

Supplementary Information:

Automated mixing of maximally localized Wannier functions into target manifolds

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S1 Gradient of single rotation

Different from Appendix A in Ref. [1], we use another definition of the gradient g for a complex function $F(z)$, by

$$F(z+h) = F(z) + 2\operatorname{Re}\langle g, h \rangle + O(h^2), \quad (1)$$

which allows a slightly more intuitive derivation of derivatives by reusing the existing rules for formal derivatives of real functions [2].

The spread functional can be written as

$$\Omega = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} f(M_{\mathbf{k}\mathbf{b}nn}^W) - \left[\frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} g(M_{\mathbf{k}\mathbf{b}nn}^W) \mathbf{b} \right]^2, \quad (2)$$

where

$$\begin{aligned} f(z) &= 1 - |z|^2 + (\operatorname{Im} \ln z)^2, \\ g(z) &= -\operatorname{Im} \ln z, \\ M_{\mathbf{k}\mathbf{b}}^W &= W^* M_{\mathbf{k}\mathbf{b}} W, \\ M_{\mathbf{k}\mathbf{b}} &= \langle u_{m,\mathbf{k}} | u_{n,\mathbf{k}+\mathbf{b}} \rangle, \end{aligned} \quad (3)$$

and $\mathbf{b}$'s are the the vectors connecting neighboring k -points, satisfying the completeness condition

$$\sum_{\mathbf{b}} w_{\mathbf{b}} \mathbf{b} \mathbf{b}^T = I_3, \quad (4)$$

where I_3 is the 3×3 identity matrix; $w_{\mathbf{b}}$ are the weights. The derivatives of $f(z)$ and $g(z)$ are

$$\begin{aligned} f'(z) &= \frac{\partial f}{\partial z^*} = -z + \frac{i \operatorname{Im} \ln z}{z^*}, \\ g'(z) &= \frac{\partial g}{\partial z^*} = -\frac{i}{2z^*}. \end{aligned} \quad (5)$$

Suppose a function F has a form of $F = \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} f(M_{\mathbf{k}\mathbf{b}nn}^W)$, then the change of F w.r.t. W is given by

$$\begin{aligned} \Delta F &= 2\operatorname{Re} \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} f'(M_{\mathbf{k}\mathbf{b}nn}^W)^* \Delta M_{\mathbf{k}\mathbf{b}nn}^W \\ &= 2\operatorname{Re} \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} f'(M_{\mathbf{k}\mathbf{b}nn}^W)^* (\Delta W^* M_{\mathbf{k}\mathbf{b}} W)_{nn} + f'(M_{\mathbf{k}\mathbf{b}nn}^W)^* (W^* M_{\mathbf{k}\mathbf{b}} \Delta W)_{nn} \\ &= 2\operatorname{Re} \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} f'(M_{\mathbf{k}\mathbf{b}nn}^W)^* (\Delta W^* M_{\mathbf{k}\mathbf{b}} W)_{nn} + f'(M_{\mathbf{k}\mathbf{b}nn}^W) (\Delta W^* M_{\mathbf{k}\mathbf{b}}^* W)_{nn} \\ &= 2\operatorname{Re} \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} f'(M_{\mathbf{k}\mathbf{b}nn}^W)^* (\Delta W^* M_{\mathbf{k}\mathbf{b}} W)_{nn} + f'(M_{\mathbf{k}-\mathbf{b}, \mathbf{b}, nn}^W) (\Delta W^* M_{\mathbf{k}-\mathbf{b}, \mathbf{b}}^* W)_{nn} \\ &= 2\operatorname{Re} \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} f'(M_{\mathbf{k}\mathbf{b}nn}^W)^* (\Delta W^* M_{\mathbf{k}\mathbf{b}} W)_{nn} + f'(M_{\mathbf{k}, -\mathbf{b}, nn}^{W*}) (\Delta W^* M_{\mathbf{k}, -\mathbf{b}} W)_{nn} \\ &= 2\operatorname{Re} \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} \left[f'(M_{\mathbf{k}\mathbf{b}nn}^W)^* + f'(M_{\mathbf{k}\mathbf{b}nn}^{W*}) \right] (\Delta W^* M_{\mathbf{k}\mathbf{b}} W)_{nn}, \end{aligned} \quad (6)$$

where the symmetry of $\mathbf{b}$ vectors are used. Therefore, the gradient is

$$(\nabla F)_{mn} = \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} \left[f'(M_{\mathbf{k}\mathbf{b}nn}^W)^* + f'(M_{\mathbf{k}\mathbf{b}nn}^{W*}) \right] (M_{\mathbf{k}\mathbf{b}} W)_{mn}. \quad (7)$$

