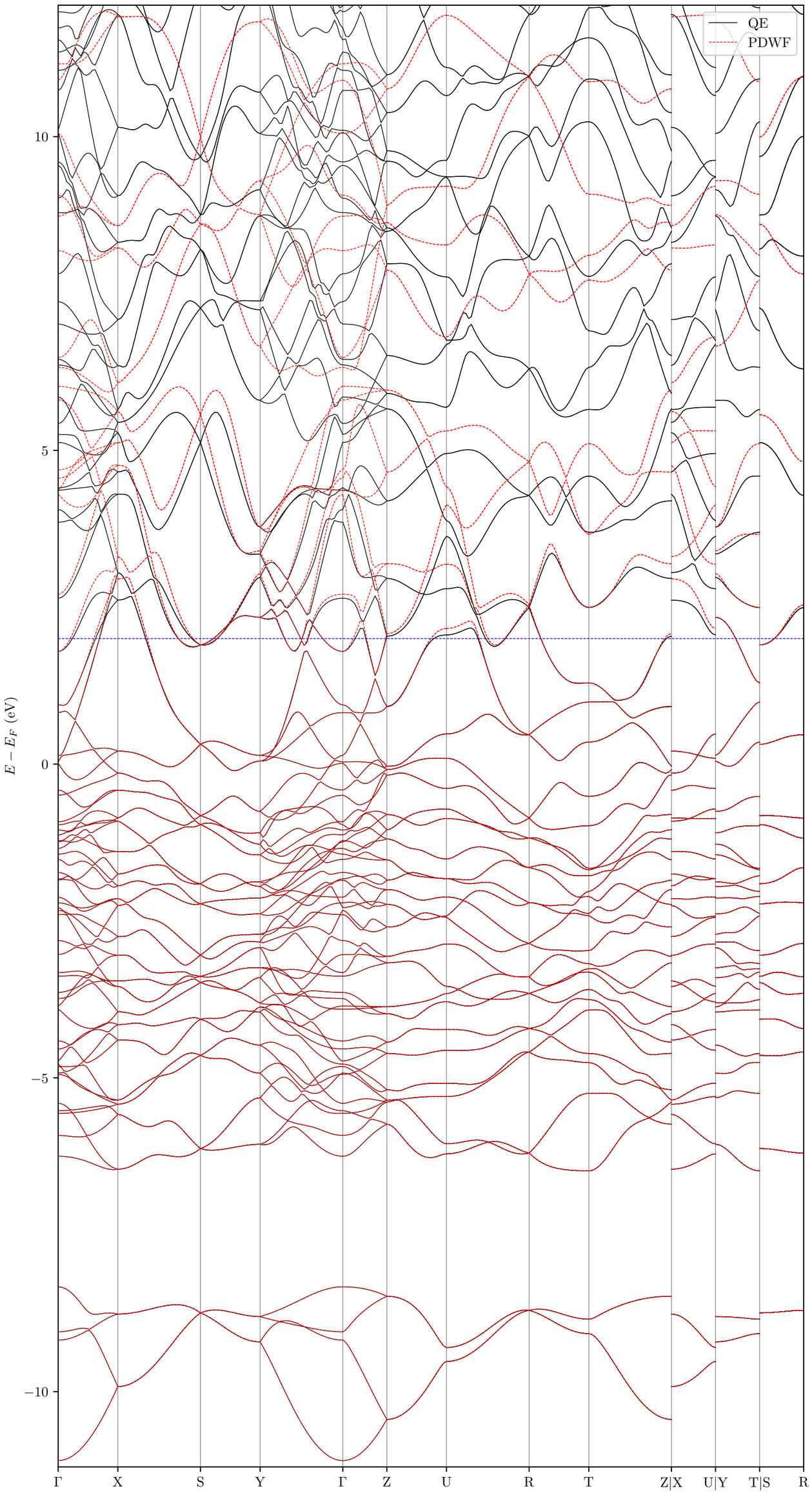

SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 6.3 | 6.7 | 7.9 | 30.4 | 39.5 | 53.5 | 2.807 |

Hamiltonian decay



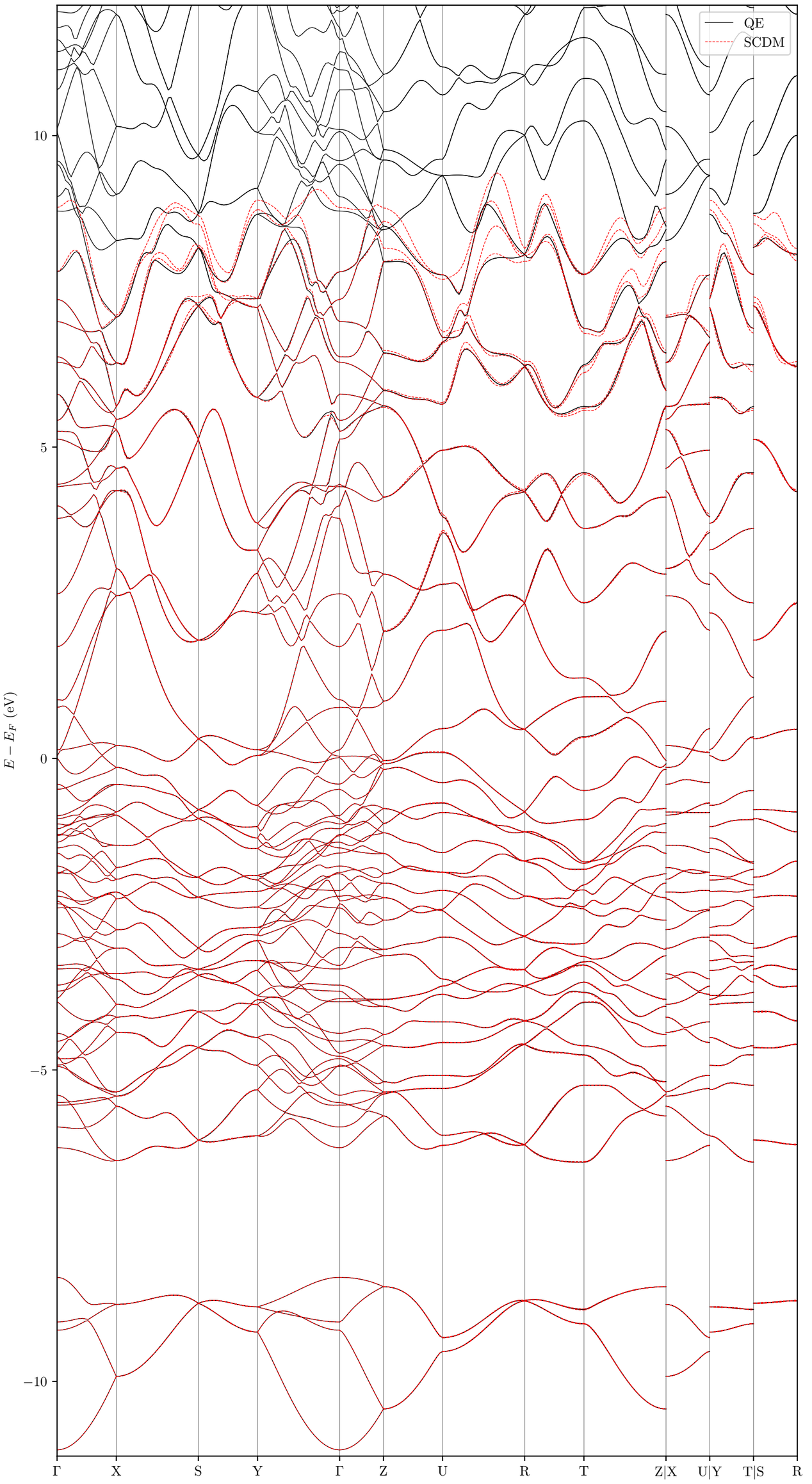
Rh8Si4 exclude semicore
PW=98a95399-f353-4605-a5bc-15884049a699
W90=ca10034a-f25d-4cd5-8b3c-f8c6e262b366




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.7 | 4.0 | 56.1 | 5.9 | 43.0 | 554.3 | 2.322 |

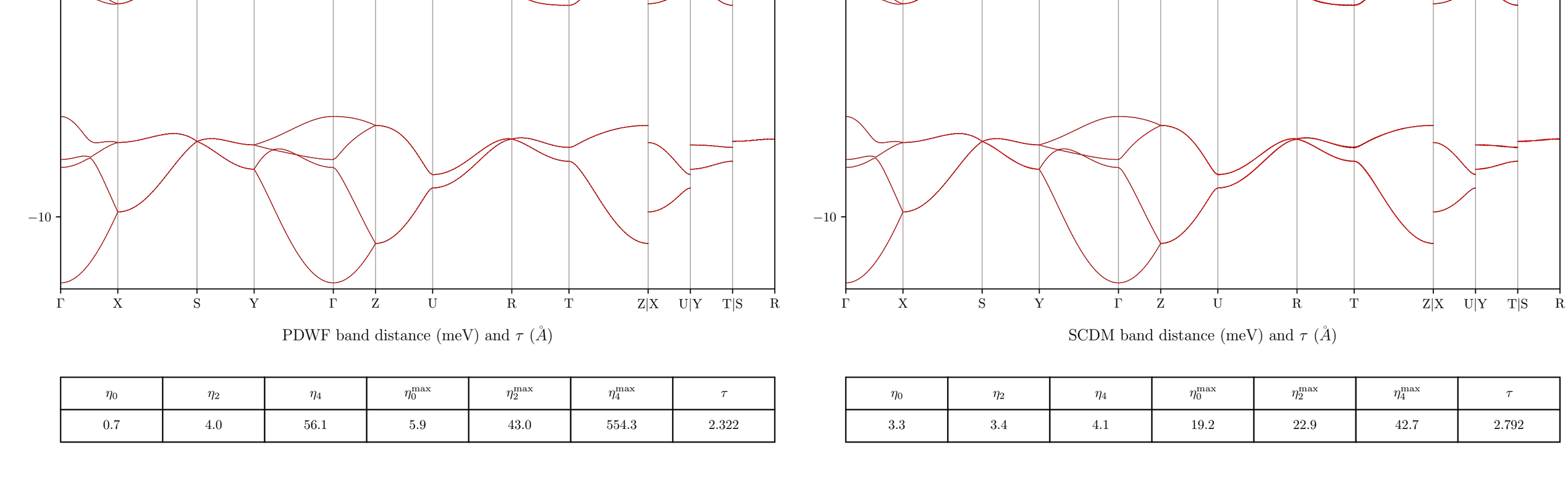
Rh8Si4 exclude semicore
PW=98a95399-f353-4605-a5bc-15884049a699
W90=f4b81a90-860b-4345-a8cc-164130cc9ab8



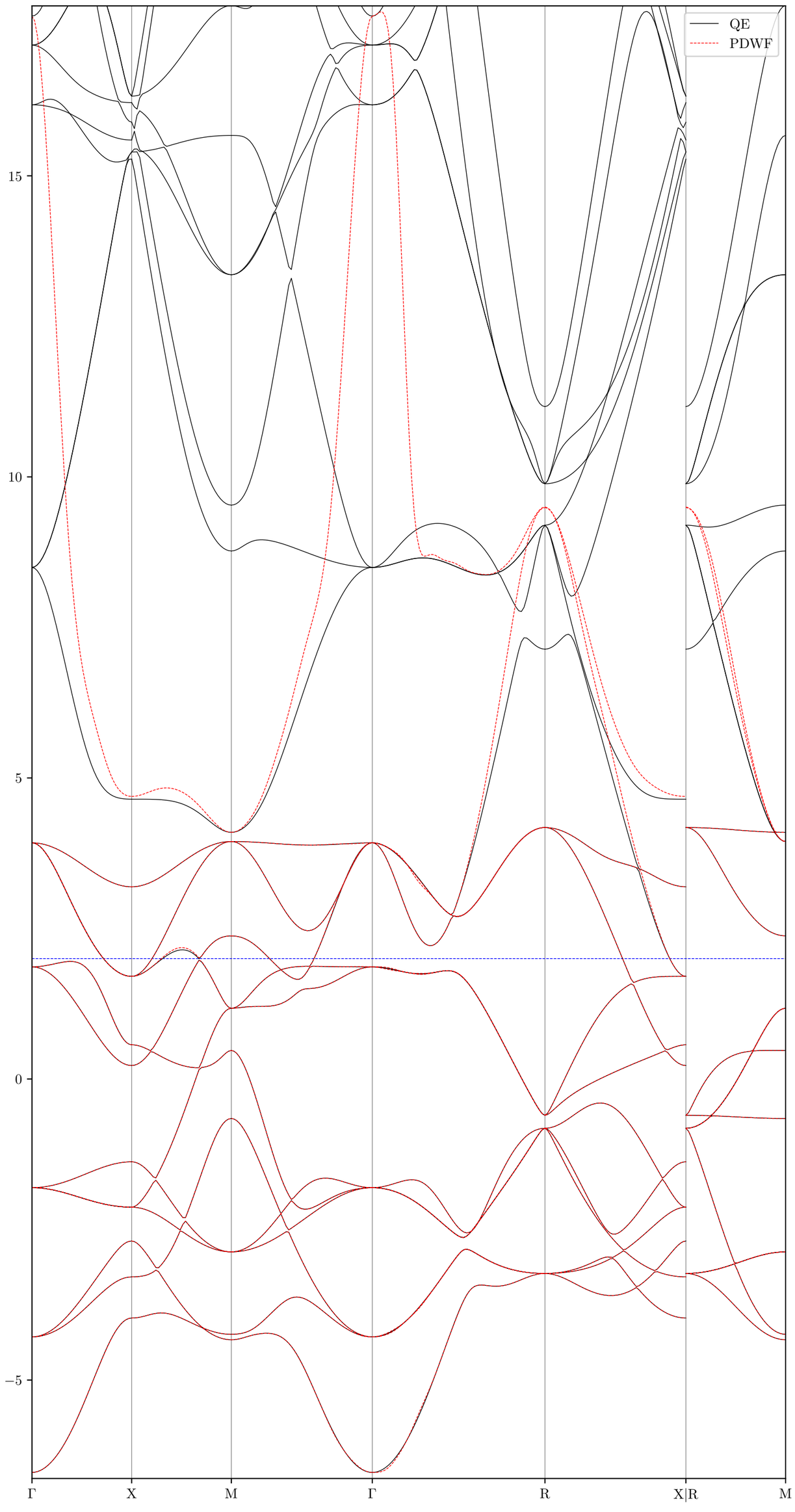

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.3 | 3.4 | 4.1 | 19.2 | 22.9 | 42.7 | 2.792 |

Hamiltonian decay



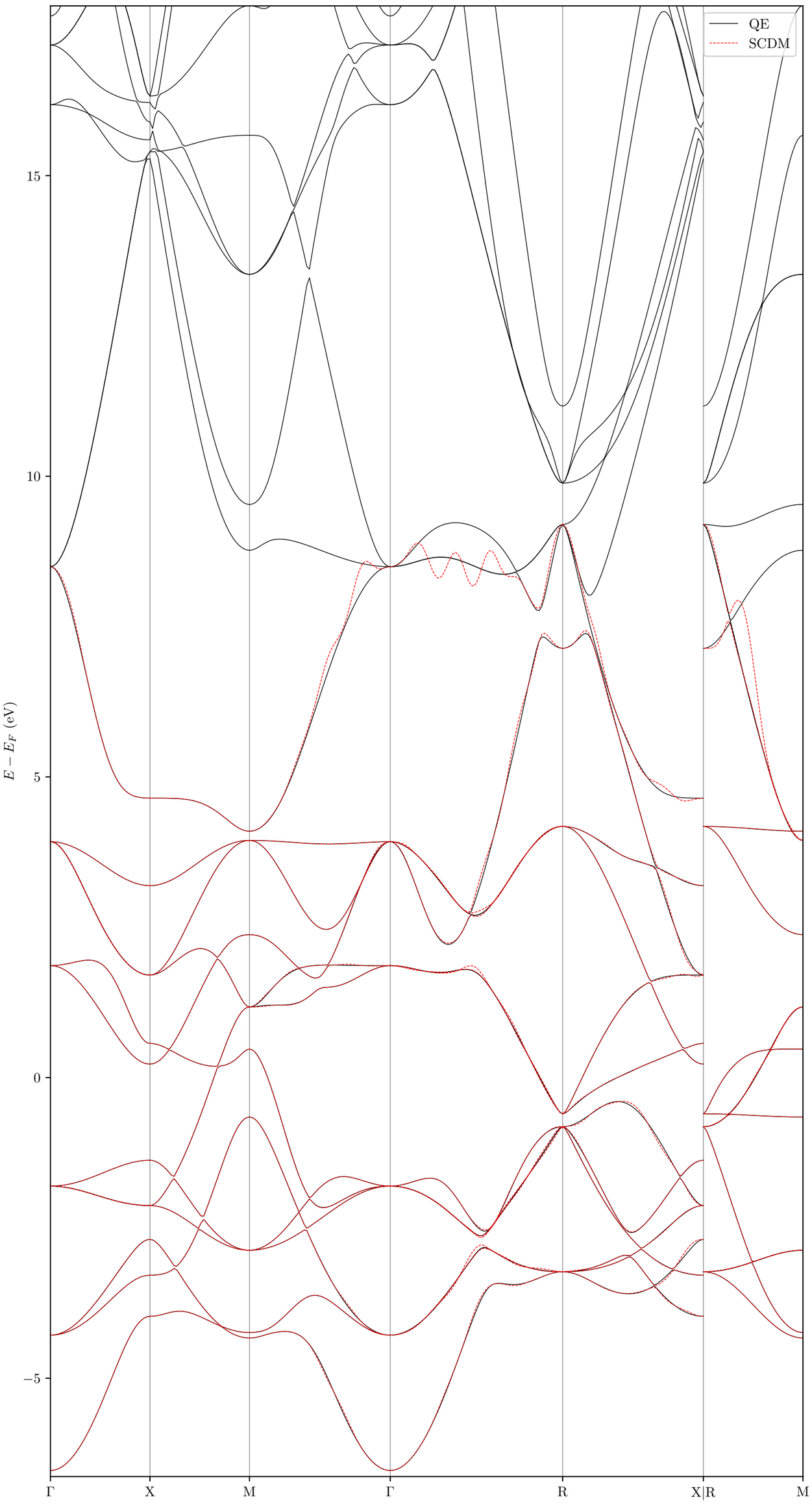
RhSc exclude semicore
PW=75b122c0-4a33-4108-88ca-1ecb3d7d1940
W90=4a0e6121-01c4-471d-b68e-8cd31a3a4966




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.5 | 3.5 | 8.2 | 40.3 | 40.3 | 135.2 | 2.105 |

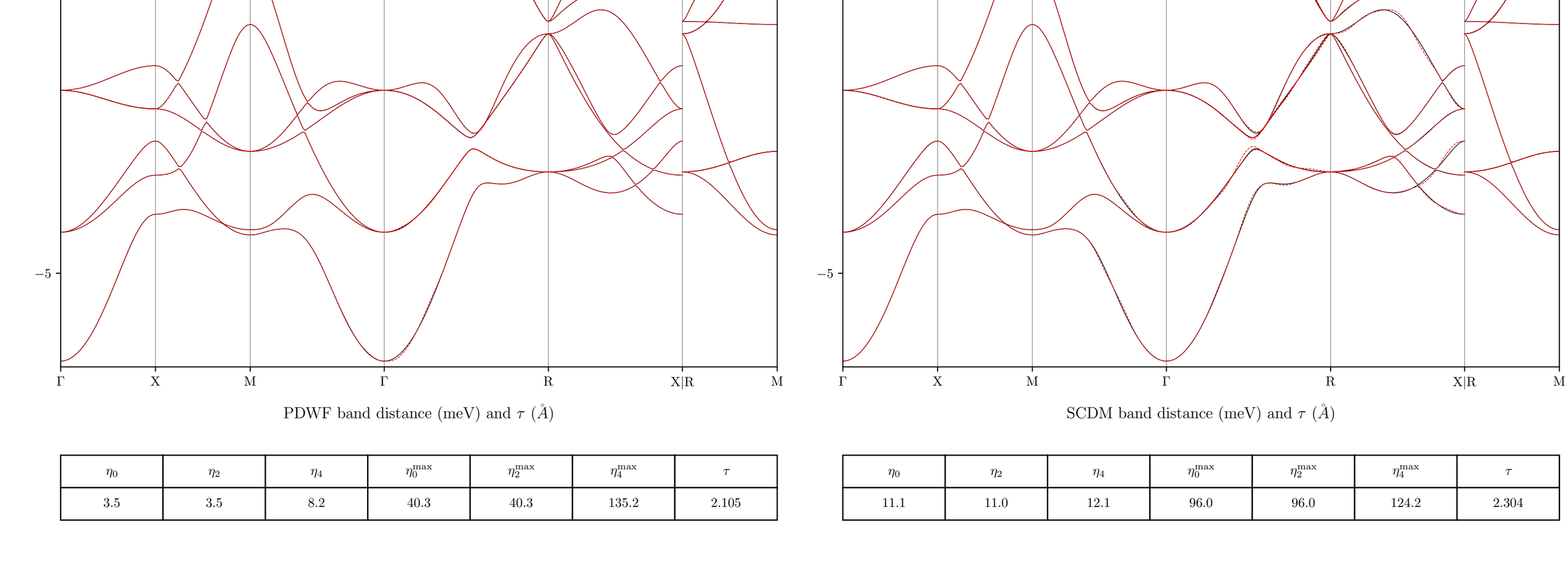
RhSc exclude semicore
PW=75b122c0-4a33-4108-88ca-1ecb3d7d1940
W90=44b18eb2-a7eb-473a-b39e-6e0fb569e72b



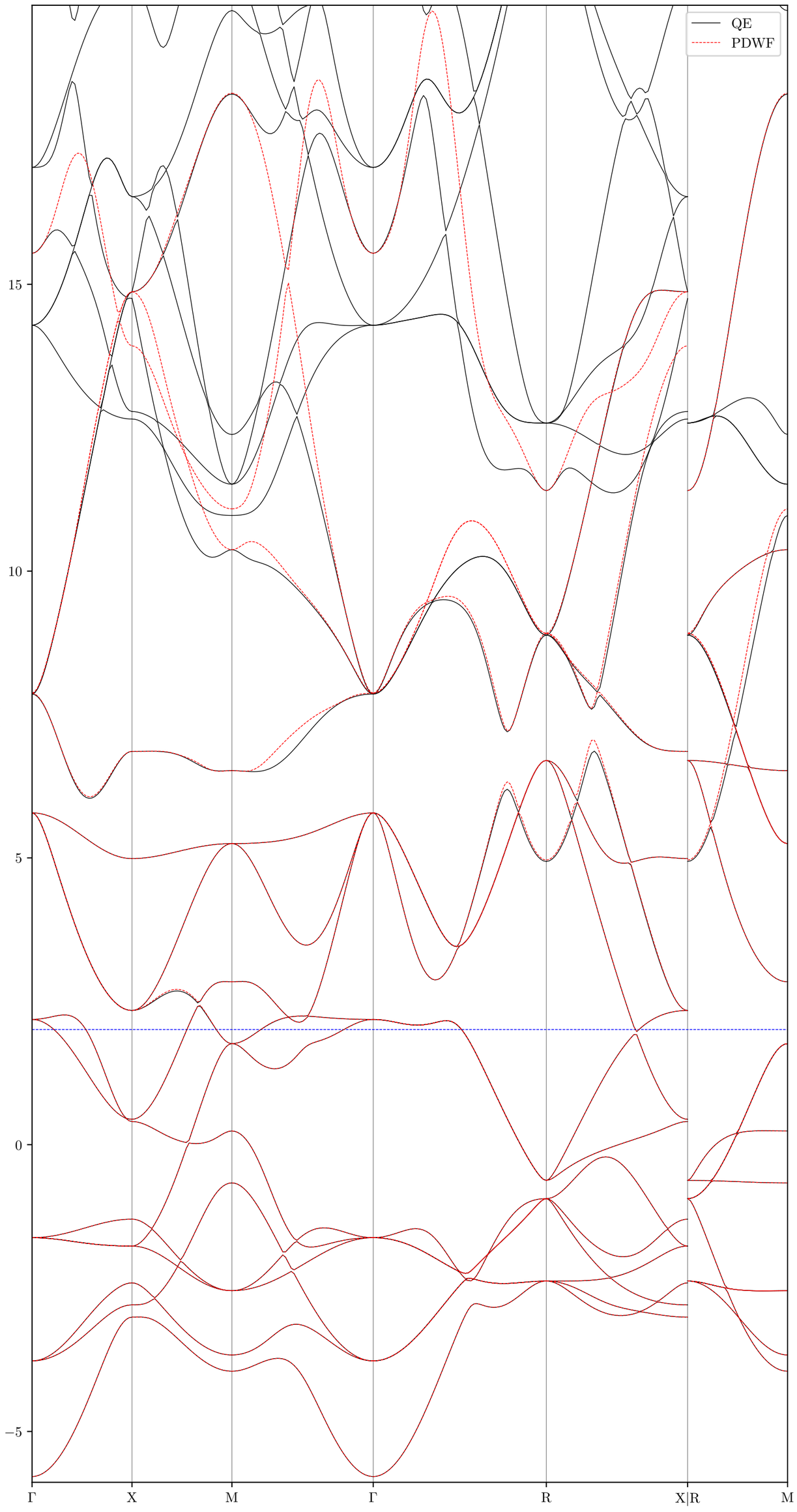

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 11.1 | 11.0 | 12.1 | 96.0 | 96.0 | 124.2 | 2.304 |

Hamiltonian decay



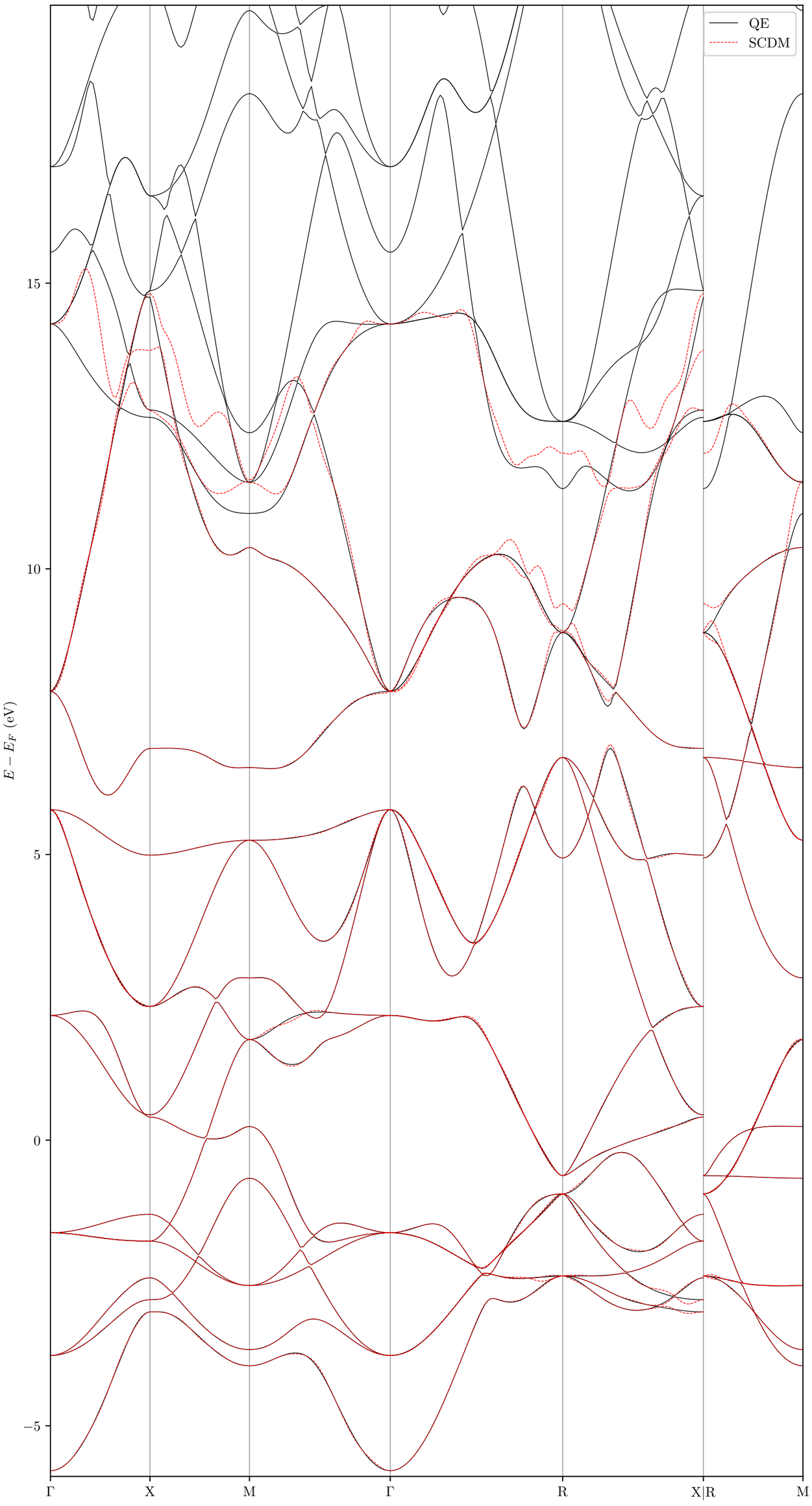
RhY exclude semicore
PW=8a89d5e6-b964-4f2f-b23c-fa30940378d6
W90=d61efacd-ecdc-48ad-83de-4edc69ded7ea




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 0.7 | 2.7 | 3.1 | 3.7 | 28.9 | 1.861 |

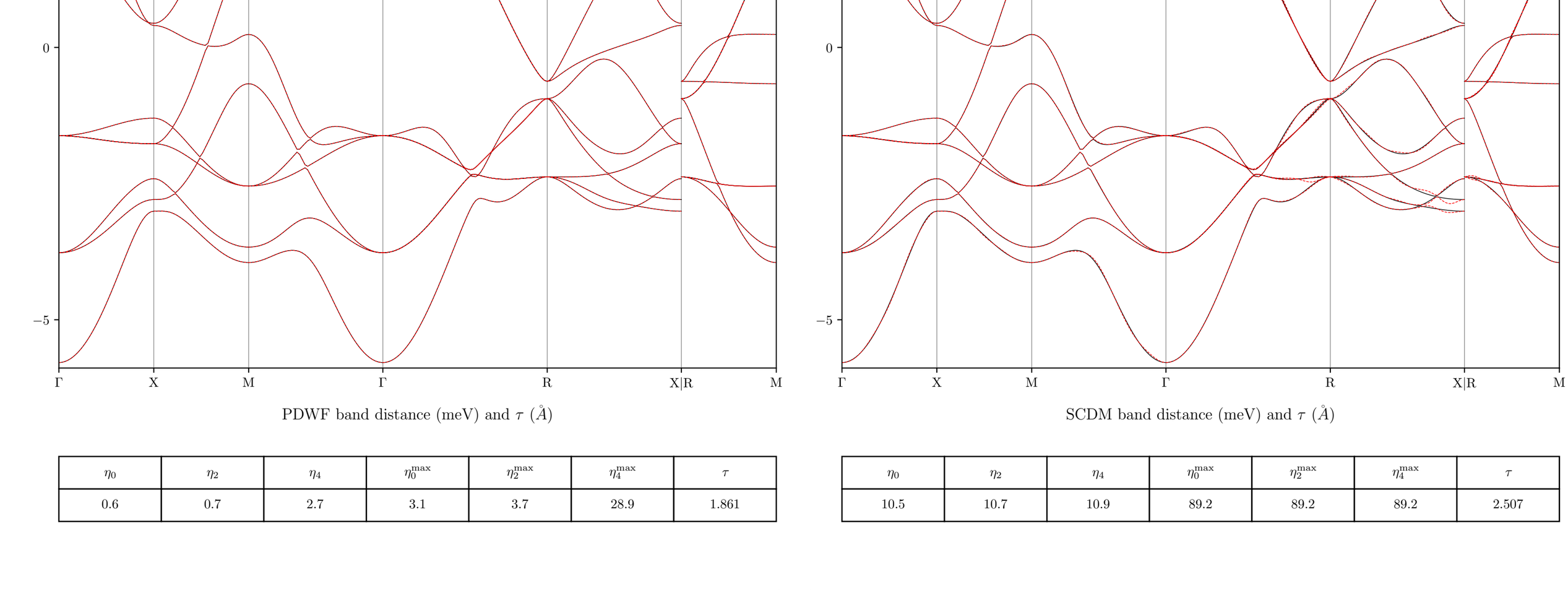
RhY exclude semicore
PW=8a89d5e6-b964-4f2f-b23c-fa30940378d6
W90=425cf049-1257-48d7-b836-06c542b93266



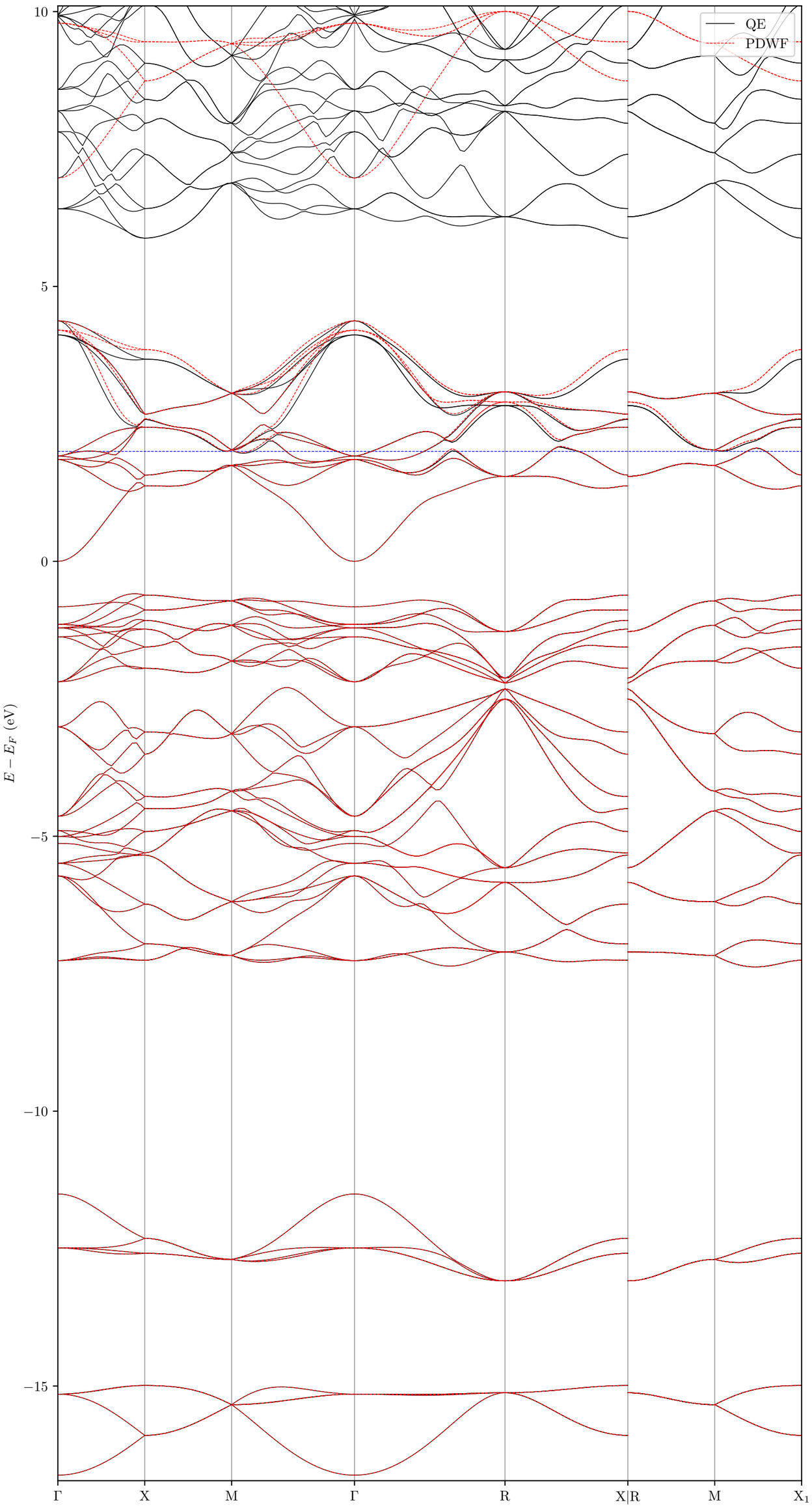

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 10.5 | 10.7 | 10.9 | 89.2 | 89.2 | 89.2 | 2.507 |

Hamiltonian decay



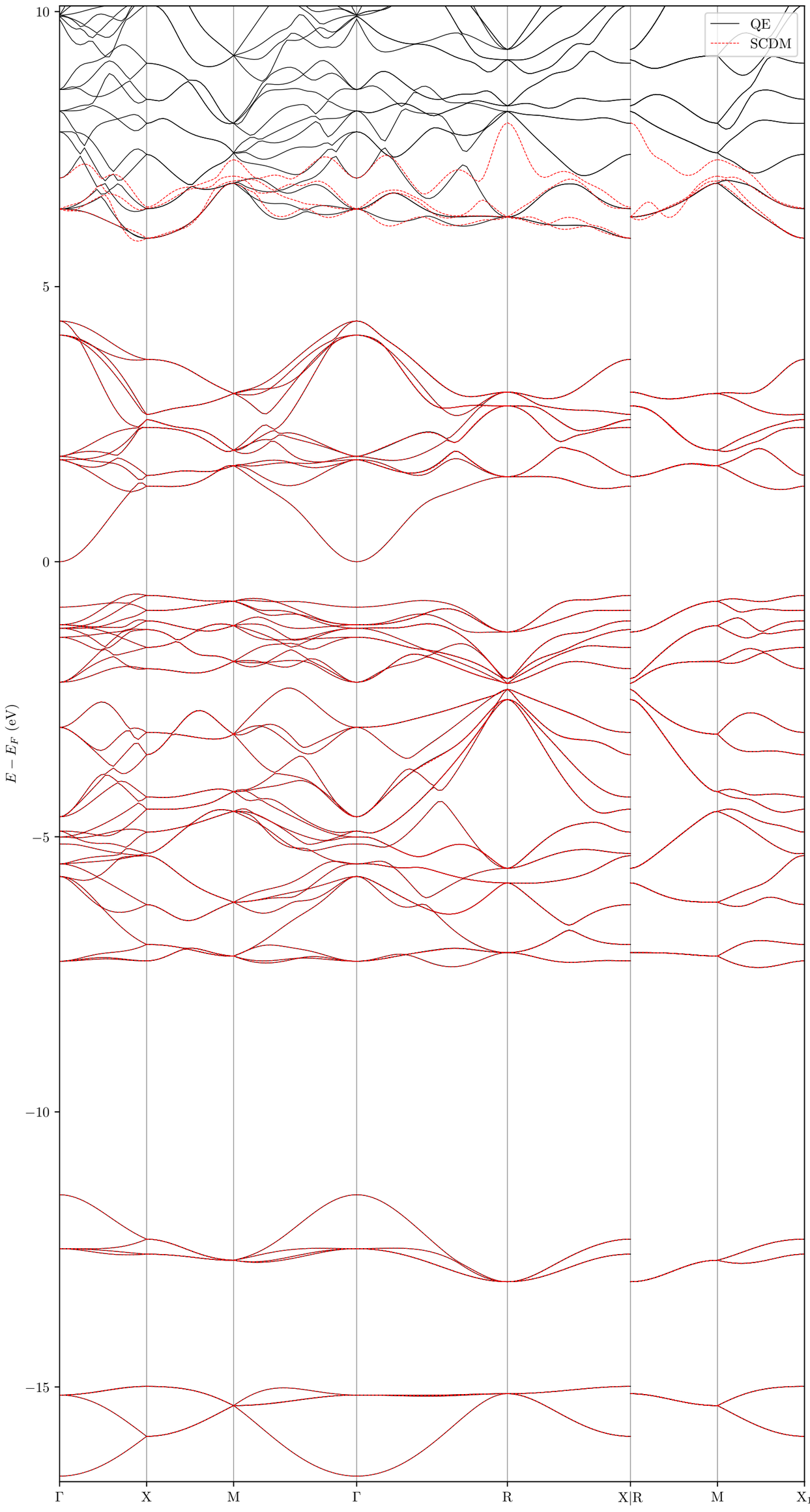
Ru4S8 exclude semicore
PW=455b7d24-4566-49de-abb7-8b575d8dbd1c
W90=86c681b7-5958-4c0c-81ca-2b3e2efcc9d7




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.4 | 1.1 | 24.1 | 3.4 | 12.6 | 221.3 | 2.314 |

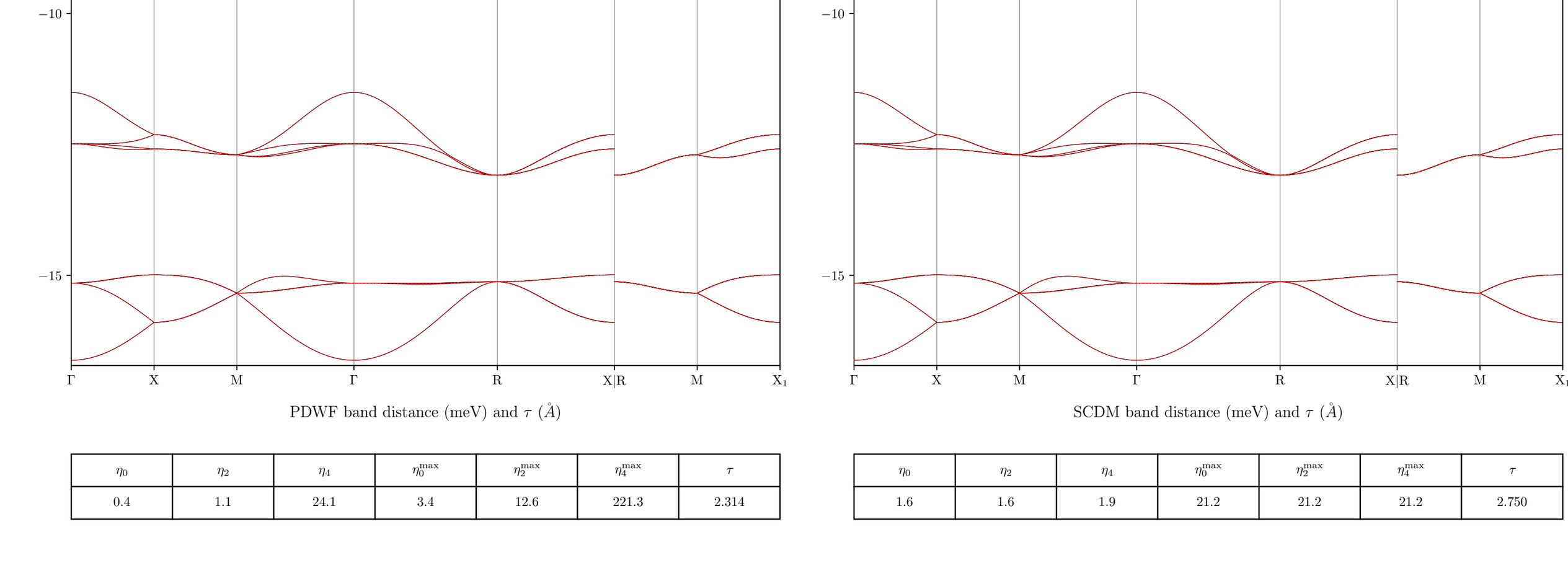
Ru4S8 exclude semicore
PW=455b7d24-4566-49de-abb7-8b575d8dbd1c
W90=73851ea8-36b2-42ff-9fe2-1a3edab46370

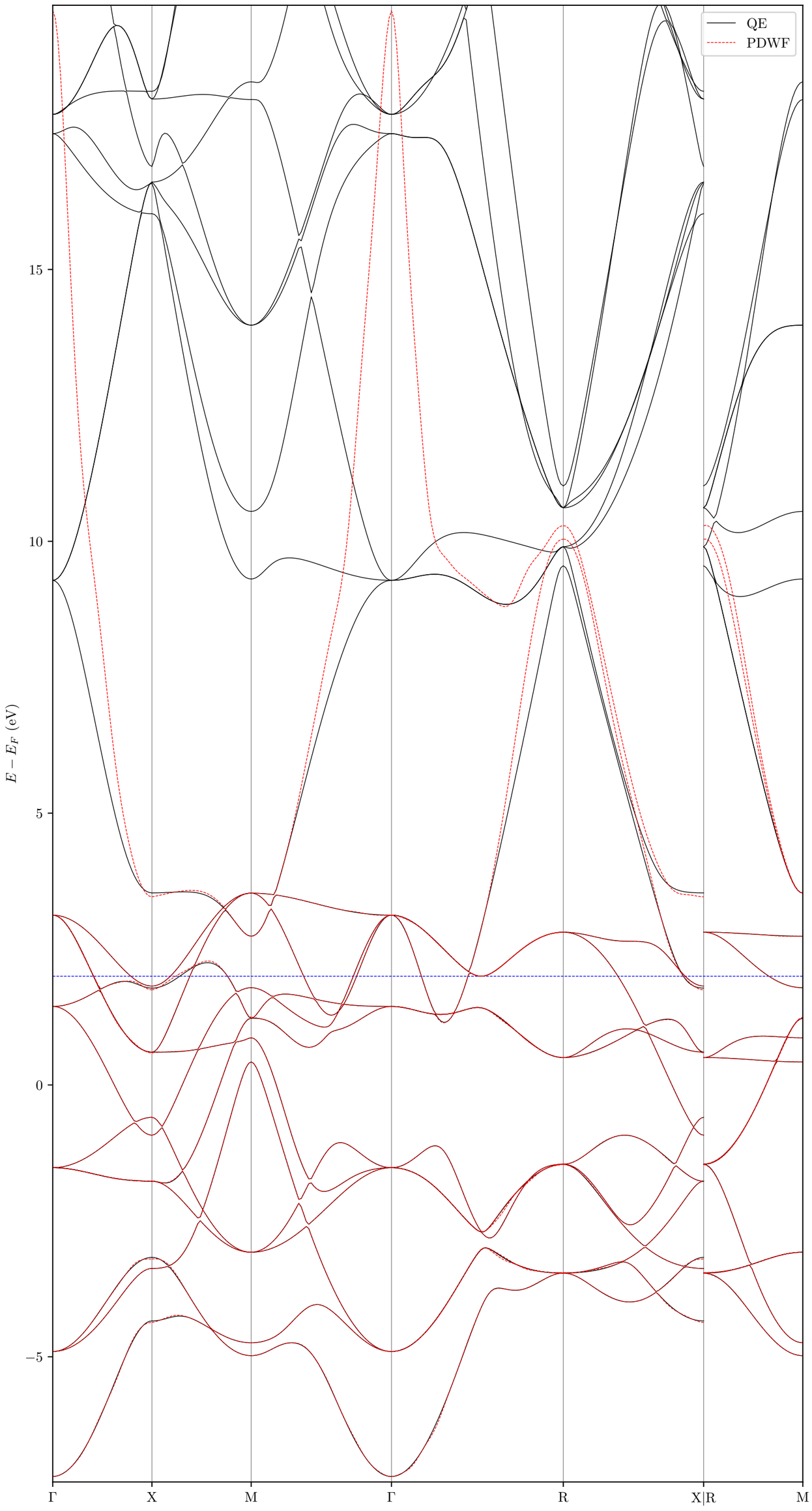



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.6 | 1.6 | 1.9 | 21.2 | 21.2 | 21.2 | 2.750 |