For the second term of the spread functional, suppose $F = \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} \mathbf{b} g(M_{\mathbf{k}\mathbf{b}nn}^W)$, we then obtain

$$(\nabla F)_{mn} = \sum_{\mathbf{k}, \mathbf{b}} w_{\mathbf{b}} \left[g'(M_{\mathbf{k}\mathbf{b}nn}^W)^* - g'(M_{\mathbf{k}\mathbf{b}nn}^{W*}) \right] (M_{\mathbf{k}\mathbf{b}} W)_{mn}. \quad (8)$$

However, since the `Optim.jl` package [3] uses the convention $F(z+h) = F(z) + \text{Re} \langle g, h \rangle + O(h^2)$, the final gradient we pass to the optimizer is

$$\begin{aligned} 2(\nabla\Omega)_{mn} &= 2 \sum_{\mathbf{kb}} w_{\mathbf{b}} \left\{ f' (M_{\mathbf{kbnn}}^W)^* + f' (M_{\mathbf{kbnn}}^{W*}) - 2 \langle \mathbf{r} \rangle \cdot \mathbf{b} \left[g' (M_{\mathbf{kbnn}}^W)^* - g' (M_{\mathbf{kbnn}}^{W*}) \right] \right\} (M_{\mathbf{kb}} W)_{mn} \\ &= 4 \sum_{\mathbf{kb}} w_{\mathbf{b}} \left[-M_{\mathbf{kbnn}}^{W*} - i \frac{\text{Im} \ln M_{\mathbf{kbnn}}^W + \langle \mathbf{r} \rangle_n \cdot \mathbf{b}}{M_{\mathbf{kbnn}}^W} \right] (M_{\mathbf{kb}} W)_{mn} \end{aligned} \quad (9)$$

S2 **b**-vectors for parallel transport

In most cases, the default **b**-vectors generated according to Eq. (4) already contain the 6 neighbors of a given k -point, i.e., $\mathbf{k} \pm \Delta\mathbf{k}$, where $\Delta\mathbf{k}$ can be $(\Delta k_x, 0, 0)$, $(0, \Delta k_y, 0)$, or $(0, 0, \Delta k_z)$, and the $\Delta k_x, \Delta k_y, \Delta k_z$ are the spacings of the k -point sampling. Thus, the parallel transport step can directly use the same overlap matrices $M_{\mathbf{kb}}$ as in the computation of the spread functional. In some rare cases, we find that the default **b**-vectors do not include the 6 neighbors for some special structures. In such cases, we generate a special set of **b**-vectors only including the 6 neighbors, so that the parallel transport works on different overlap matrices than that for computing the spread functional. Then, the gauge matrices $U_{\mathbf{k}}$ generated by the parallel transport step can be used for interpolating band structure, or as input for further maximal localization, etc.

S3 Gauge matrix of MRWF

Here we show that the valence MRWFs exactly span the original DFT valence manifold. This is justified by the following fact: the final gauge matrix after the MRWF procedure is block diagonal,

$$U(\mathbf{k}) = \begin{bmatrix} U_{\text{VB}}(\mathbf{k}) & 0 \\ 0 & U_{\text{CB}}(\mathbf{k}) \end{bmatrix}, \quad (10)$$

where $U_{\text{VB}}(\mathbf{k}) \in \mathbb{C}^{P \times P}$ are unitary transformation for the valence bands, $U_{\text{CB}}(\mathbf{k}) \in \mathbb{C}^{(M-P) \times Q}$ are semi-unitary transformation for the conduction bands, P is the number of valence bands (also number of valence WFs), M is the number of DFT bands, Q is the number of conduction WFs, $N = P + Q$ is the total number of WFs. Thus, the DFT Bloch states are partitioned into two groups: the valence MRWF are unitary transformations, thus span the same space as the valence Bloch states; the disentanglement procedure of VCB Wannierization does not introduce any errors in the valence MRWF, but rather encodes all the disentanglement information in the conduction MRWF, which will be affected by the error of VCB disentanglement procedure. This partly explains why in main text Fig. 5, the band distance of VB-DFT can be smaller than that of VB(VCB)-DFT—since the valence MRWF are unaffected by the disentanglement procedure, no error is introduced in the valence MRWF. Another factor or improved accuracy can be attributed to the fact that the valence MRWFs are more localized, thus can be more accurate in terms of Fourier interpolation.