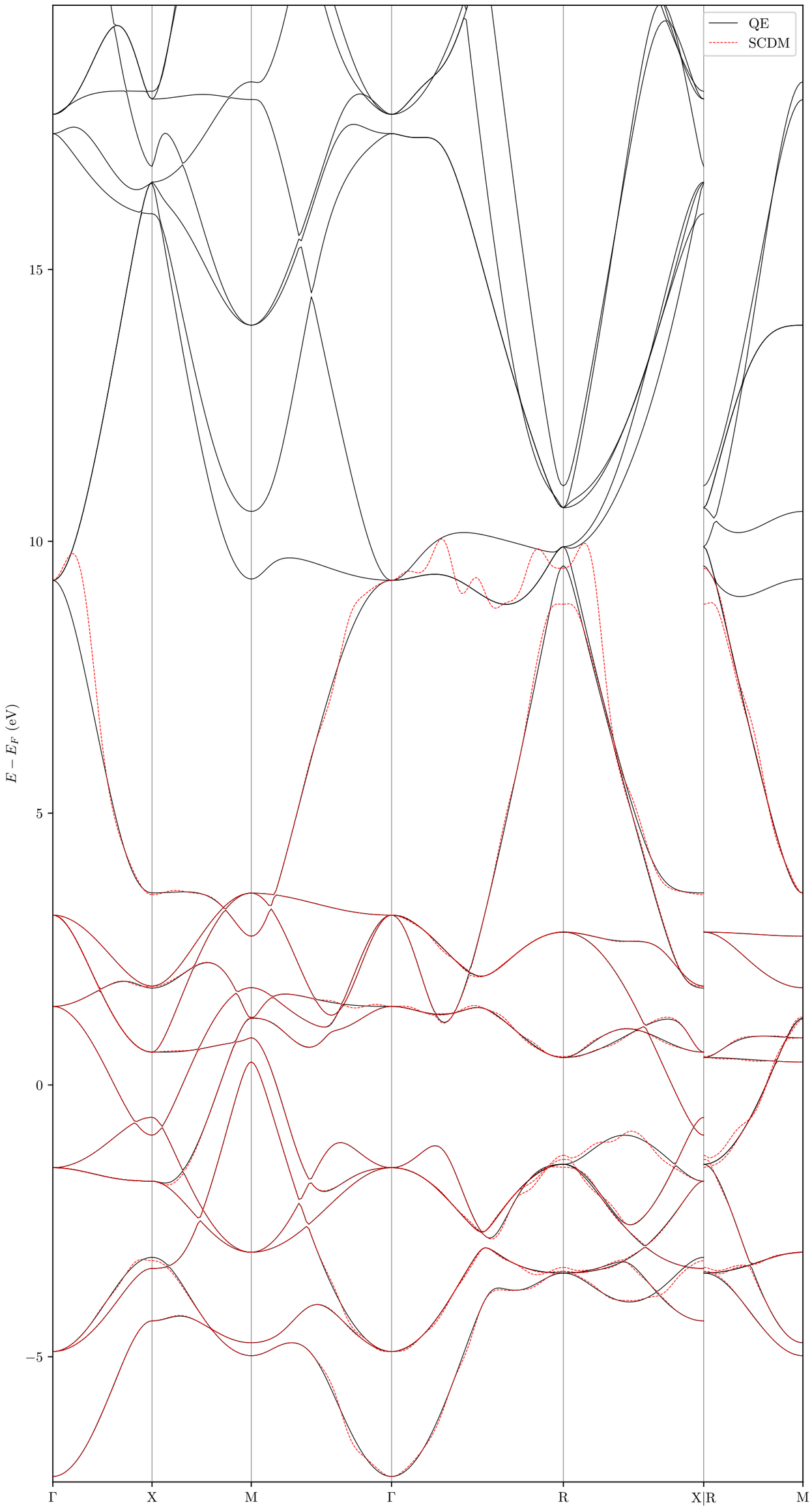
Hamiltonian decay





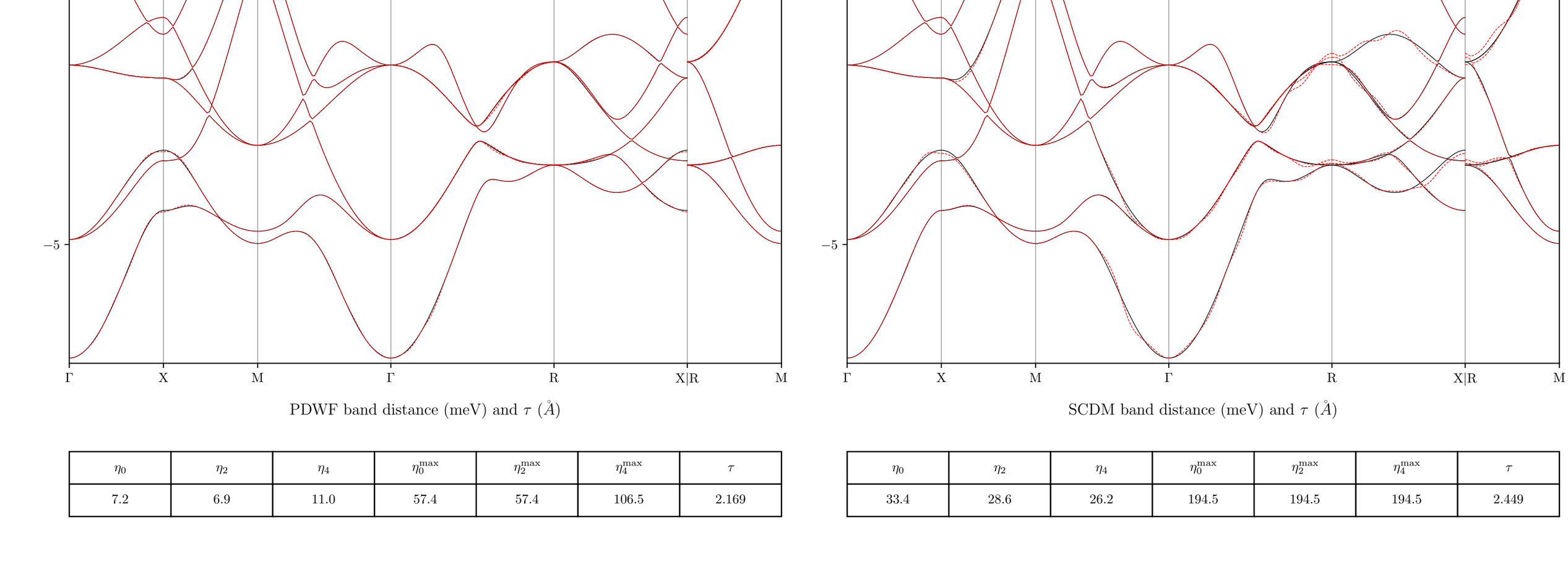

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 7.2 | 6.9 | 11.0 | 57.4 | 57.4 | 106.5 | 2.169 |

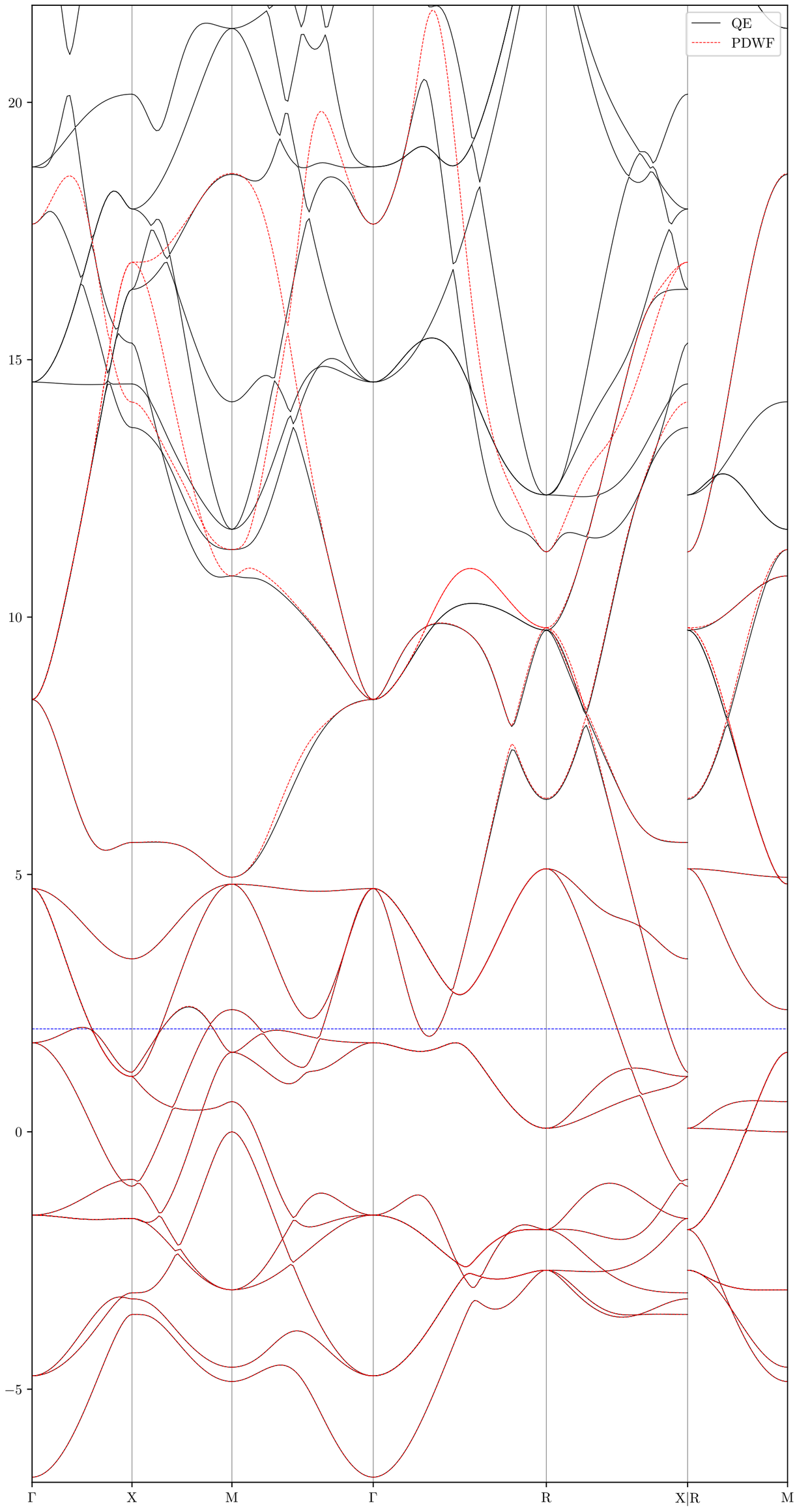



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 33.4 | 28.6 | 26.2 | 194.5 | 194.5 | 194.5 | 2.449 |



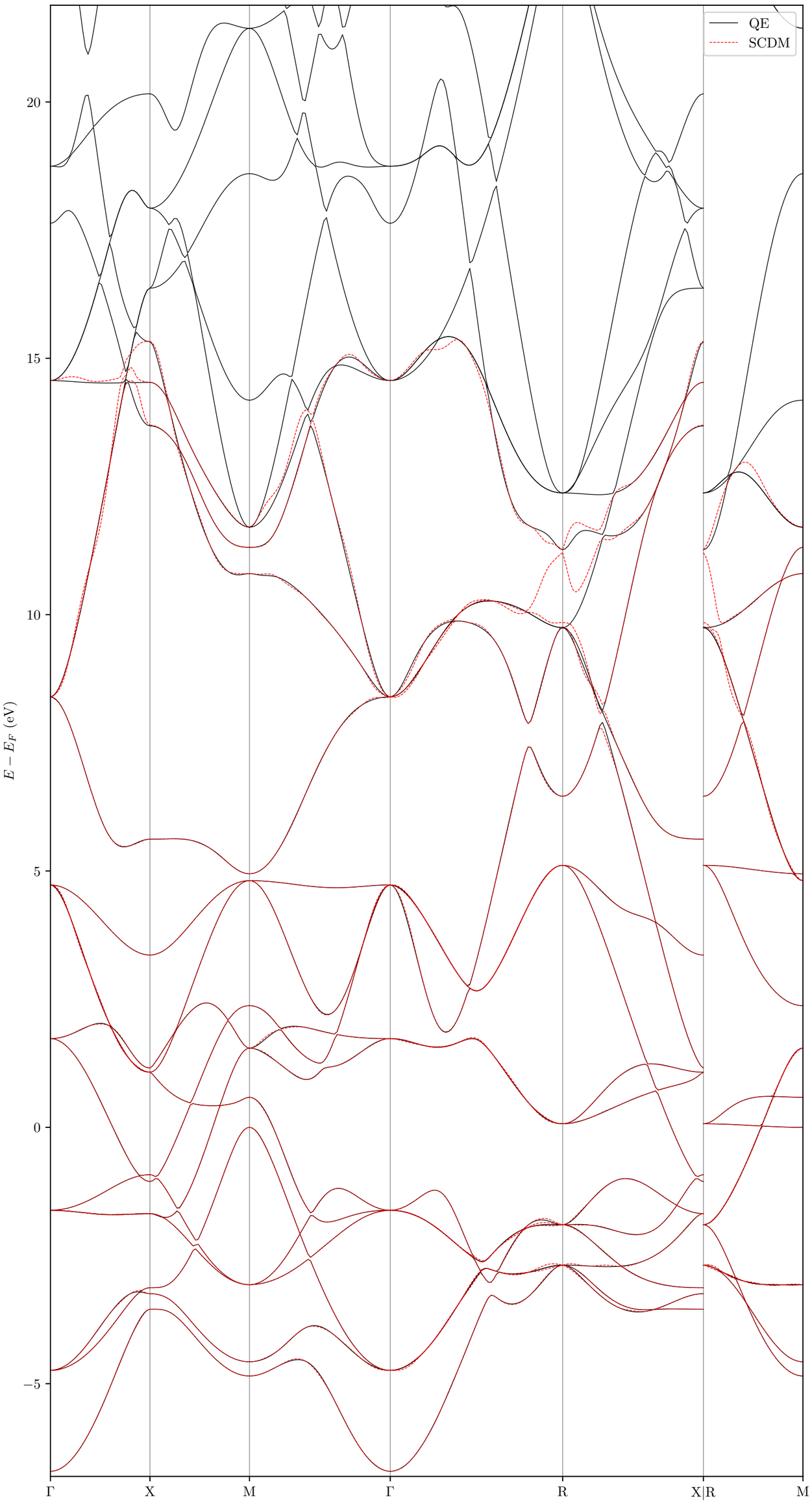
RuZr exclude semicore
PW=dfd8332a-1581-4e6d-9ba2-f05245810017
W90=ac2bd577-b1a8-481a-8c03-f8f7f18f31bf




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.8 | 0.9 | 1.4 | 4.8 | 5.8 | 12.8 | 1.879 |

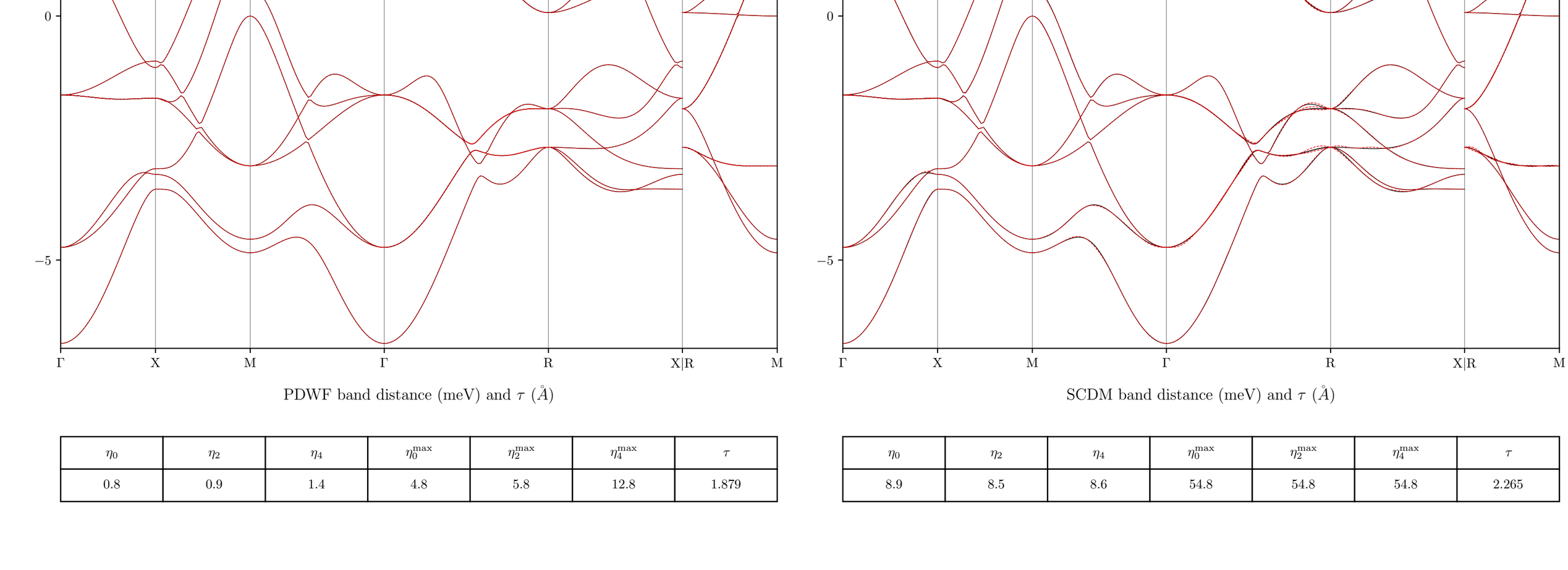
RuZr exclude semicore
PW=dfd8332a-1581-4e6d-9ba2-f05245810017
W90=2ddfdafc-0b49-4a1b-8b20-2d1a09f6ca28



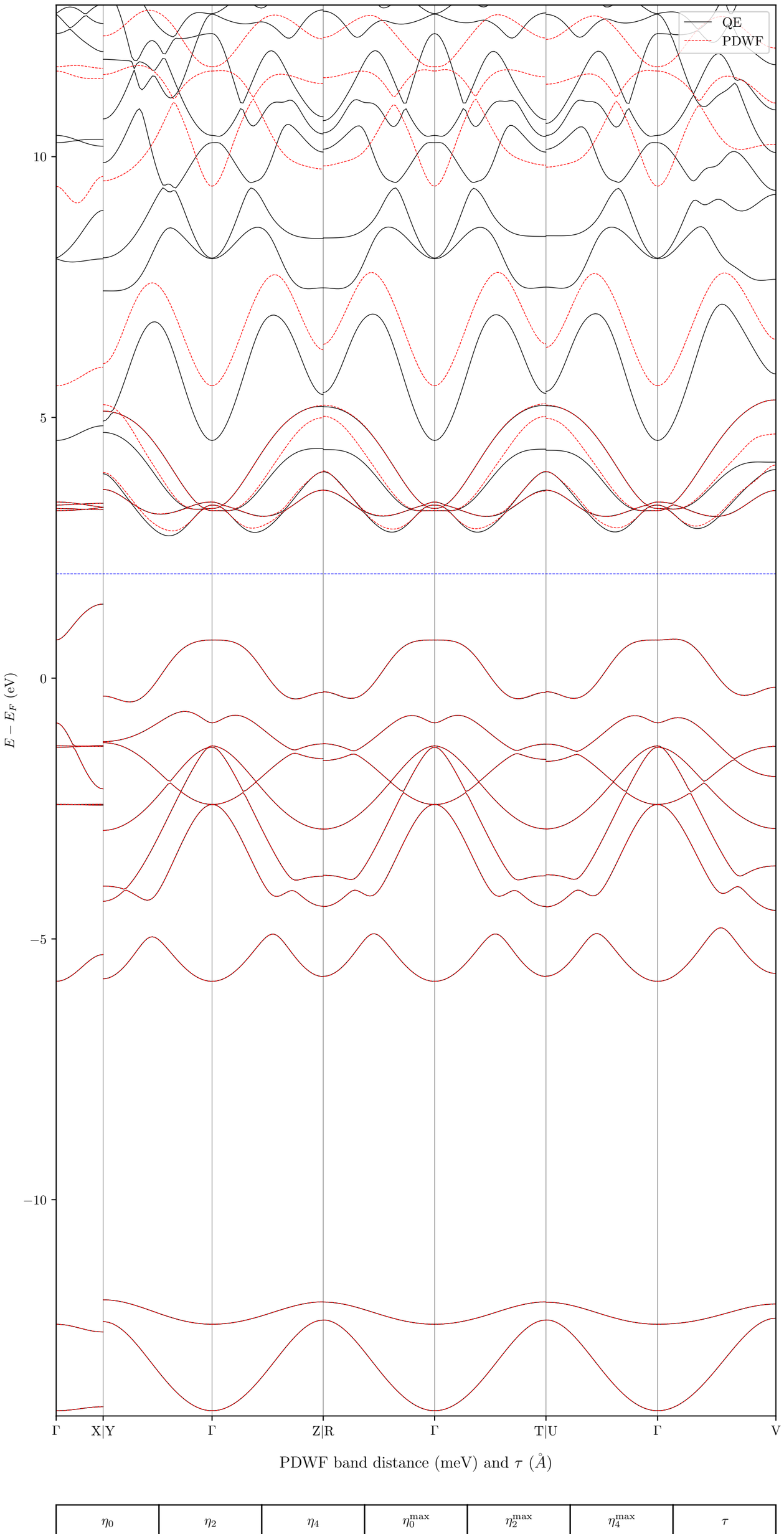

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 8.9 | 8.5 | 8.6 | 54.8 | 54.8 | 54.8 | 2.265 |

Hamiltonian decay



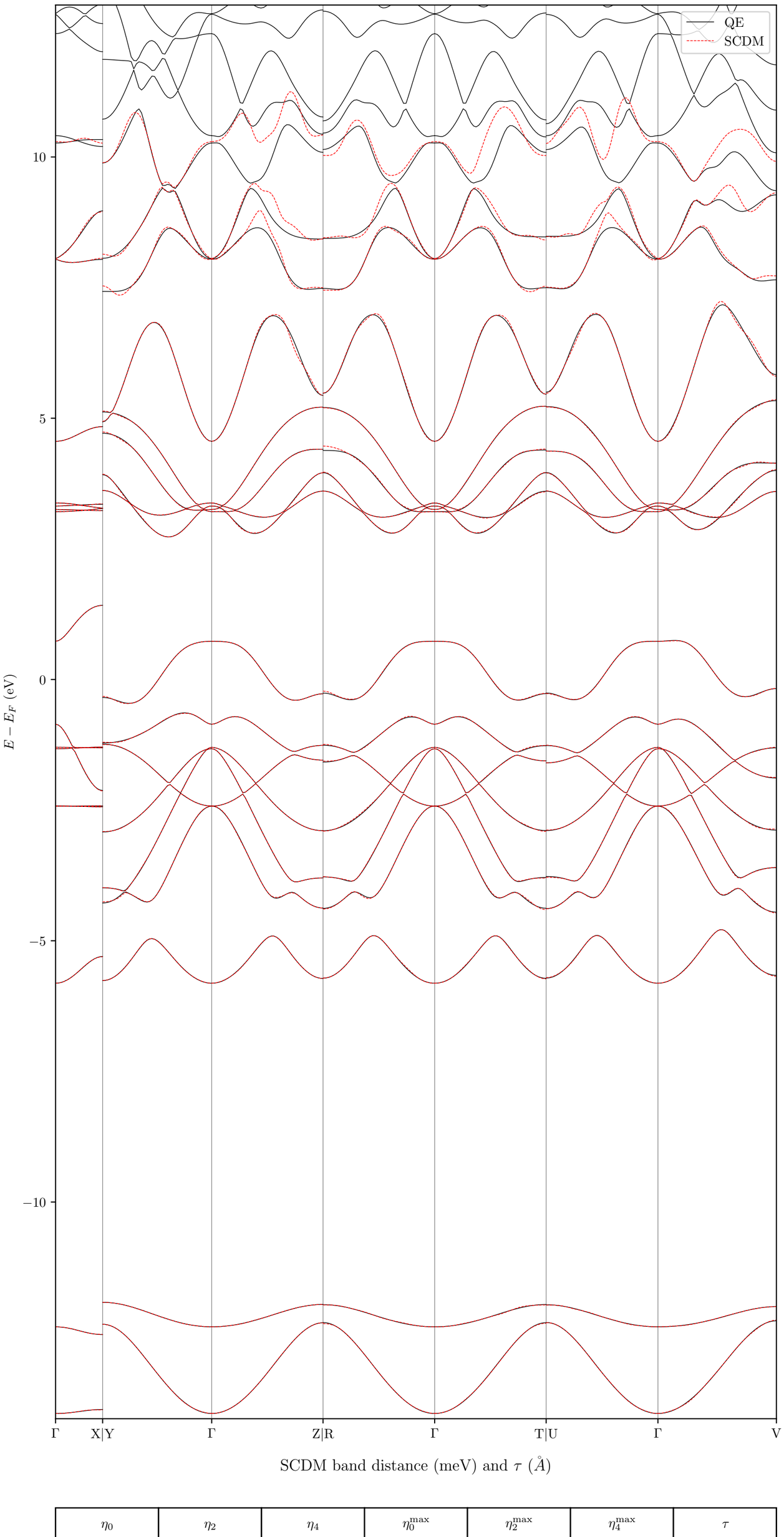
S2Ta exclude semicore
PW=a4b1b61d-8bd7-4c74-8987-6b7bd222d43b
W90=43d30fb5-139c-40a2-a9a2-bc6c35728a8b




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.4 | 1.4 | 19.1 | 7.7 | 8.0 | 114.2 | 2.337 |

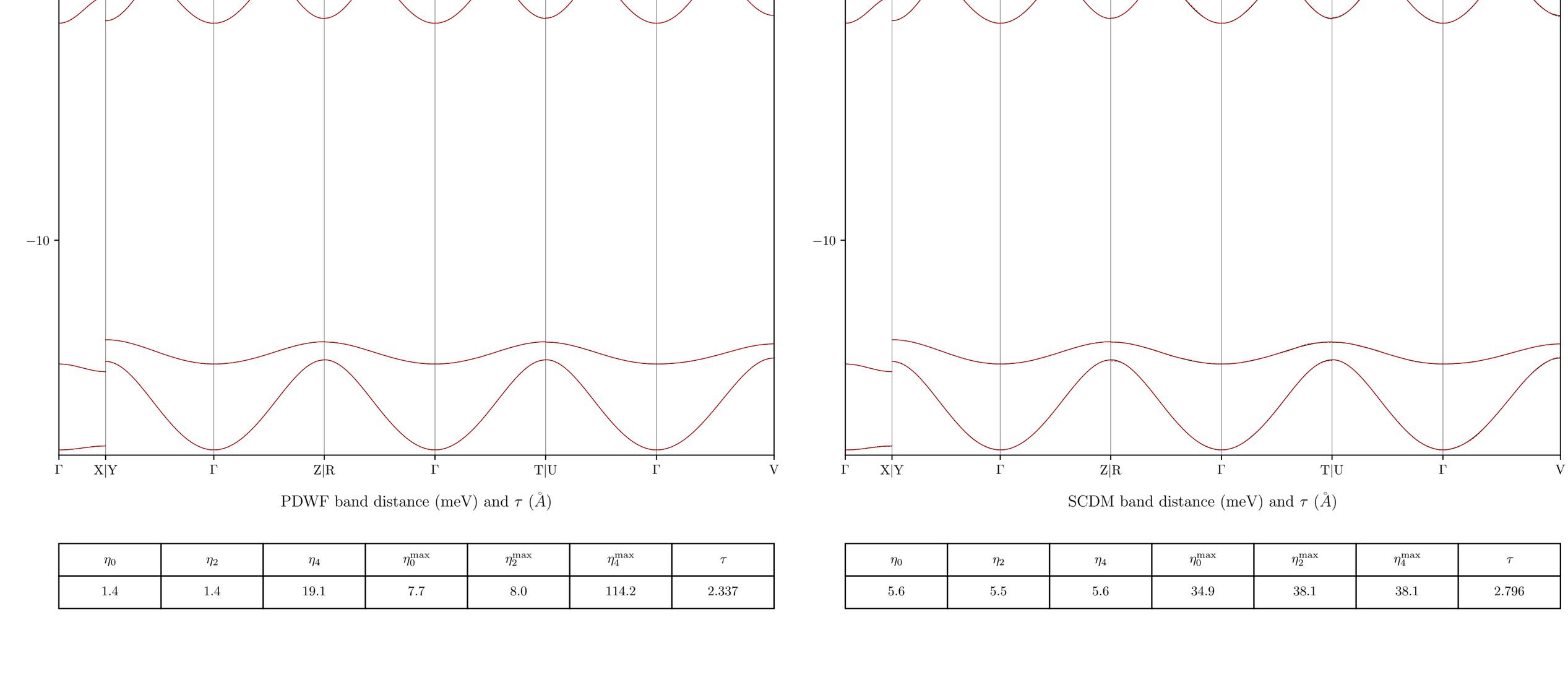
S2Ta exclude semicore
PW=a4b1b61d-8bd7-4c74-8987-6b7bd222d43b
W90=d7e27251-cabc-48f0-b34c-1647de816b3f



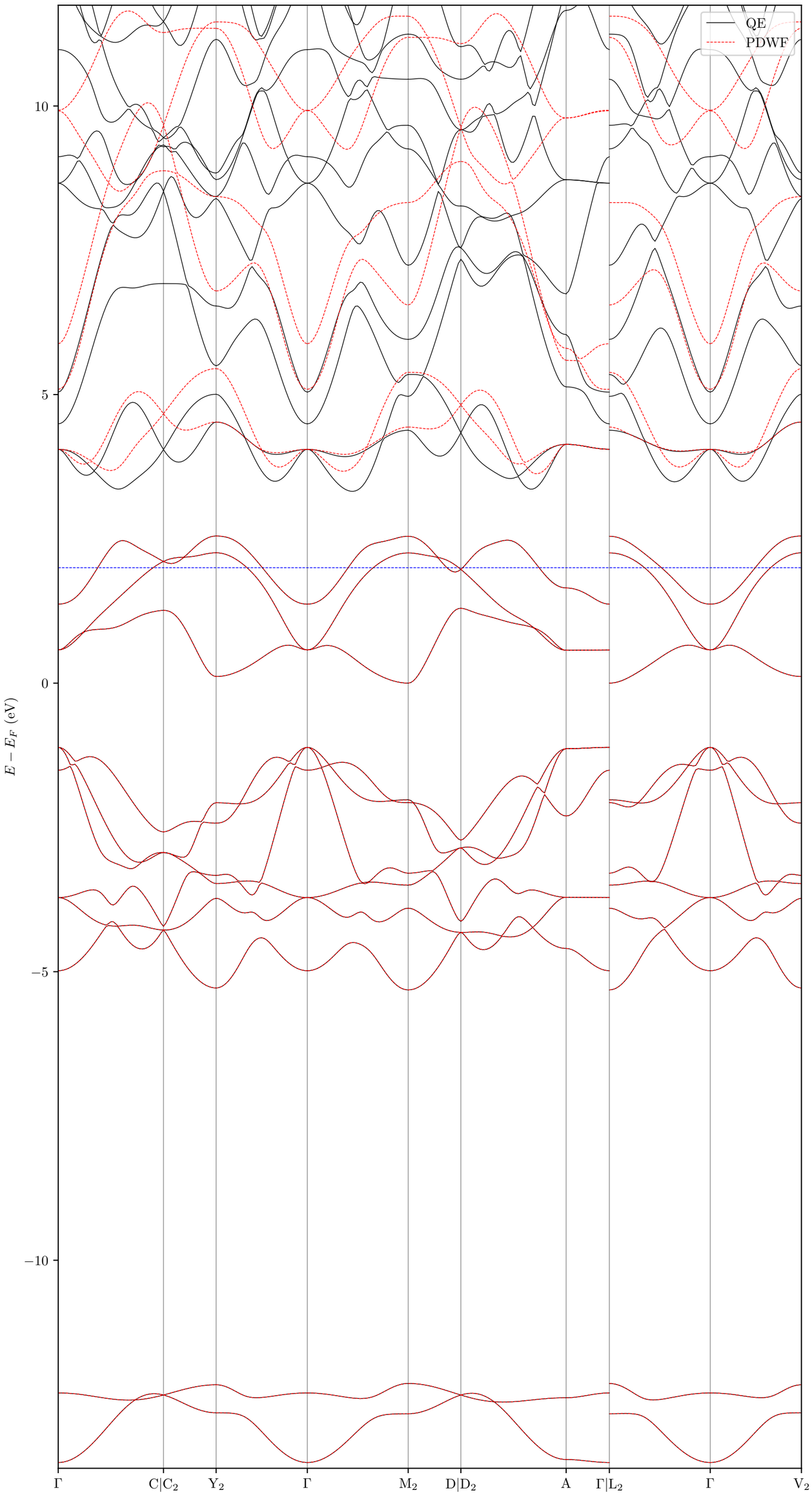

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.6 | 5.5 | 5.6 | 34.9 | 38.1 | 38.1 | 2.796 |

Hamiltonian decay



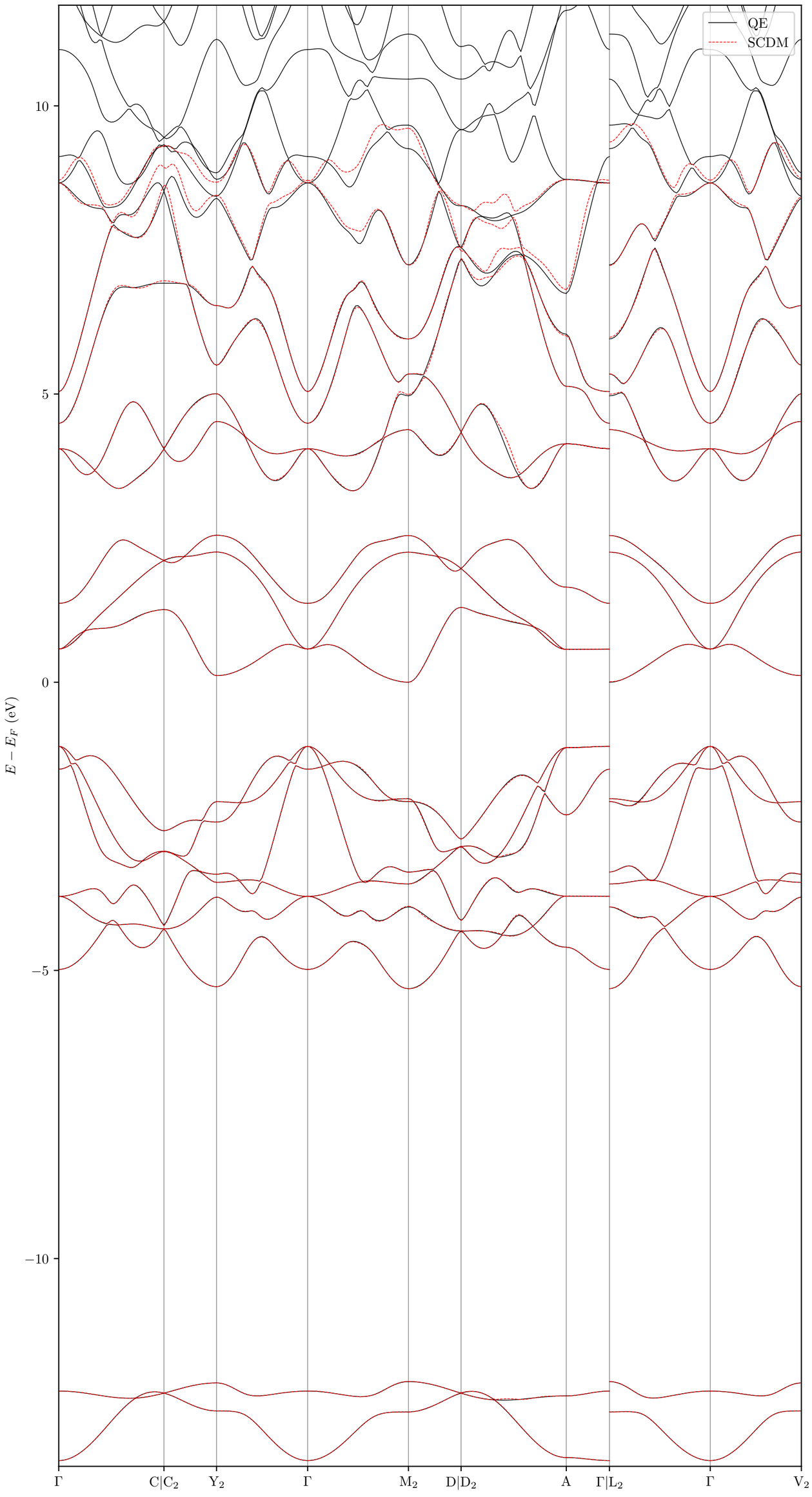
S2Zr exclude semicore
PW=d64e833a-8030-45ba-a2e8-7ffba0aab2f0
W90=990df551-0225-4d70-bc49-e85ca50ee5f1




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.1 | 20.0 | 7.9 | 7.9 | 107.4 | 2.361 |

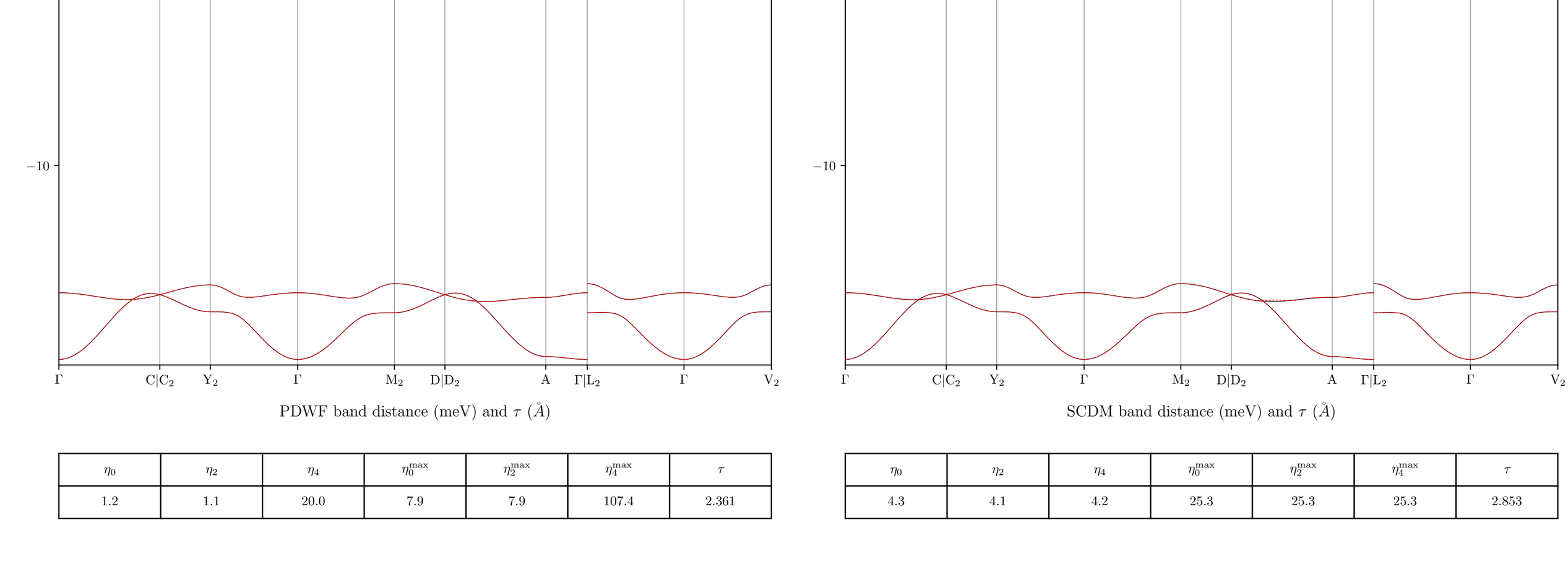
S2Zr exclude semicore
PW=d64e833a-8030-45ba-a2e8-7ffba0aab2f0
W90=0e1b8c37-5b4e-4cbd-a4c2-bd55fe84ca16

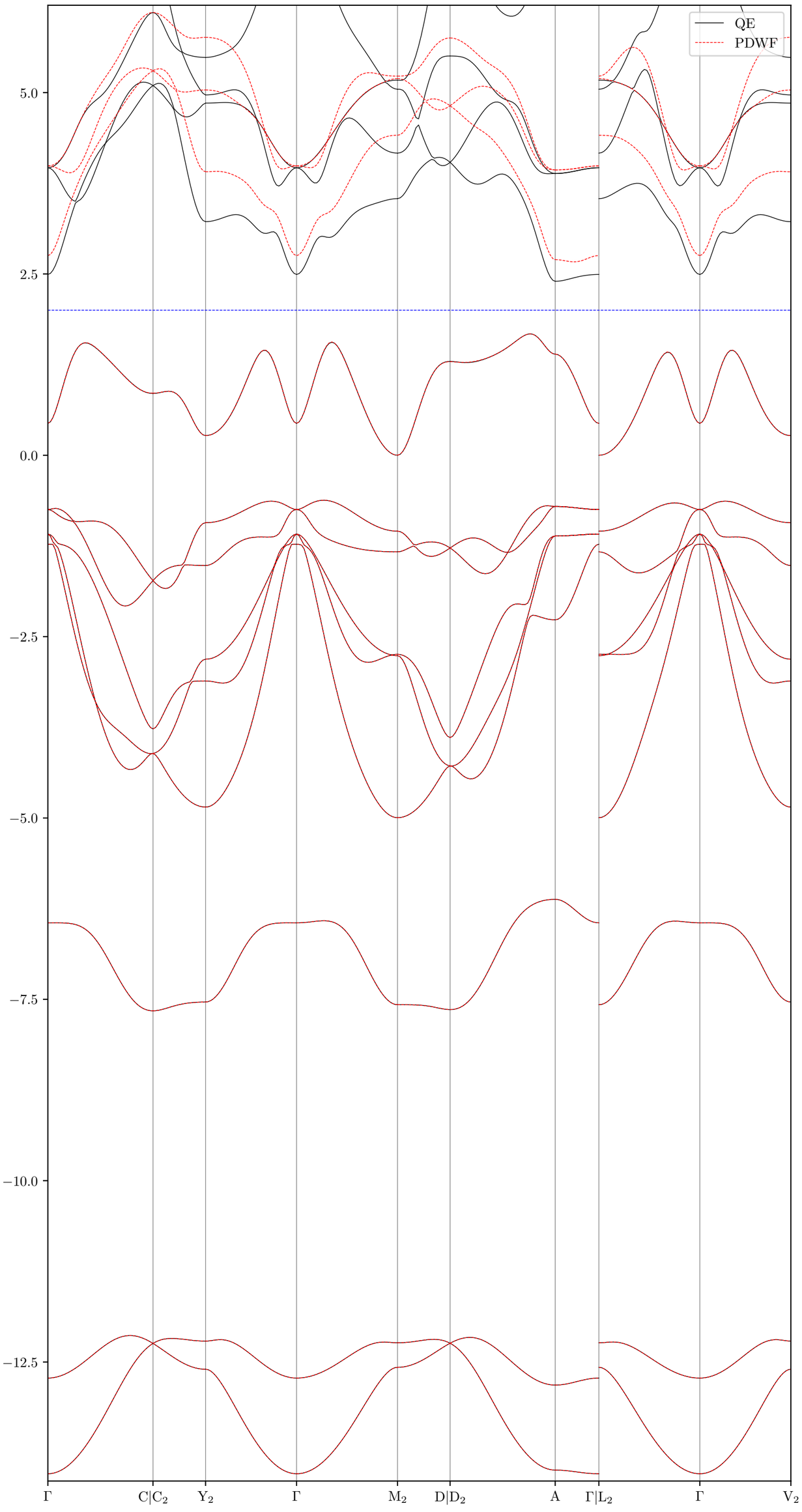



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.3 | 4.1 | 4.2 | 25.3 | 25.3 | 25.3 | 2.853 |

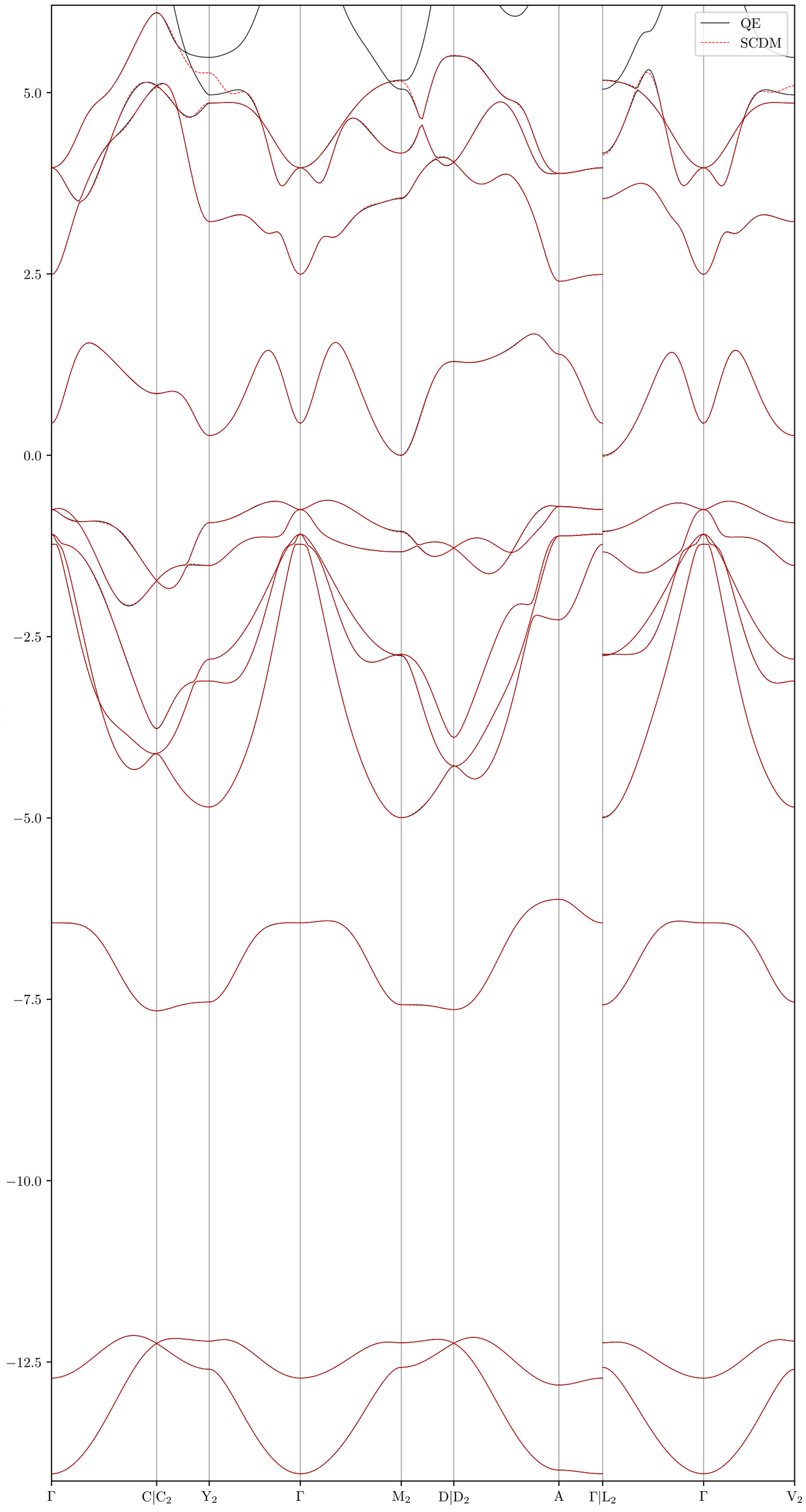
Hamiltonian decay





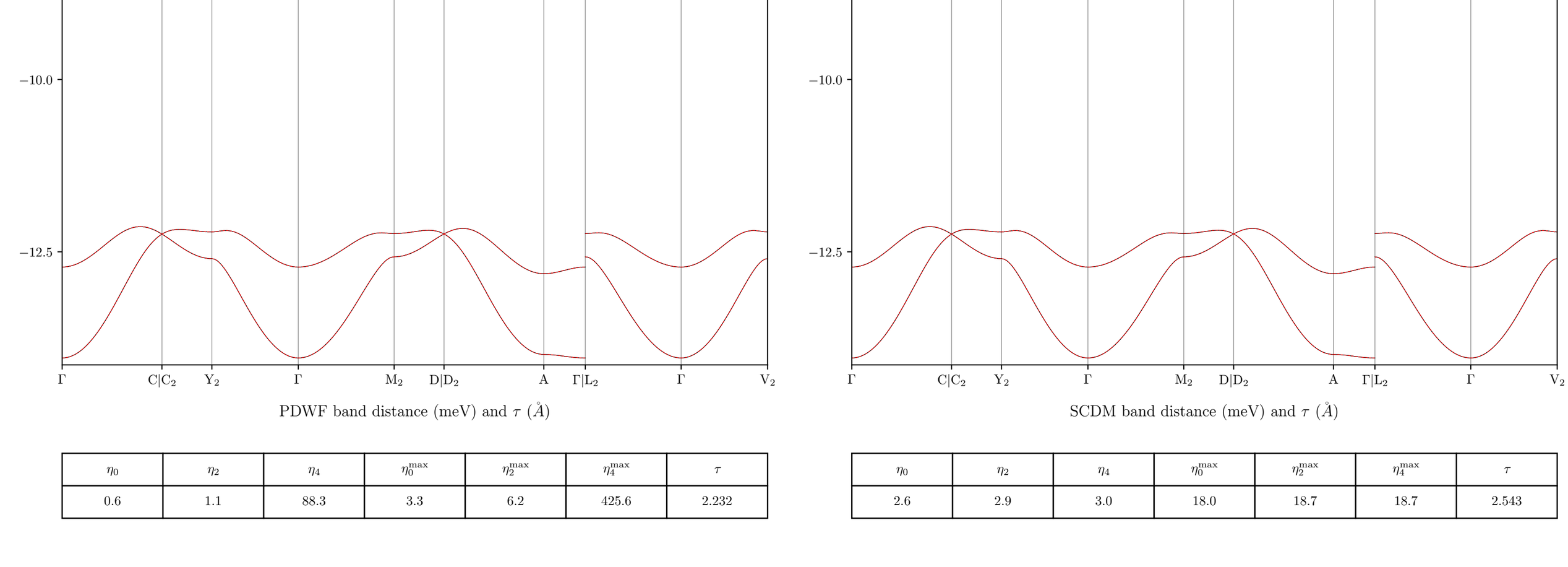

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.6 | 1.1 | 88.3 | 3.3 | 6.2 | 425.6 | 2.232 |