Now we prove Eq. (10). Again, we stress that this is not limited to the case of valence/conduction, but can be straightforwardly generalized to any groups of isolated bands.

Proof. We proceed with the following steps:

- *The (X, Y) representation of the frozen valence bands during disentanglement*

Using the (X, Y) representation [1] for the gauge matrices of VCB Wannierization, the frozen condition is equivalent to the following factorization,

$$U(\mathbf{k}) = \begin{bmatrix} I & 0 \\ 0 & Y(\mathbf{k}) \end{bmatrix} X(\mathbf{k}), \quad (11)$$

where I is the identity matrix of rank P , and $Y(\mathbf{k})$ are semi-unitary matrices of size $(M - P) \times Q$. Here for simplicity we relax the frozen condition to valence bands only. In practice, usually a larger frozen

window (e.g., including low-lying conduction bands) is used; however, this does not affect the proof since we can always partition the additional part (e.g., corresponding to the low-lying conduction bands) of the identity matrix to $Y(\mathbf{k})$, so I is still of rank P .

Remark. Here we use the (X, Y) representation for analyzing the gauge matrices, this does not mean that the disentanglement procedure must be done using the variational method of Ref. [1]—instead, one can also convert into the (X, Y) representation from gauge matrices obtained using standard disentanglement procedure [4].

- The Hamiltonian diagonalizations do not mix valence and conduction manifolds

The Wannier-gauge Hamiltonians $H^W(\mathbf{k})$ are rotations of Bloch-gauge Hamiltonians $H(\mathbf{k})$ by unitary matrices $U(\mathbf{k})$,

$$H^W(\mathbf{k}) = U^*(\mathbf{k})H(\mathbf{k})U(\mathbf{k}), \quad (12a)$$

$$H(\mathbf{k}) = \text{diag}(\varepsilon_{1\mathbf{k}}, \dots, \varepsilon_{M\mathbf{k}}). \quad (12b)$$

In the following, we always assume eigenvalues are ordered non-decreasingly, i.e., $\varepsilon_{1\mathbf{k}} \leq \dots \leq \varepsilon_{M\mathbf{k}}$. As introduced in the main text Eq. (2), $H^W(\mathbf{k})$ are diagonalized by eigenvectors $V(\mathbf{k})$, and the new gauge matrices are

$$\begin{bmatrix} I & 0 \\ 0 & Y(\mathbf{k}) \end{bmatrix} X(\mathbf{k})V(\mathbf{k}). \quad (13)$$

Since both $X(\mathbf{k})$ and $V(\mathbf{k})$ are unitary matrices of rank N , for simplicity we absorb $V(\mathbf{k})$ into $X(\mathbf{k})$, so now the $U(\mathbf{k})$ matrices diagonalize the Hamiltonians, i.e.,

$$\begin{bmatrix} \varepsilon'_1 & & & & \\ & \ddots & & & \\ & & \varepsilon'_P & & \\ & & & \varepsilon'_{P+1} & \\ & & & & \ddots \\ & & & & & \varepsilon'_N \end{bmatrix} = X^* \begin{bmatrix} I_P & 0 \\ 0 & Y^* \end{bmatrix} \begin{bmatrix} \varepsilon_1 & & & & \\ & \ddots & & & \\ & & \varepsilon_P & & \\ & & & \varepsilon_{P+1} & \\ & & & & \ddots \\ & & & & & \varepsilon_M \end{bmatrix} \begin{bmatrix} I_P & 0 \\ 0 & Y \end{bmatrix} X, \quad (14)$$

where I_P is the identity matrix of rank P , and ε'_i are the eigenvalues of $H^W(\mathbf{k})$; for simplicity of notations we drop the $\mathbf{k}$ dependence. Note that the Hamiltonian in Y gauge,