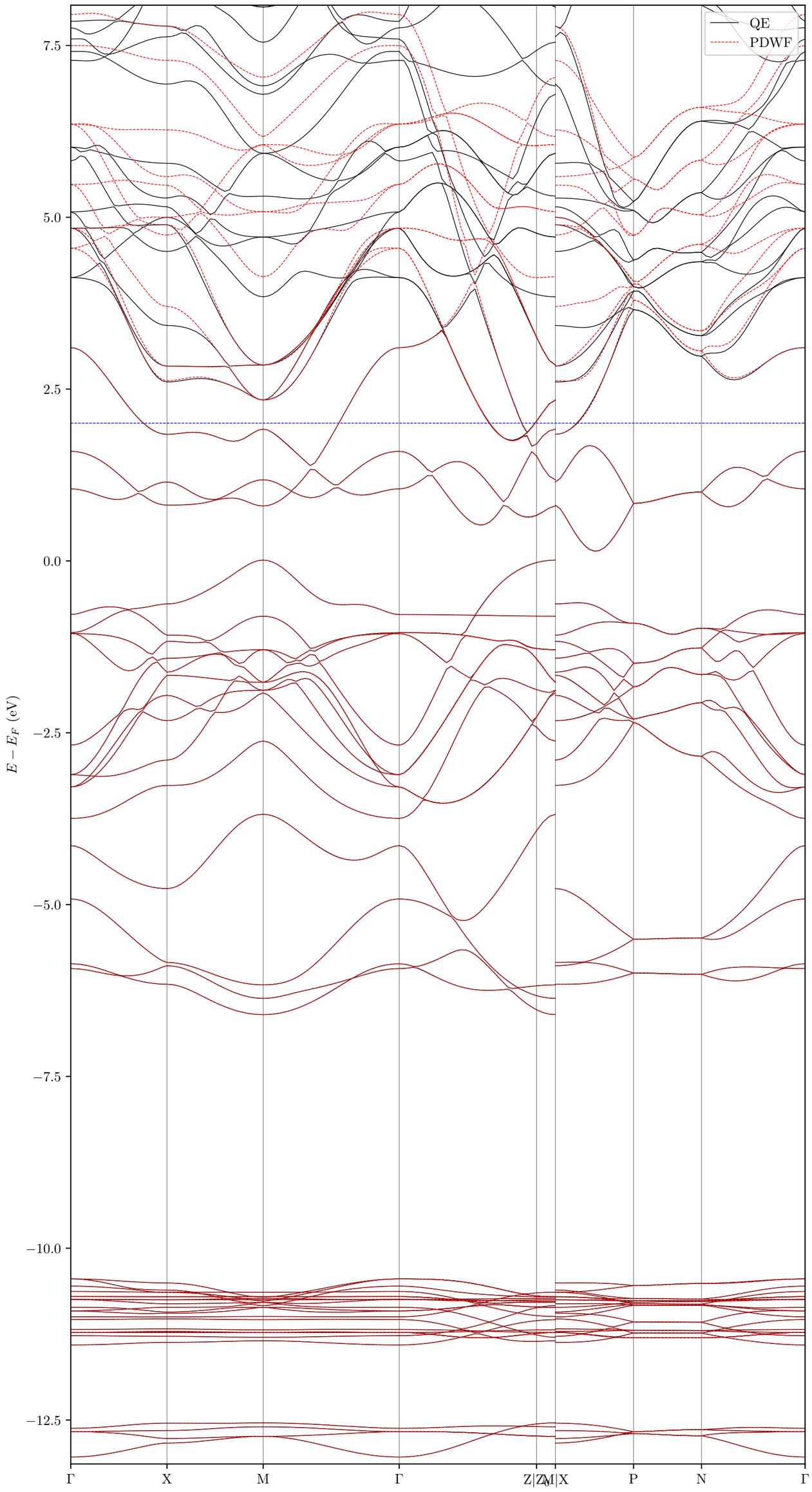



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.6 | 2.9 | 3.0 | 18.0 | 18.7 | 18.7 | 2.543 |



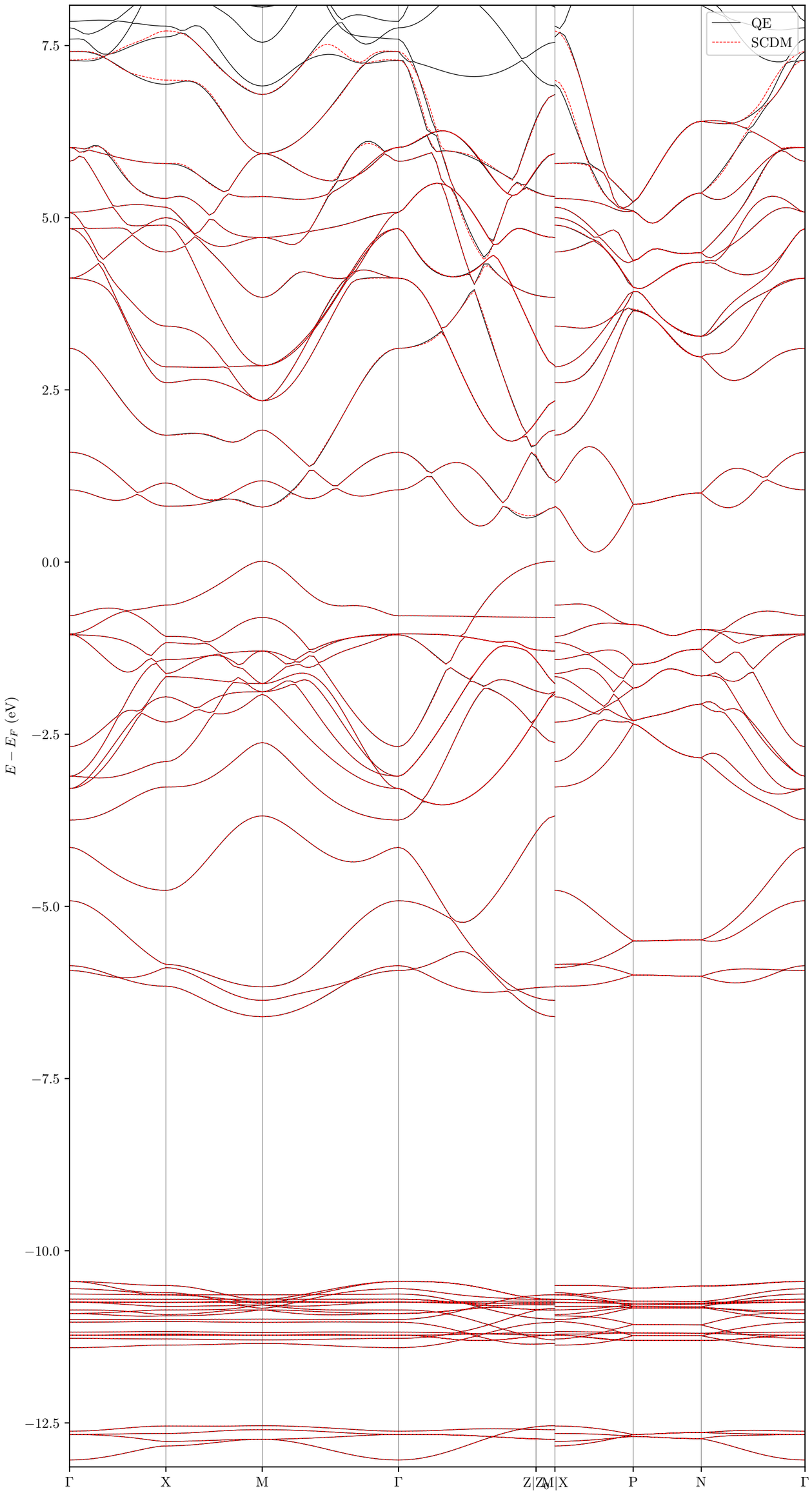
Se4Tl4 **INCLUDE** semicore
PW=d3fb7635-c456-4e15-b2c5-1a5ff999cb1d
W90=4e7a6fed-9317-4064-bed6-35724d691c2b




PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.0 | 1.2 | 27.4 | 7.2 | 9.9 | 354.8 | 2.644 |

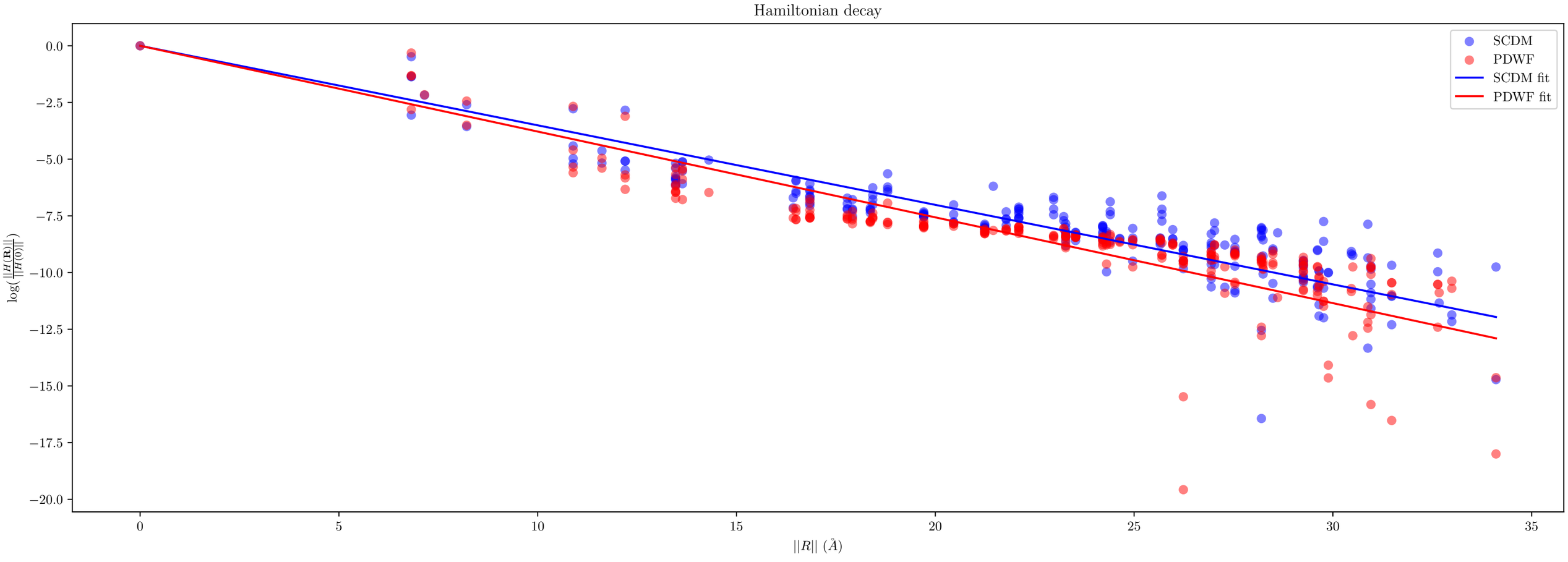
Se4Tl4 **INCLUDE** semicore
PW=d3fb7635-c456-4e15-b2c5-1a5ff999cb1d
W90=42891181-f5a5-4afd-a006-7ce76d762b9a

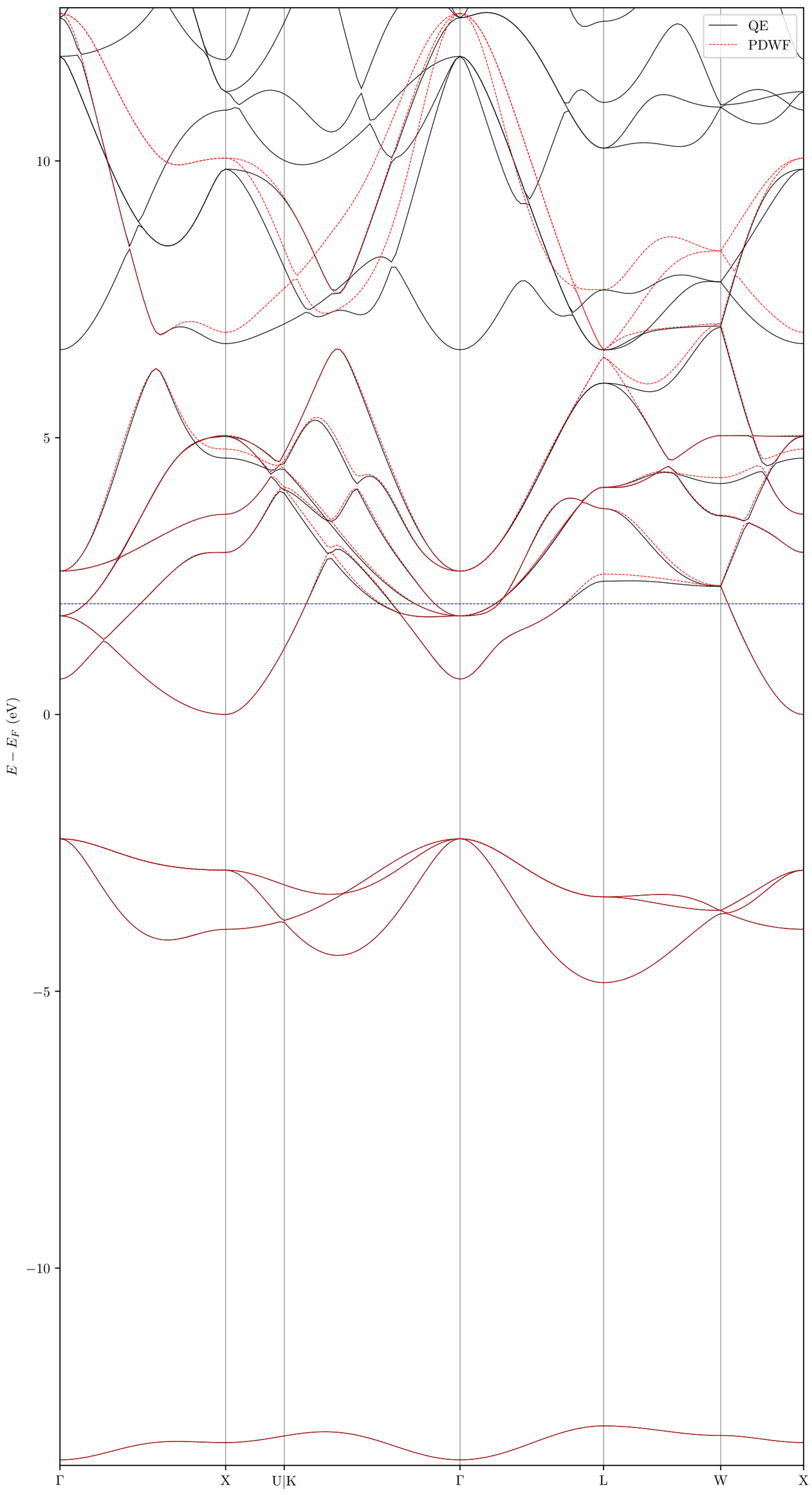



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.9 | 2.4 | 17.7 | 37.9 | 41.4 | 2.851 |

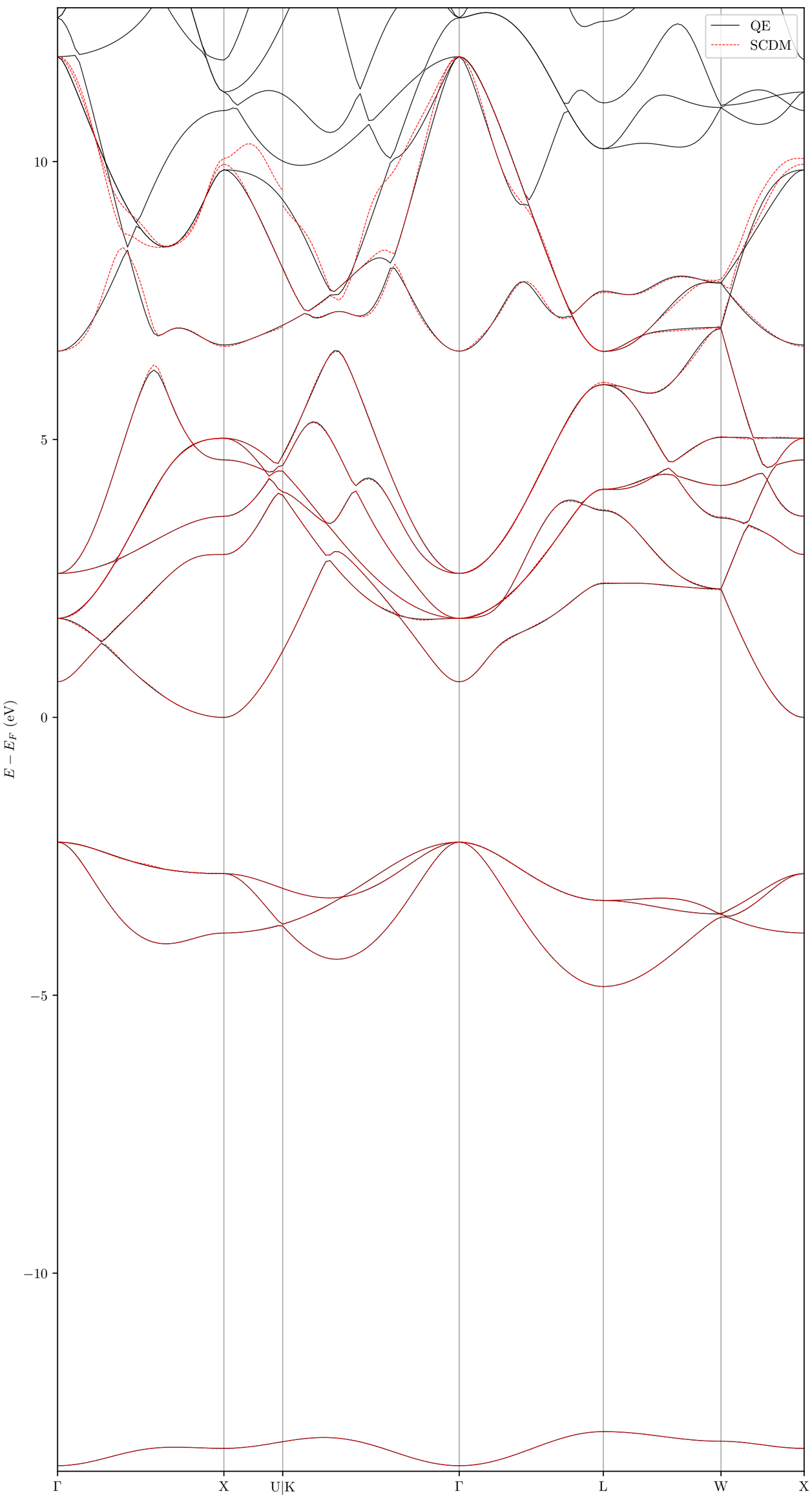
Hamiltonian decay





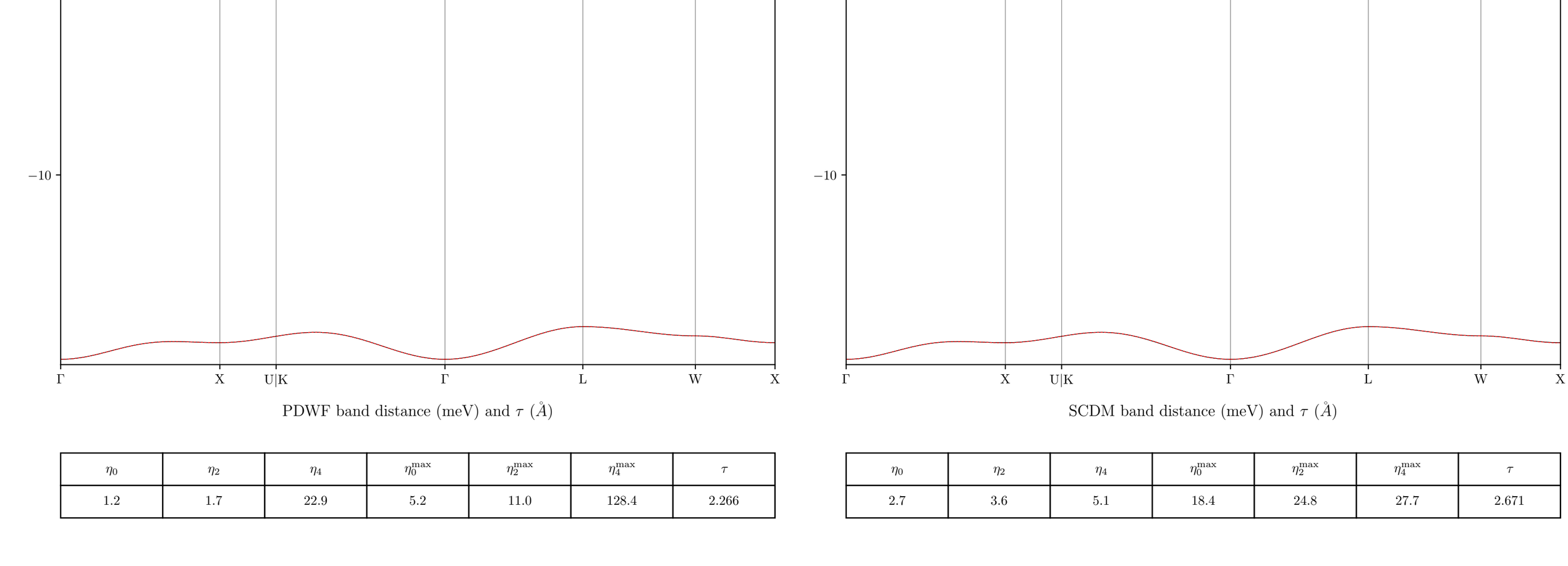

PDWF band distance (meV) and $\tau$ ($\AA$)