$$H^Y := \begin{bmatrix} I_P & 0 \\ 0 & Y^* \end{bmatrix} \begin{bmatrix} \varepsilon_1 & & \\ & \ddots & \\ & & \varepsilon_M \end{bmatrix} \begin{bmatrix} I_P & 0 \\ 0 & Y \end{bmatrix} = \begin{bmatrix} \text{diag}(\varepsilon_1, \dots, \varepsilon_P) & 0 \\ 0 & Y^* \text{diag}(\varepsilon_{P+1}, \dots, \varepsilon_M)Y \end{bmatrix}, \quad (15)$$

clearly has P eigenvalues $\varepsilon_1, \dots, \varepsilon_P$ same as original DFT ones. Now we consider the remaining Q eigenvalues of $Y^* \text{diag}(\varepsilon_{P+1}, \dots, \varepsilon_M)Y$.

Lemma S3.1. Suppose $Y \in \mathbb{C}^{m \times n}$ is a semi-unitary matrix with $m > n$, then its singular values are 1.

Proof. For a full singular value decomposition $Y = U\Sigma V^*$, where $U \in \mathbb{C}^{m \times m}$, $V \in \mathbb{C}^{n \times n}$ are unitary matrices, and $\Sigma \in \mathbb{R}^{m \times n}$ is a diagonal matrix with $0 \leq \sigma_i \in \mathbb{R}$ on the diagonal. Since $Y^*Y = I_n$, we have $V\Sigma^2V^* = I_n$, thus $\sigma_i = 1$ for $i = 1, \dots, n$ because σ_i is real and non-negative. $\square$

Using Lemma S3.1, we have

$$Y^* \text{diag}(\varepsilon_{P+1}, \dots, \varepsilon_M)Y = V\Sigma^*U^* \text{diag}(\varepsilon_{P+1}, \dots, \varepsilon_M)U\Sigma V^*. \quad (16)$$

Let us denote

$$A = U^* \text{diag}(\varepsilon_{P+1}, \dots, \varepsilon_M)U, \quad (17)$$

then A has the same eigenvalues of $\varepsilon_{P+1}, \dots, \varepsilon_M$. Since

$$\Sigma = \begin{bmatrix} I_{N-P} \\ 0 \end{bmatrix}_{(M-P) \times (N-P)}, \quad (18)$$

$\Sigma^* A \Sigma$ is just the upper-left $(N-P) \times (N-P)$ block of A .

Lemma S3.2. *For a Hermitian matrix $A \in \mathbb{C}^{m \times m}$ and its partition*

$$A = \begin{bmatrix} B & C \\ C^* & D \end{bmatrix}, \quad (19)$$

where $B \in \mathbb{C}^{n \times n}$, $D \in \mathbb{C}^{(m-n) \times (m-n)}$, $C \in \mathbb{C}^{n \times (m-n)}$, if the eigenvalues of A and B are ordered non-decreasingly (i.e., $\lambda_1(A) \leq \dots \leq \lambda_m(A)$, $\lambda_1(B) \leq \dots \leq \lambda_n(B)$), then the eigenvalues of A and B have the following relation:

$$\lambda_i(A) \leq \lambda_i(B) \leq \lambda_{i+m-n}(A), \quad (20)$$

for $i = 1, \dots, n$.

Proof. This is Theorem 4.3.28 on page 246 of Ref. [5]. □

Using Lemma S3.2, we now know that the eigenvalues of Eq. (17) are bounded by ε_{P+1} and ε_M . Thus, the eigenvalues of Eq. (16) have the same bounds since V is unitary. Since the valence and conduction manifolds are gapped in energy, i.e., $\varepsilon_P < \varepsilon_{P+1}$, the intersection of the two sets of eigenvalues $\{\varepsilon_1, \dots, \varepsilon_P\}$ and $\{\varepsilon_{P+1}, \dots, \varepsilon_M\}$ is empty. Note that the additional X matrix in Eq. (14) is unitary and does not change the eigenvalues, and we know the eigenvalues of Eq. (15) can be separated into two sets without intersection, thus $\varepsilon'_i = \varepsilon_i$ for $i = 1, \dots, P$, and $\varepsilon_{P+1} \leq \varepsilon'_i \leq \varepsilon_M$ for $i = P+1, \dots, N$.