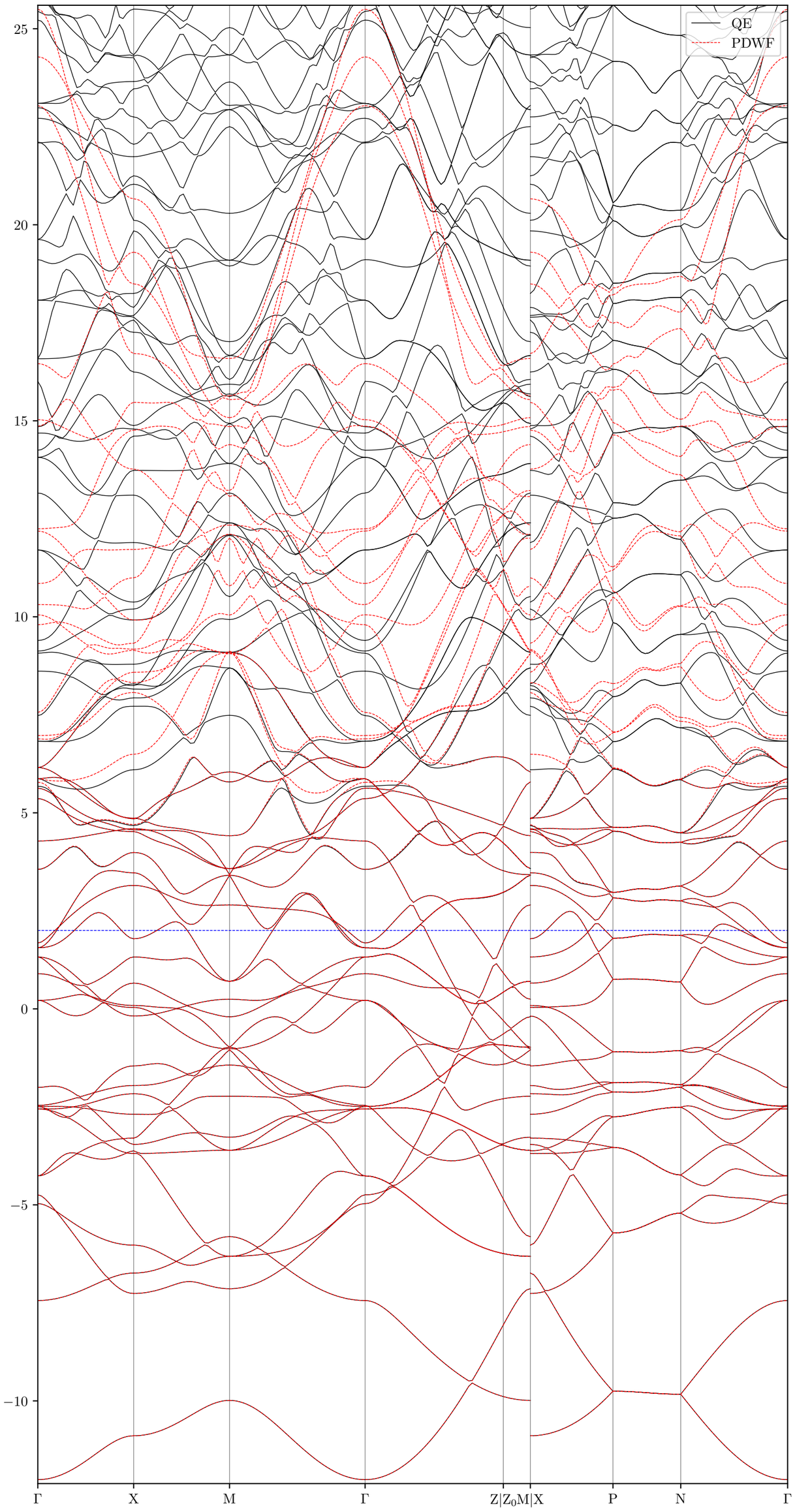
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.2 | 1.7 | 22.9 | 5.2 | 11.0 | 128.4 | 2.266 |




SCDM band distance (meV) and $\tau$ ($\AA$)

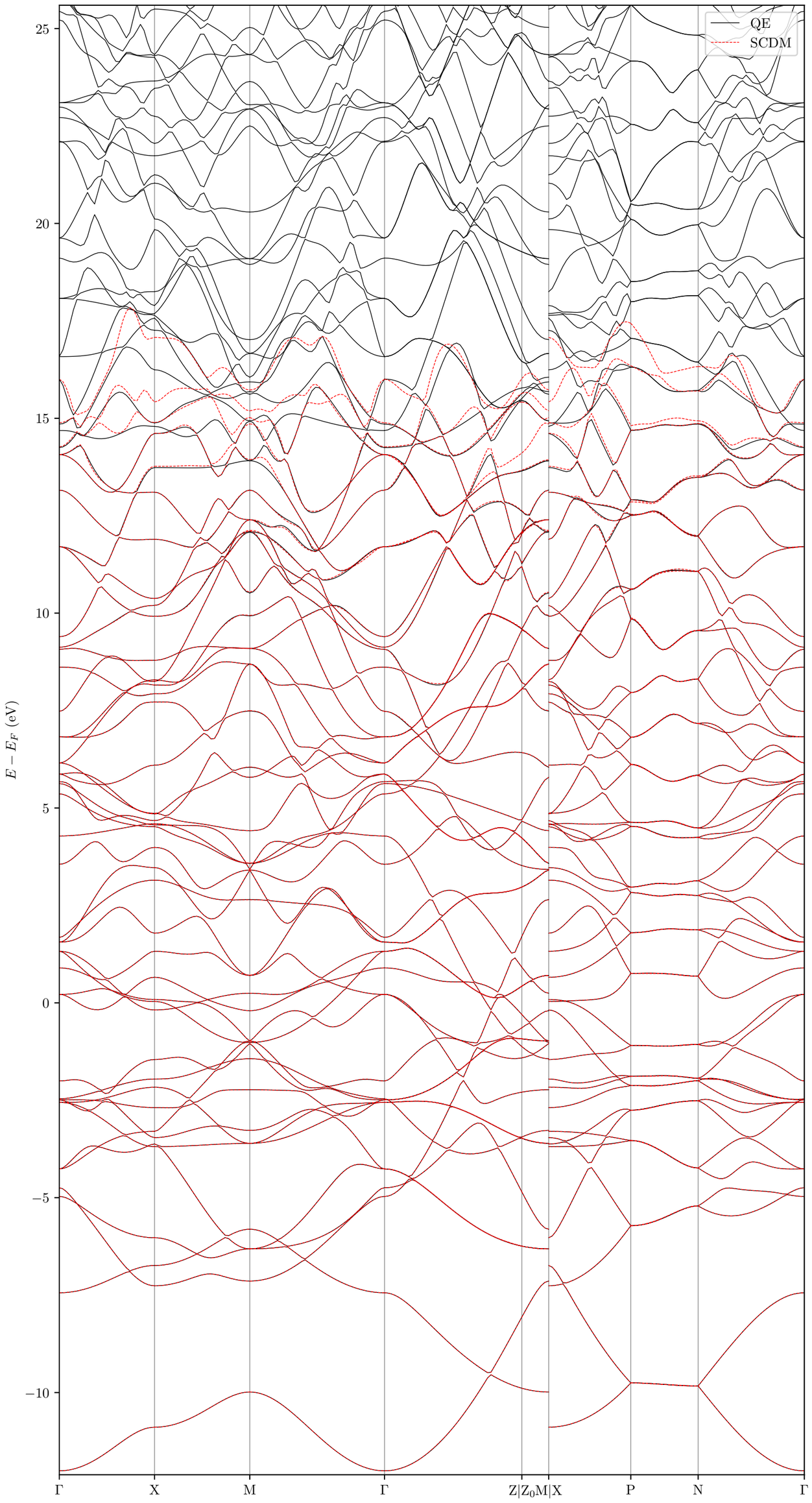
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.7 | 3.6 | 5.1 | 18.4 | 24.8 | 27.7 | 2.671 |





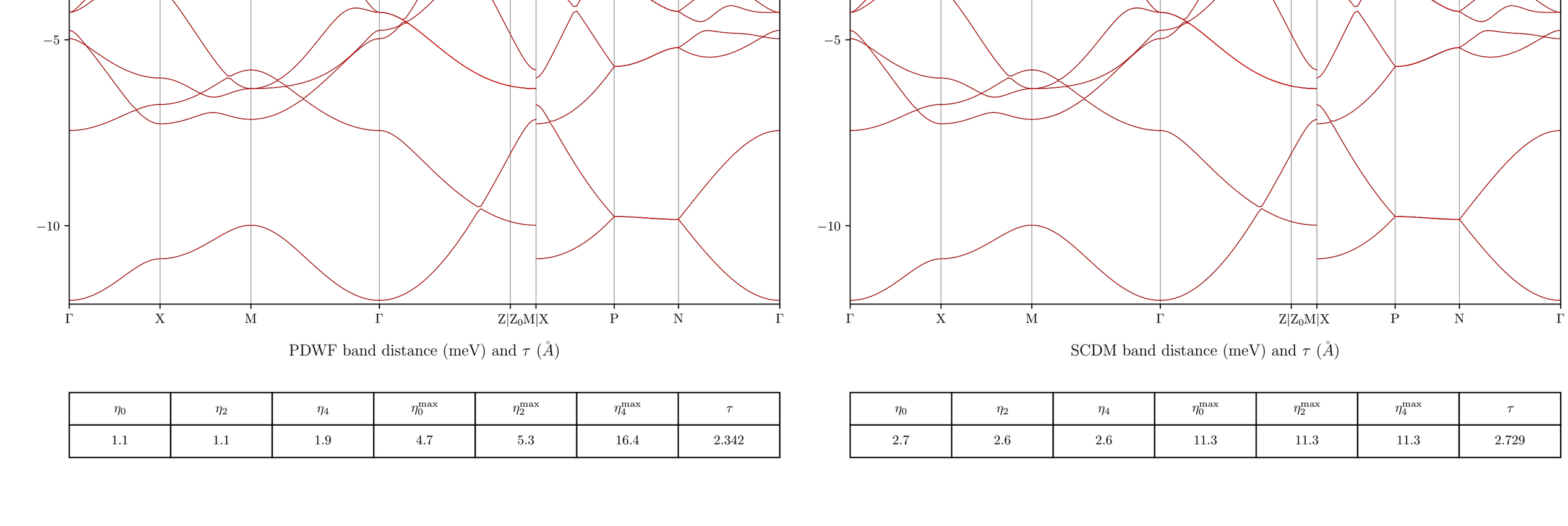

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

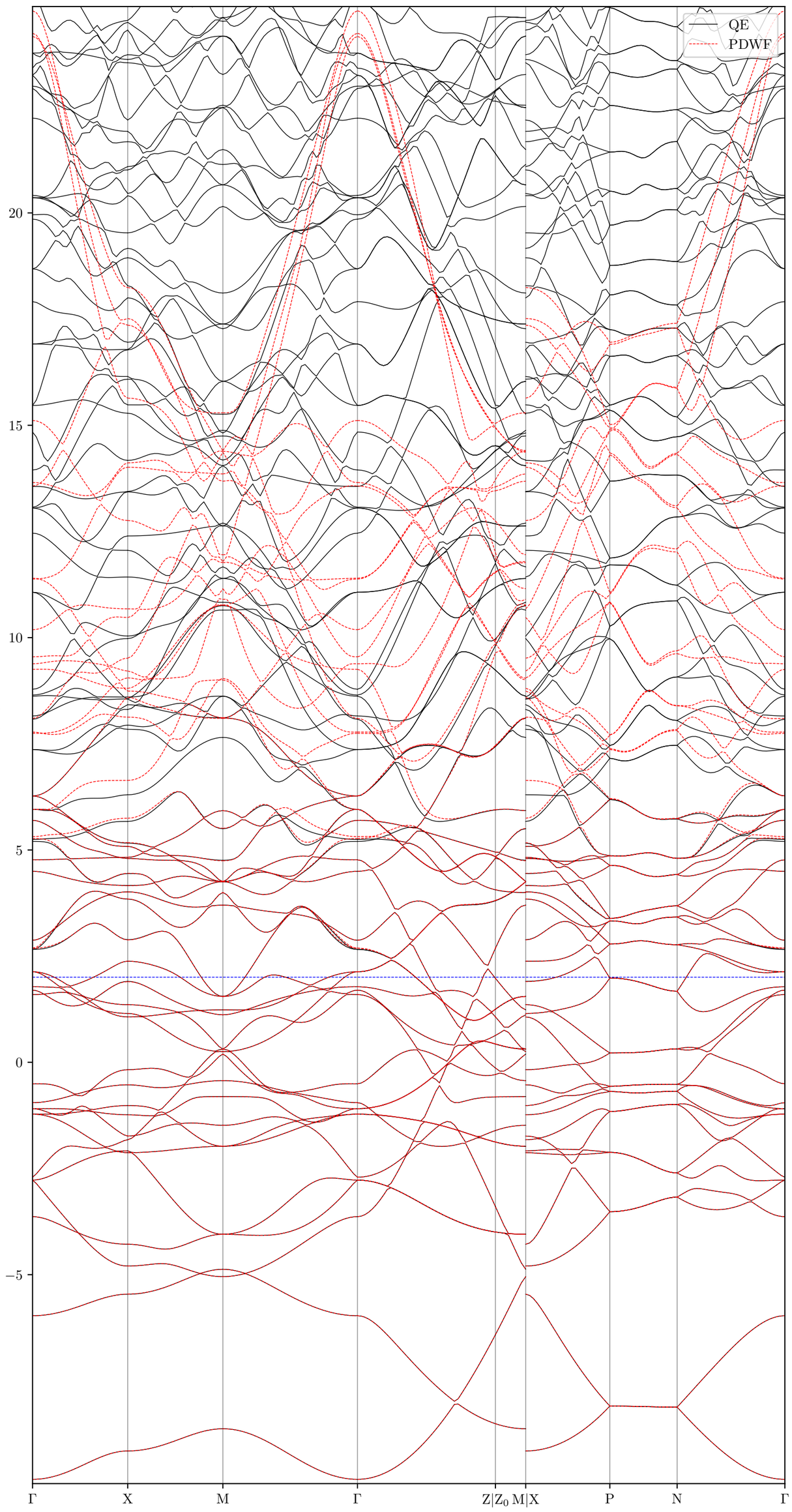
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.1 | 1.1 | 1.9 | 4.7 | 5.3 | 16.4 | 2.342 |




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

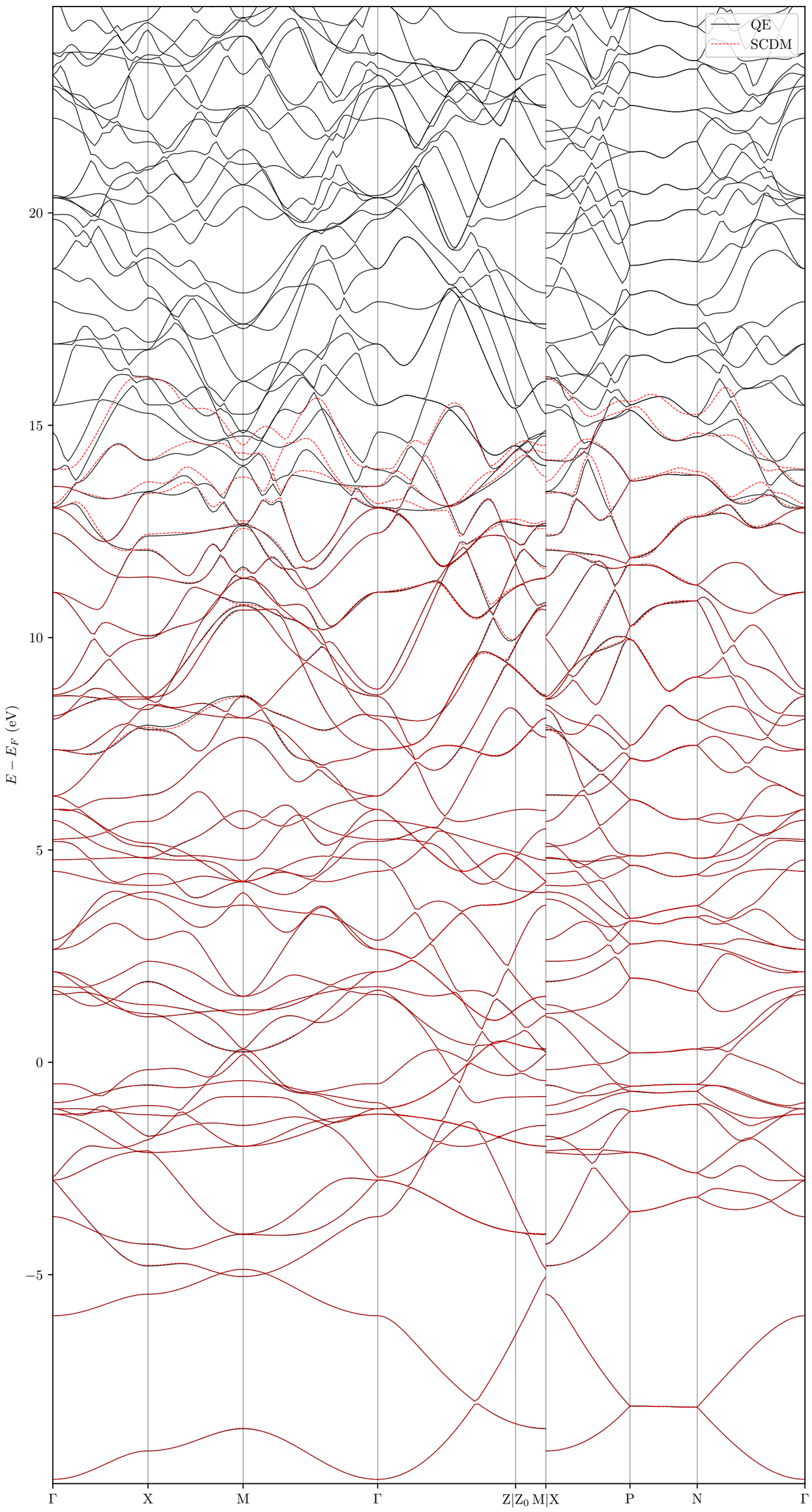
| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.7 | 2.6 | 2.6 | 11.3 | 11.3 | 11.3 | 2.729 |





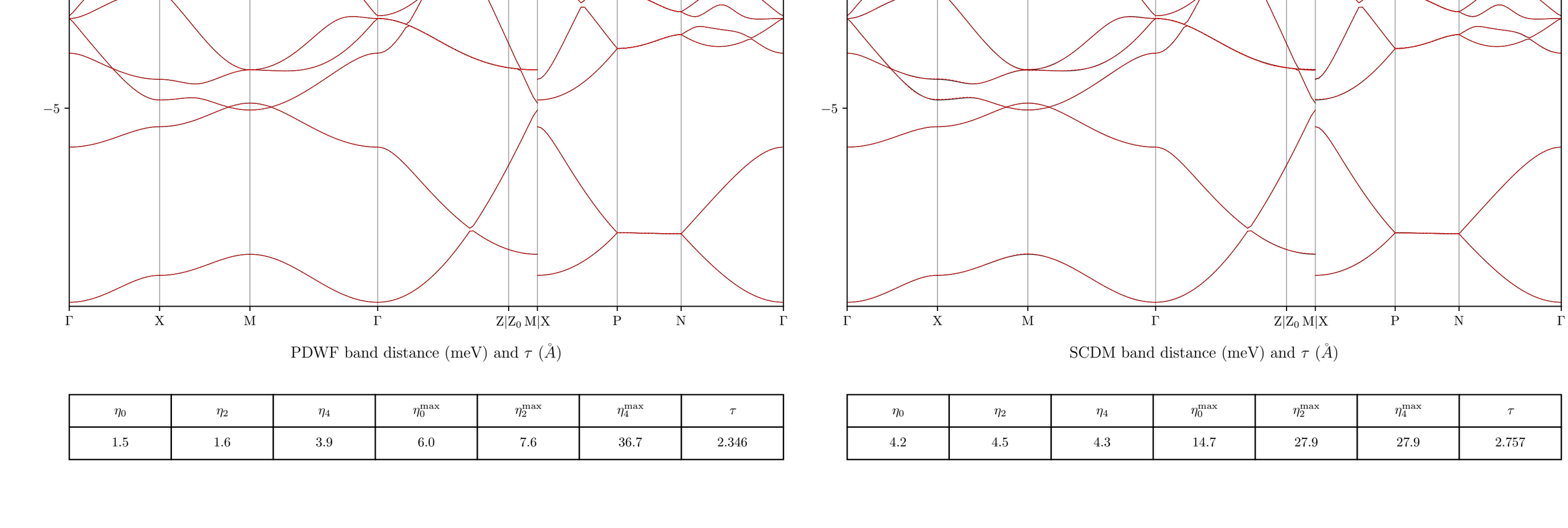

PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.5 | 1.6 | 3.9 | 6.0 | 7.6 | 36.7 | 2.346 |

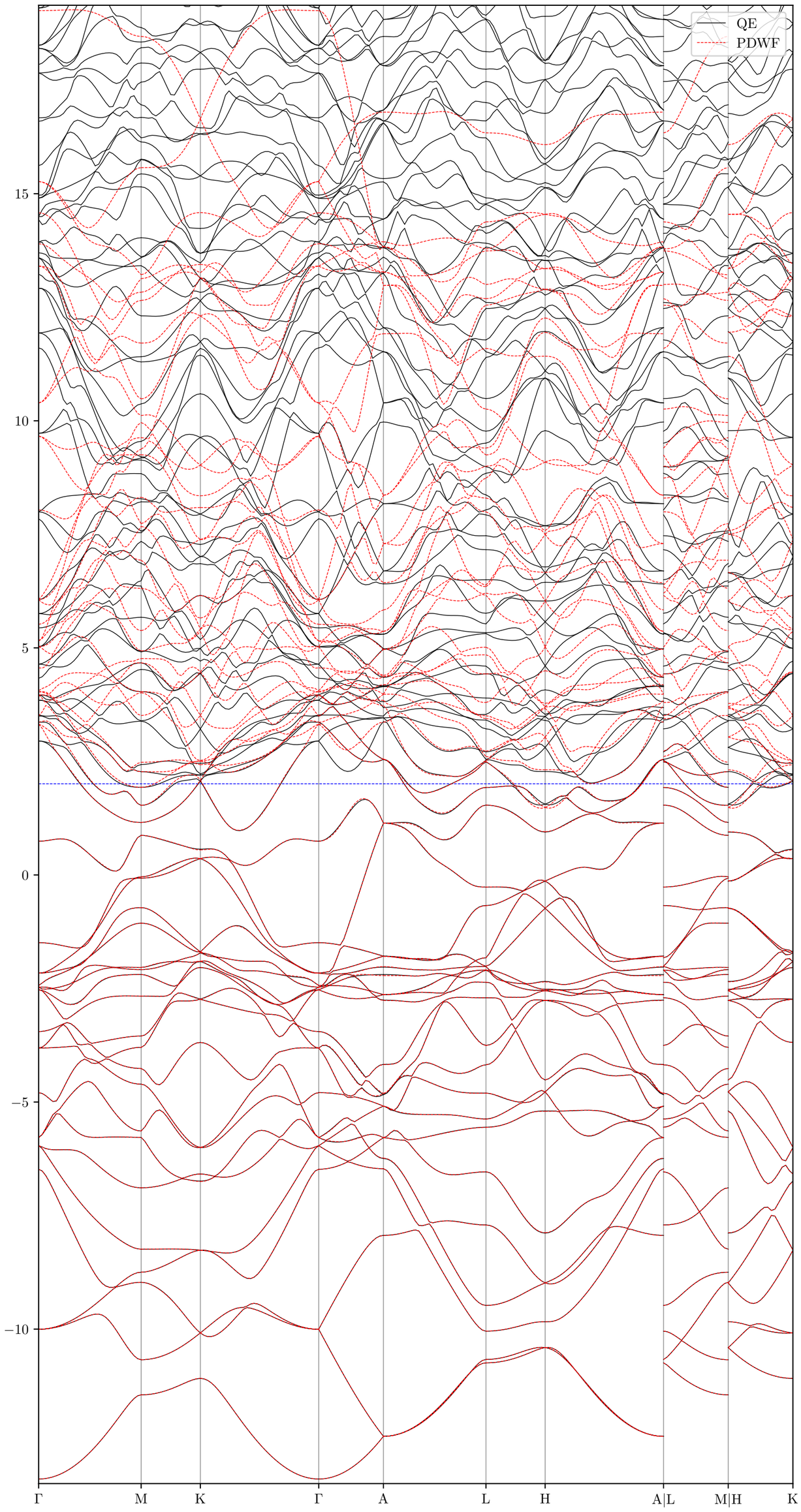



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.2 | 4.5 | 4.3 | 14.7 | 27.9 | 27.9 | 2.757 |



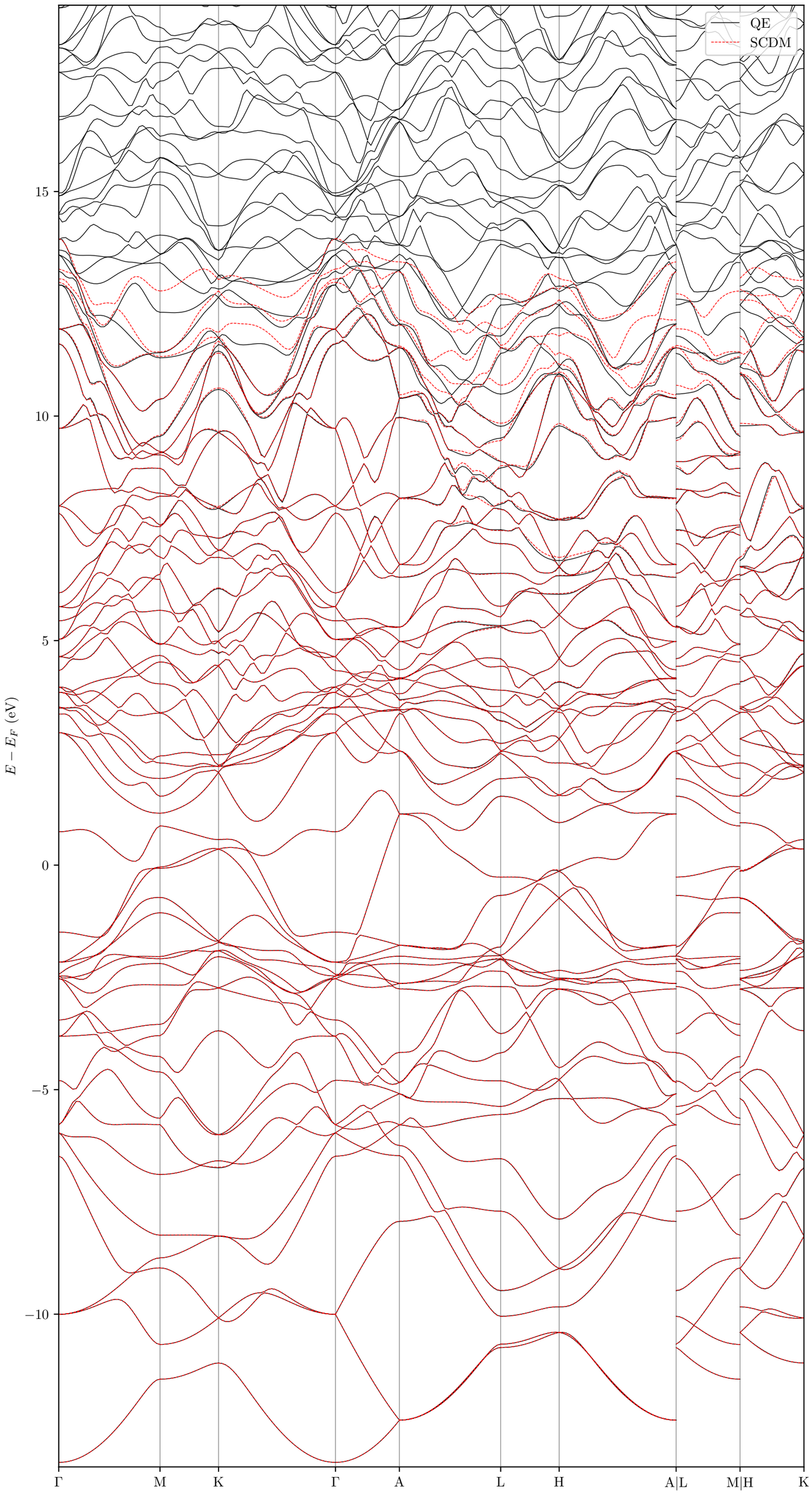
Si6Ta3 exclude semicore
PW=40c24e80-f38b-41cd-b863-2a8b86c35759
W90=d86265a2-fcbf-422b-a8b1-b258d45dd5e4




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.2 | 8.9 | 98.3 | 24.2 | 73.7 | 584.8 | 2.488 |

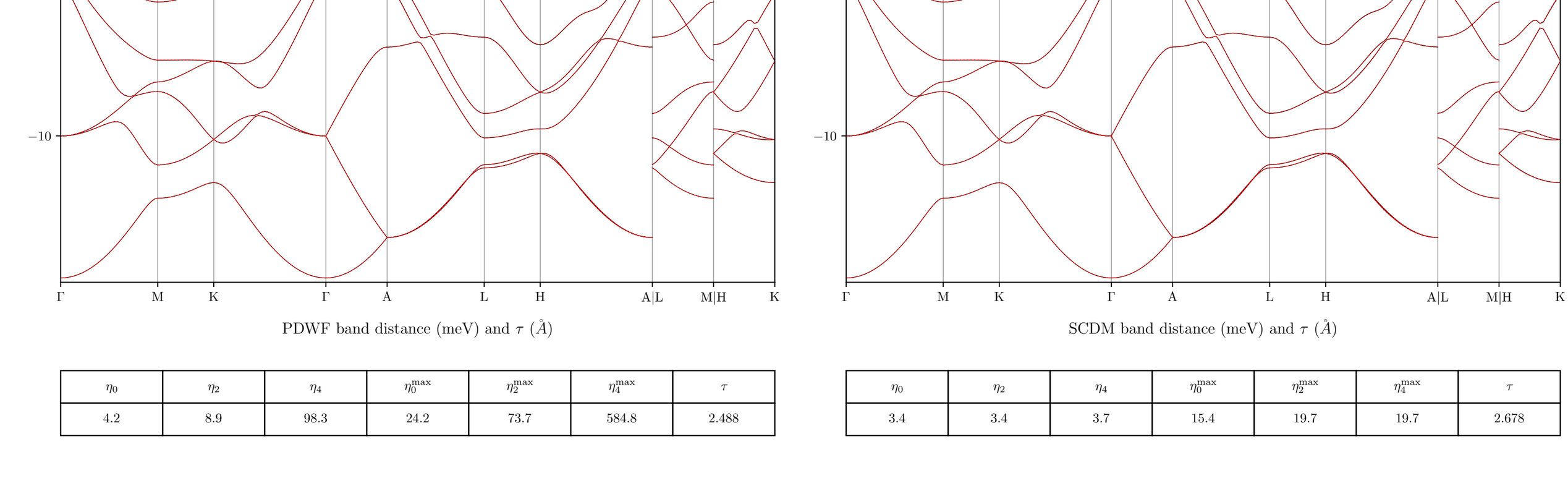
Si6Ta3 exclude semicore
PW=40c24e80-f38b-41cd-b863-2a8b86c35759
W90=ab2d061d-a71f-4035-aec6-df7d359c451f



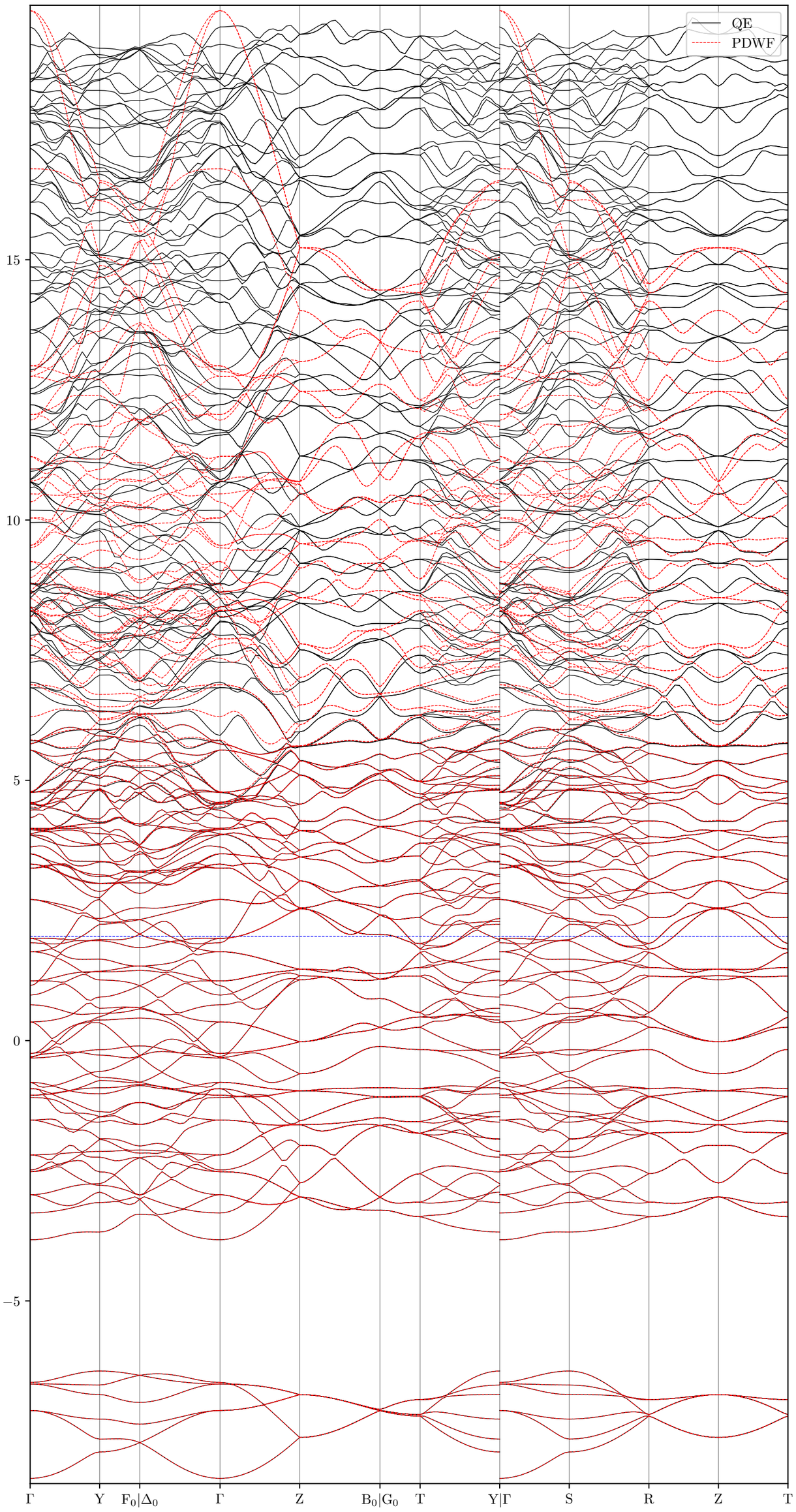

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 3.4 | 3.4 | 3.7 | 15.4 | 19.7 | 19.7 | 2.678 |

Hamiltonian decay



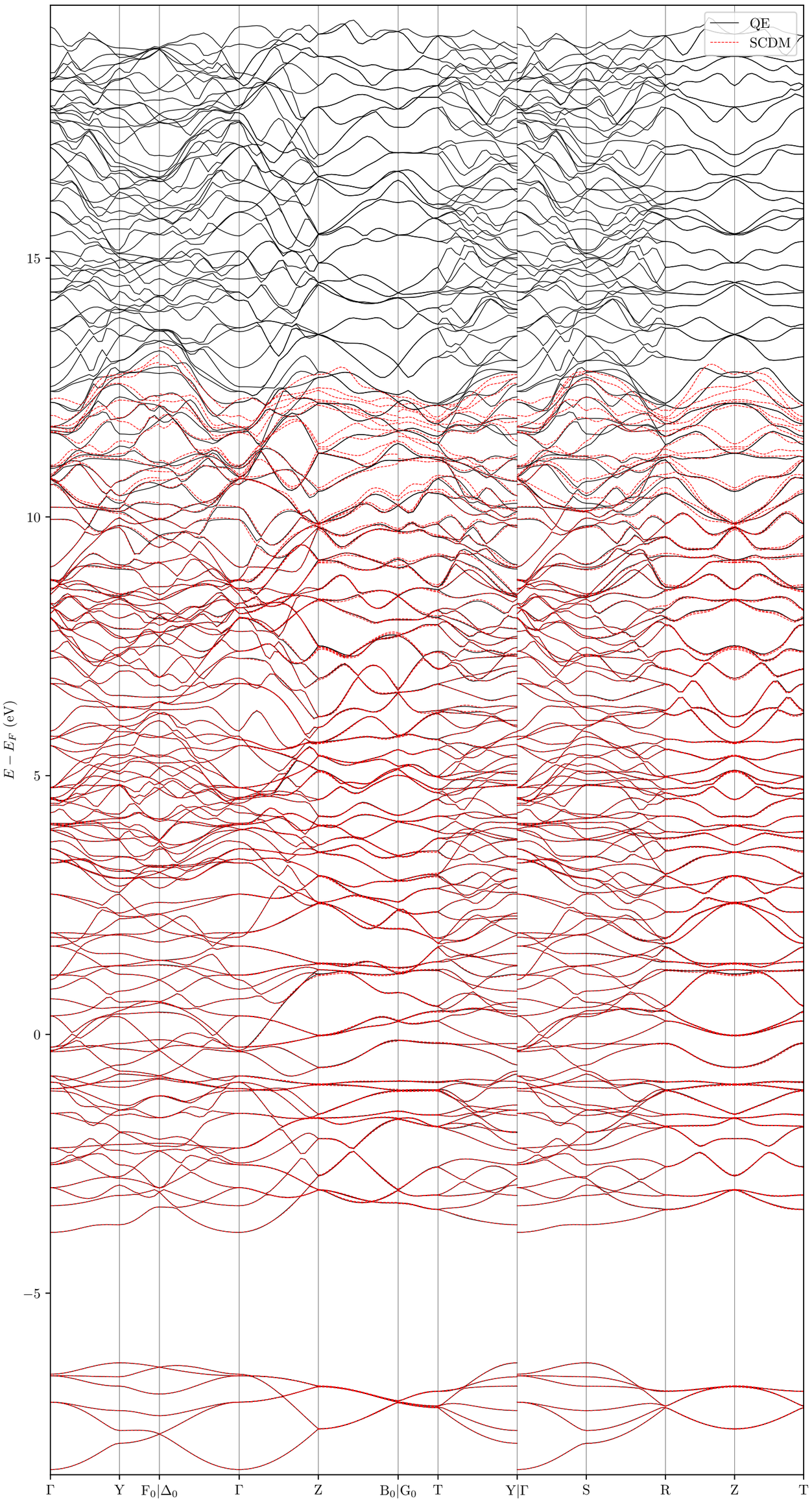
Si6Y10 exclude semicore
PW=d346891d-e361-40f7-86b8-d130f73745f7
W90=8c600b2d-a991-4df5-86a7-c1e78ace10dc




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 0.9 | 0.9 | 1.4 | 4.8 | 4.8 | 16.0 | 2.710 |

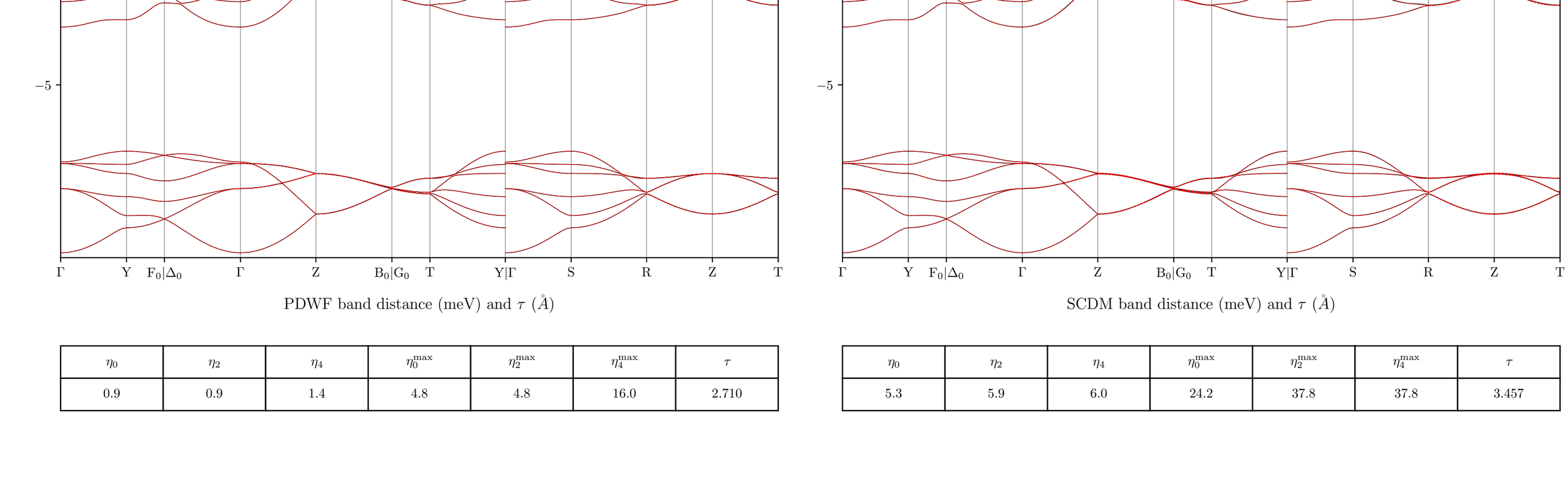
Si6Y10 exclude semicore
PW=d346891d-e361-40f7-86b8-d130f73745f7
W90=b3363142-418d-4088-9900-a94029c9d259



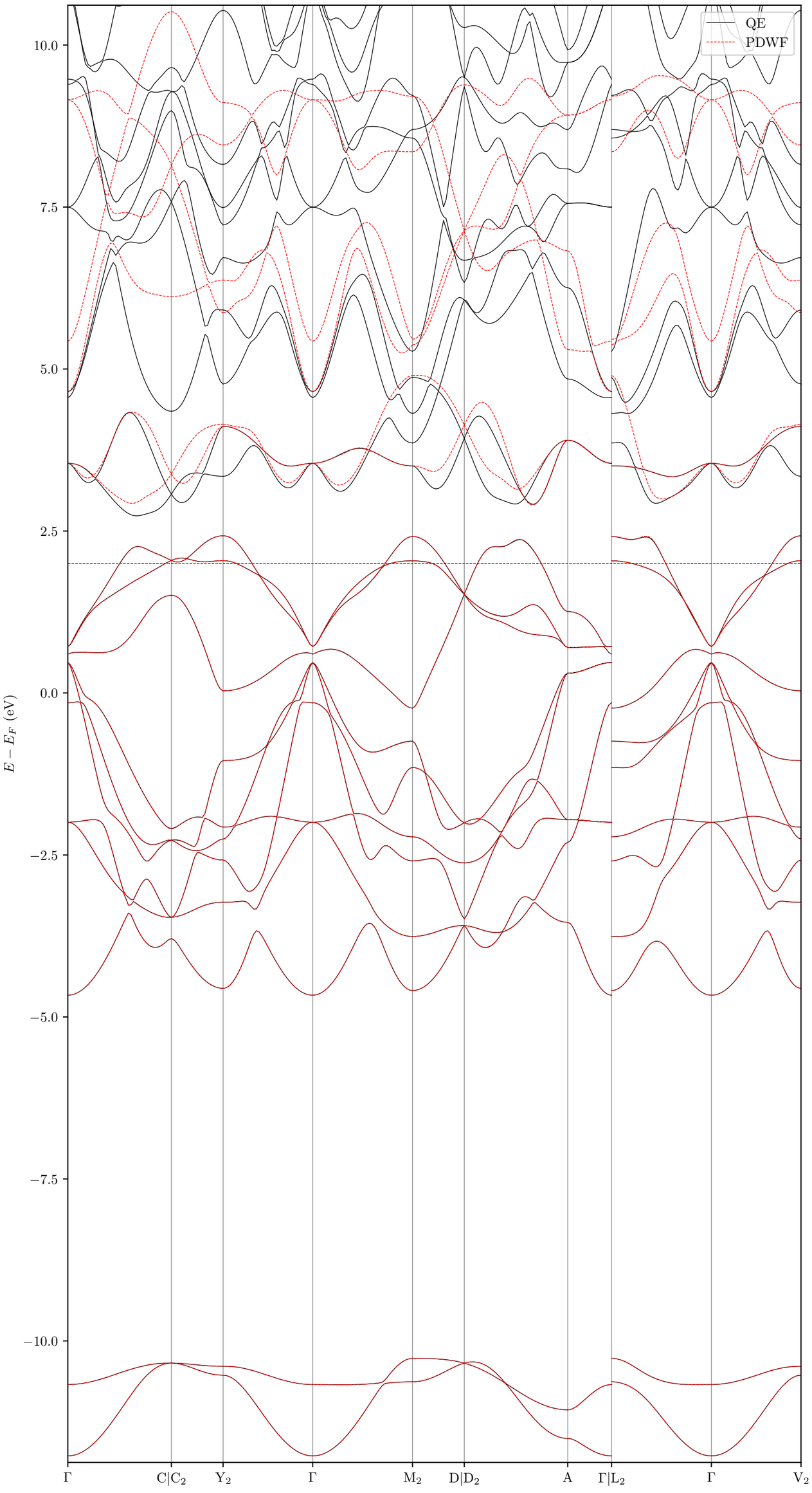

SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.3 | 5.9 | 6.0 | 24.2 | 37.8 | 37.8 | 3.457 |

Hamiltonian decay



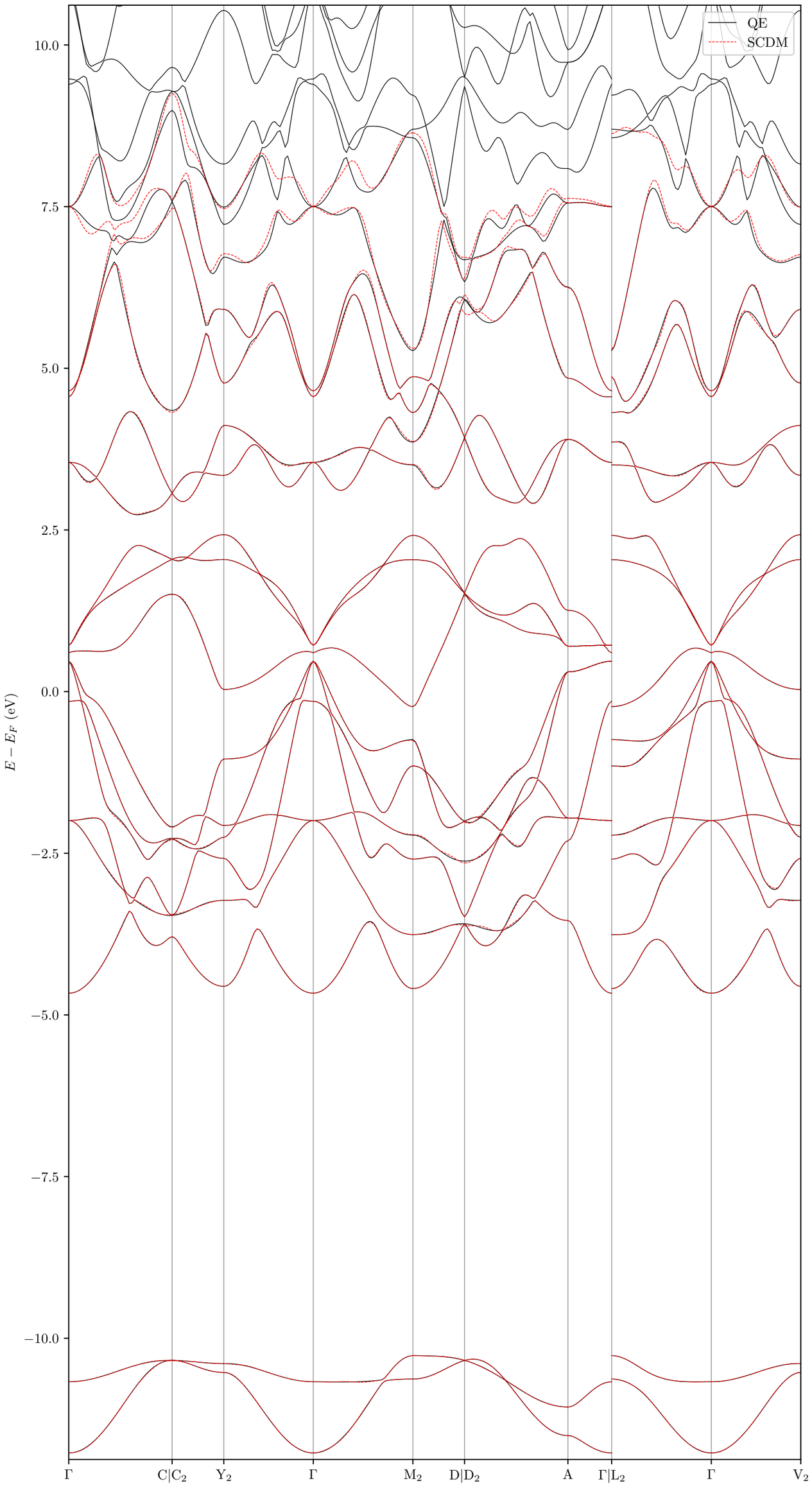
Te2Zr exclude semicore
PW=9f8f9cad-aa10-4a1d-a71c-10ea93a53c9c
W90=7c515442-babe-4476-b843-15d88731a1b0




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 1.5 | 1.6 | 66.9 | 8.7 | 8.7 | 450.3 | 2.541 |

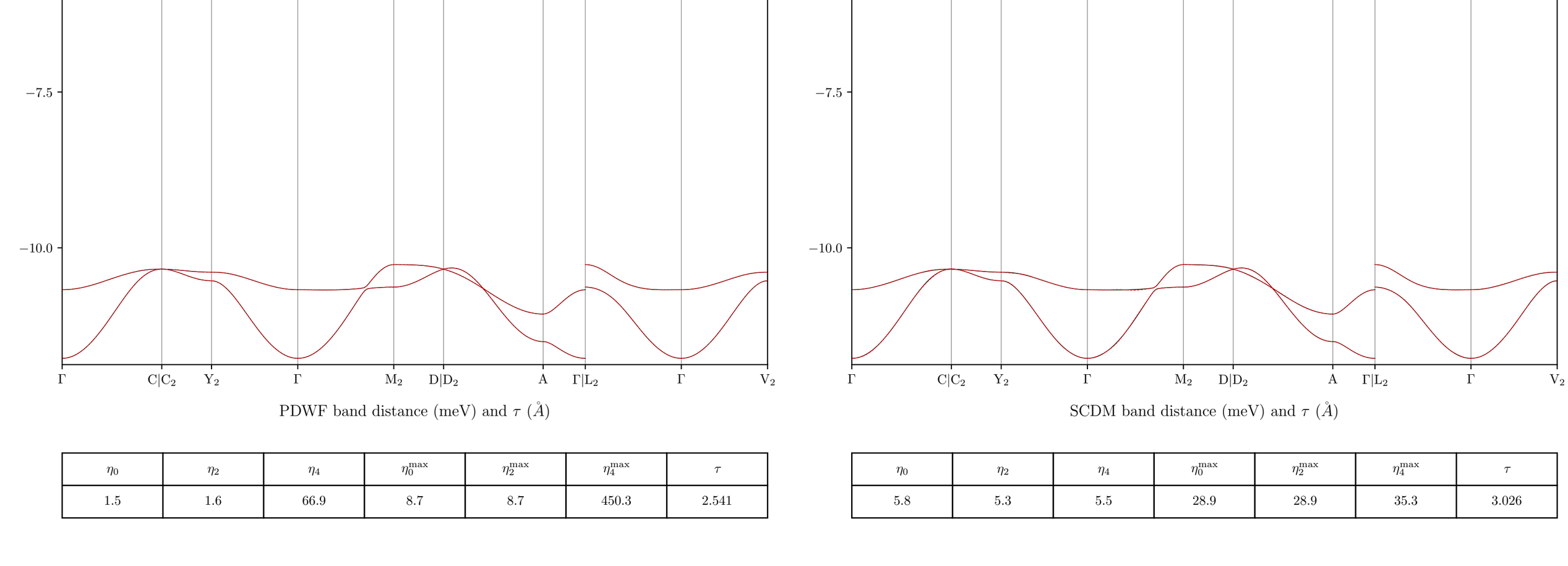
Te2Zr exclude semicore
PW=9f8f9cad-aa10-4a1d-a71c-10ea93a53c9c
W90=c1ebb384-78e5-4fbd-bda2-0cf089cf65d5

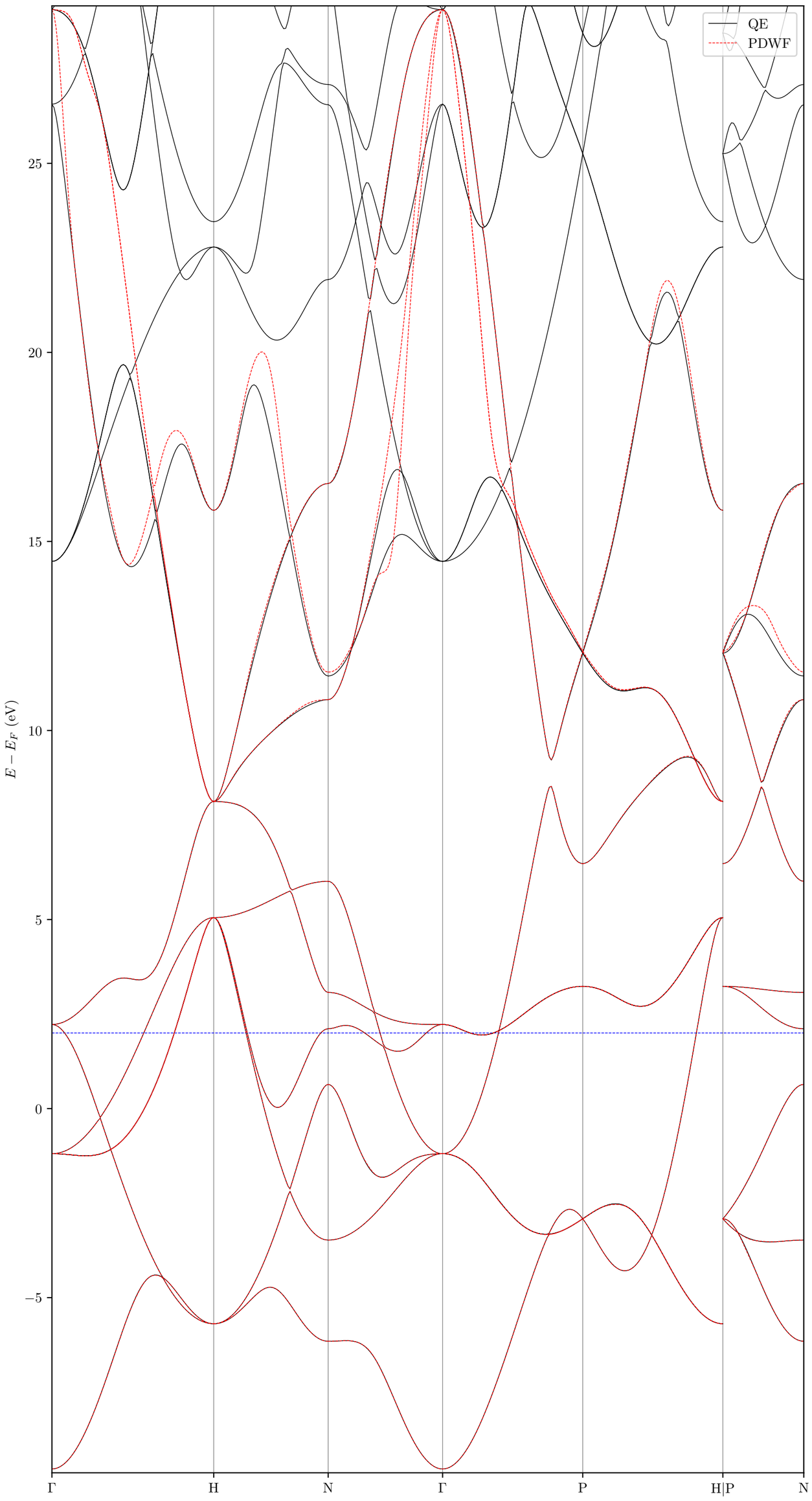



SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 5.8 | 5.3 | 5.5 | 28.9 | 28.9 | 35.3 | 3.026 |

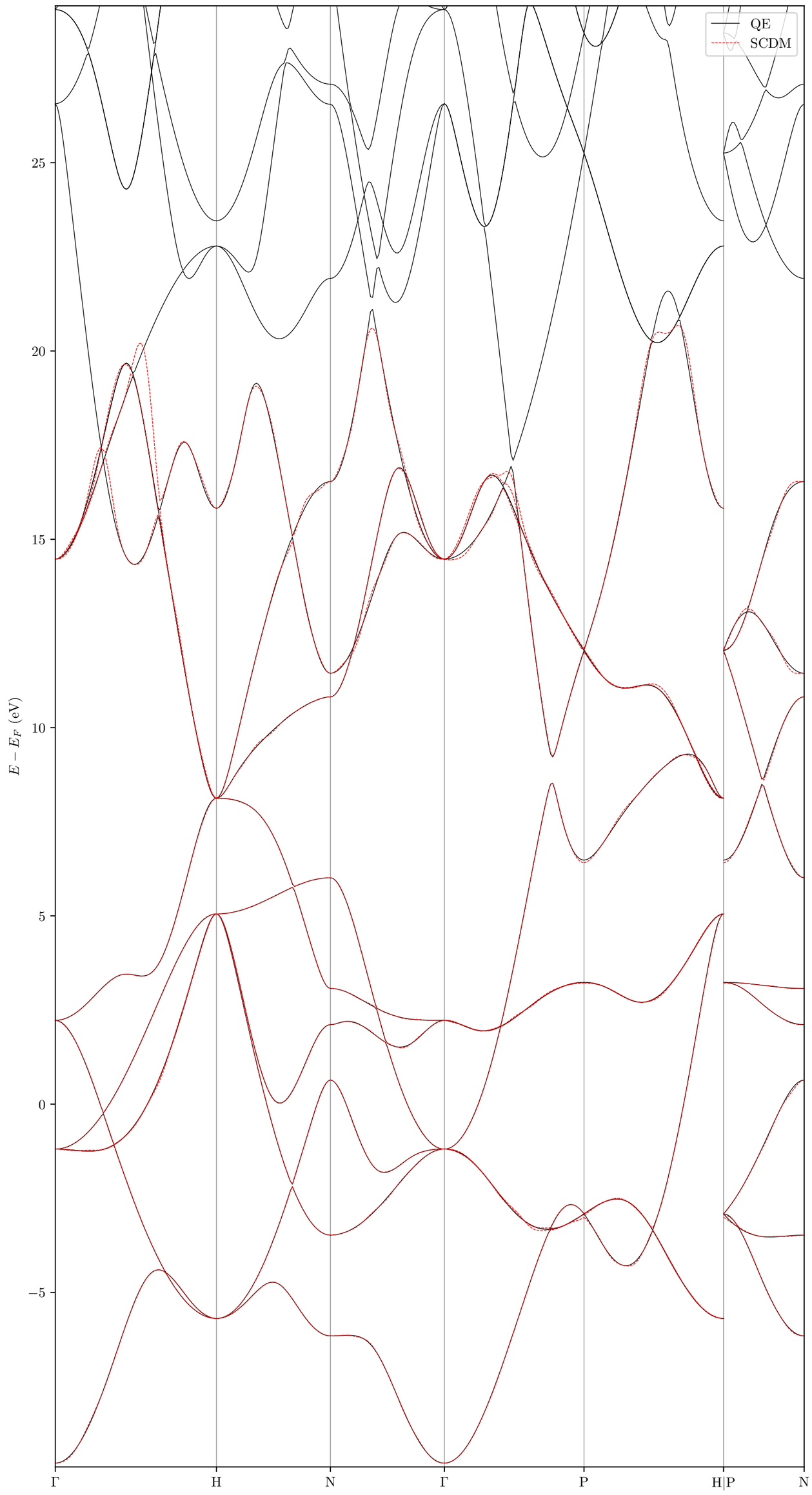
Hamiltonian decay





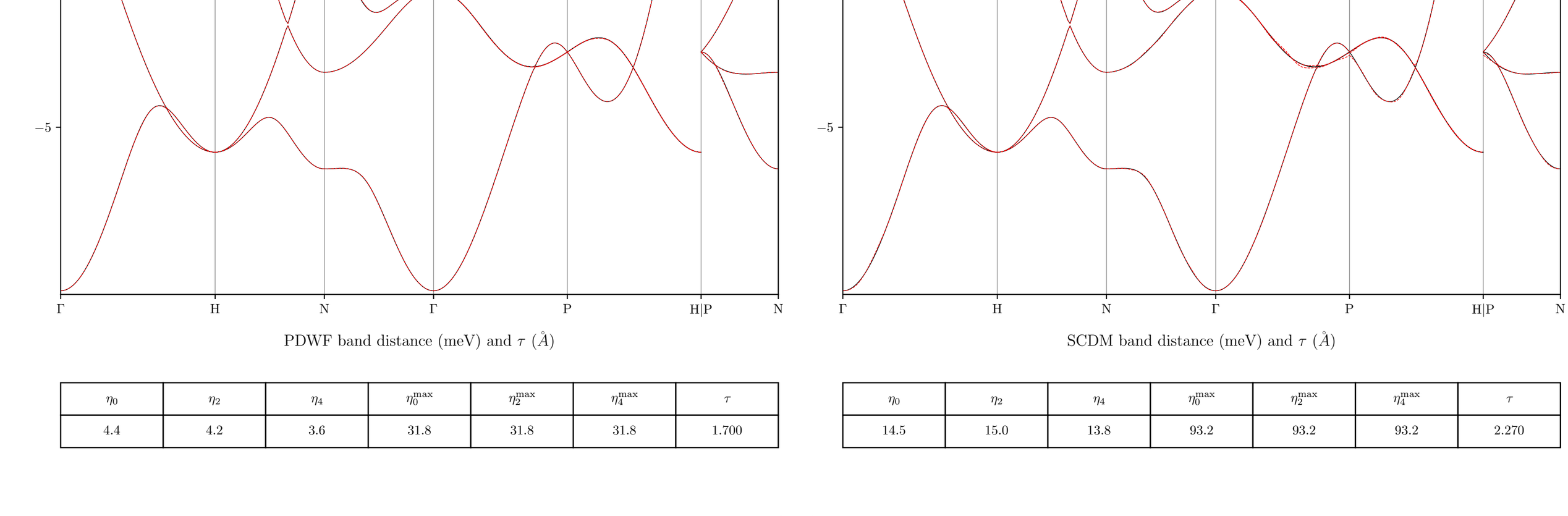

PDWF band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.4 | 4.2 | 3.6 | 31.8 | 31.8 | 31.8 | 1.700 |

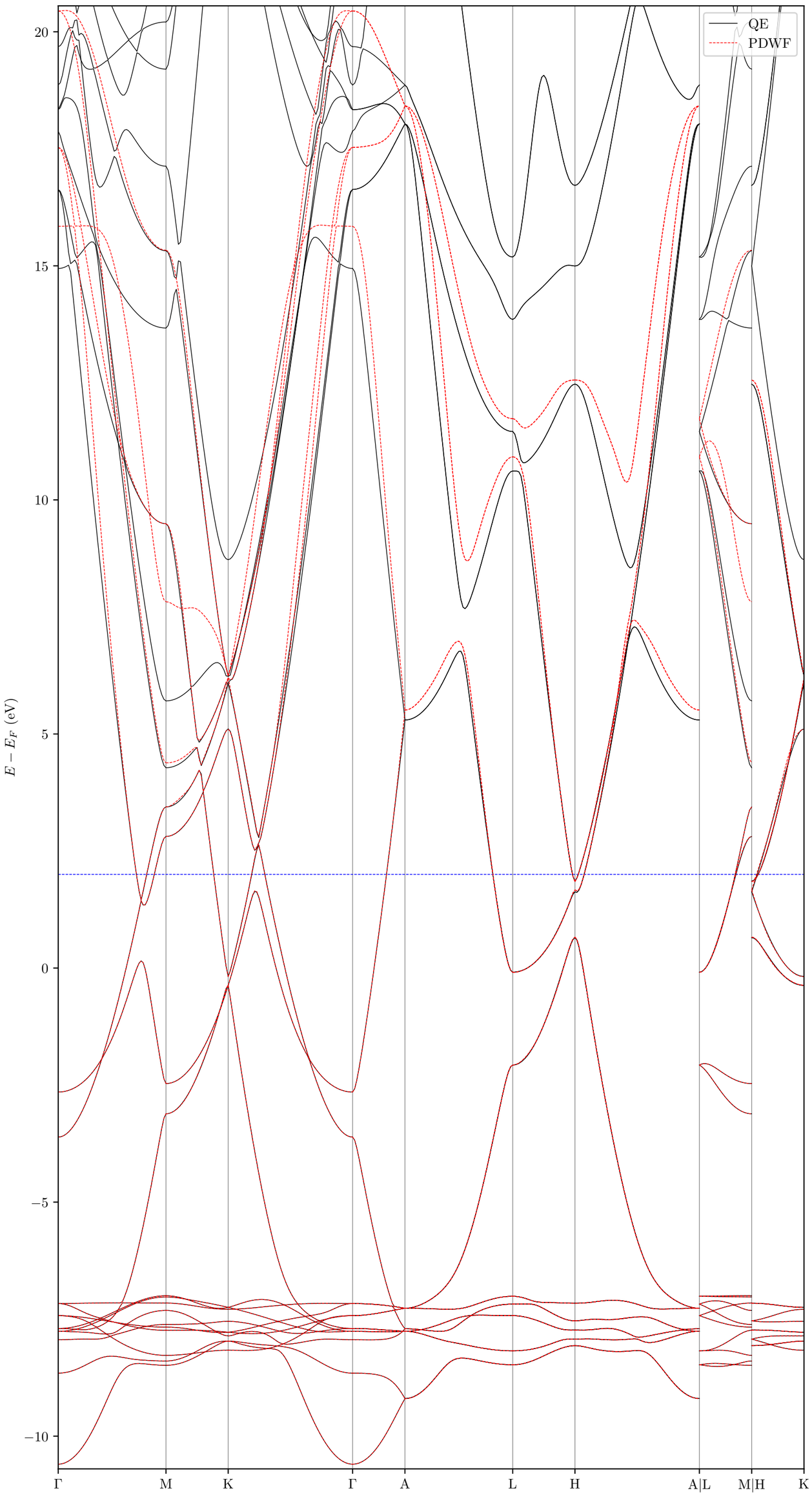



SCDM band distance (meV) and $\tau$ ($\AA$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 14.5 | 15.0 | 13.8 | 93.2 | 93.2 | 93.2 | 2.270 |



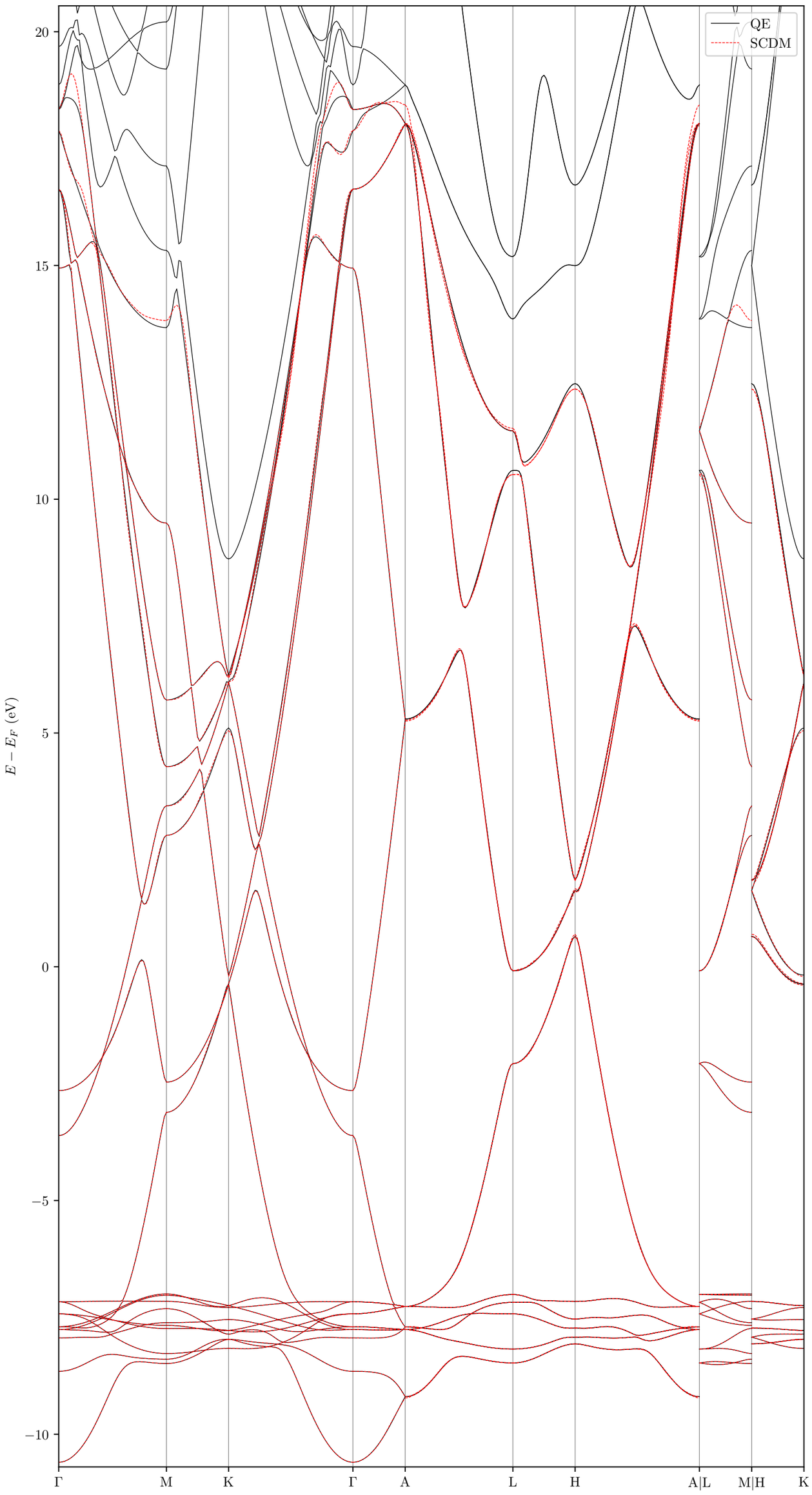
Zn2 exclude semicore
PW=d1e2b170-4edb-45e5-b6f1-e40f9229162f
W90=40173783-70c7-43d2-8336-a80575ff94e6




PDWF band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 2.2 | 3.5 | 7.5 | 18.2 | 43.5 | 125.6 | 2.075 |

Zn2 exclude semicore
PW=d1e2b170-4edb-45e5-b6f1-e40f9229162f
W90=72eb6f4a-cf8a-420b-aeb1-0497a0261d46




SCDM band distance (meV) and $\tau$ ($\mathring{A}$)

| $\eta_0$ | $\eta_2$ | $\eta_4$ | $\eta_0^{\max}$ | $\eta_2^{\max}$ | $\eta_4^{\max}$ | $\tau$ |
|---|---|---|---|---|---|---|
| 4.9 | 6.8 | 8.9 | 48.5 | 52.8 | 75.2 | 2.330 |

Hamiltonian decay