Lemma S3.3. *Let $A, B \in \mathbb{C}^{m \times m}$ be two block diagonal matrices with the same block structure, i.e.,*

$$A = \begin{bmatrix} A_1 & & \\ & \ddots & \\ & & A_k \end{bmatrix}, B = \begin{bmatrix} B_1 & & \\ & \ddots & \\ & & B_k \end{bmatrix}, \quad (21)$$

where A_i, B_i have the same size for $i = 1, \dots, k$. Suppose the eigenvalues of A_i and B_j have no intersection, i.e., $\lambda(A_i) \cap \lambda(B_j) = \emptyset$ whenever $i \neq j$. If $C \in \mathbb{C}^{m \times m}$ and $AC = CB$, then C is also block diagonal with the same block structure, and C_i satisfies $A_i C_i = C_i B_i$ for each $i = 1, \dots, k$.

Proof. This is Corollary 2.4.4.2 on page 112 of Ref. [5]. □

Note that we can rewrite Eq. (14) into block diagonal form:

$$\begin{bmatrix} \text{diag}(\varepsilon'_1, \dots, \varepsilon'_P) & \\ & \text{diag}(\varepsilon'_{P+1}, \dots, \varepsilon'_M) \end{bmatrix} = X^* H^Y X, \quad (22)$$

where H^Y is also block diagonal, partitioned as in Eq. (15). After multiplying X on both sides of Eq. (22), by Lemma S3.3 we know X is also block diagonal with the same block structure,

$$X = \begin{bmatrix} X_1 & \\ & X_2 \end{bmatrix}, \quad (23)$$

where X_1 and X_2 are unitary matrices with ranks of P and Q , respectively.

Finally, our unitary transformation U is block diagonal,

$$U = \begin{bmatrix} I_P & \\ & Y \end{bmatrix} \begin{bmatrix} X_1 & \\ & X_2 \end{bmatrix} = \begin{bmatrix} X_1 & \\ & Y X_2 \end{bmatrix}. \quad (24)$$

- *The final gauge transformation is block diagonal*

After Hamiltonian diagonalization, we use parallel transport and maximal localization to construct ML-WFs for the two submanifolds, respectively, i.e., multiplying two additional gauge matrices Z_1 and Z_2 on Eq. (24),

$$\begin{bmatrix} X_1 & \\ & Y X_2 \end{bmatrix} \begin{bmatrix} Z_1 & \\ & Z_2 \end{bmatrix} = \begin{bmatrix} X_1 Z_1 & \\ & Y X_2 Z_2 \end{bmatrix}. \quad (25)$$

This does not alter the block diagonal structure, thus the final MRWF gauge is block diagonal as Eq. (10). □

References

- [1] Anil Damle, Antoine Levitt, and Lin Lin. Variational Formulation for Wannier Functions with Entangled Band Structure. *Multiscale Model. Simul.*, 17(1):167–191, jan 2019.
- [2] Ken Kreutz-Delgado. The Complex Gradient Operator and the CR-Calculus. 2009.
- [3] Patrick K Mogensen and Asbjørn N Riseth. Optim: A mathematical optimization package for Julia. *J. Open Source Software*, 3(24):615, apr 2018.
- [4] Ivo Souza, Nicola Marzari, and David Vanderbilt. Maximally localized Wannier functions for entangled energy bands. *Phys. Rev. B*, 65(3):035109, dec 2001.
- [5] Roger A. Horn. *Matrix Analysis: Second Edition*. Cambridge University Press, 2012.

S4 Evolution of WF spreads and centers for silicon valence

Figure S1 shows the evolution of WF spreads and centers for the valence manifold of silicon. Note that in our test of the random gauge case (Fig. S1a), maximal localization always fail due to zeros in the diagonal of the overlap matrices. To bypass this limitation, we generate another series of random unitary matrices as the initial gauge, and maximally localize the WFs. The new random matrices are still comparable to the random gauge directly after the Hamiltonian diagonalization, since the total spreads ($1454.34 \text{ \AA}^2$) is still on the same order as the previous one ($1091.30 \text{ \AA}^2$). Overall parallel transport generates the best starting gauge, leading to much faster convergence for maximal localization. Especially, the case of parallel transport + single rotation results in the smoothest evolution of both spreads and centers.

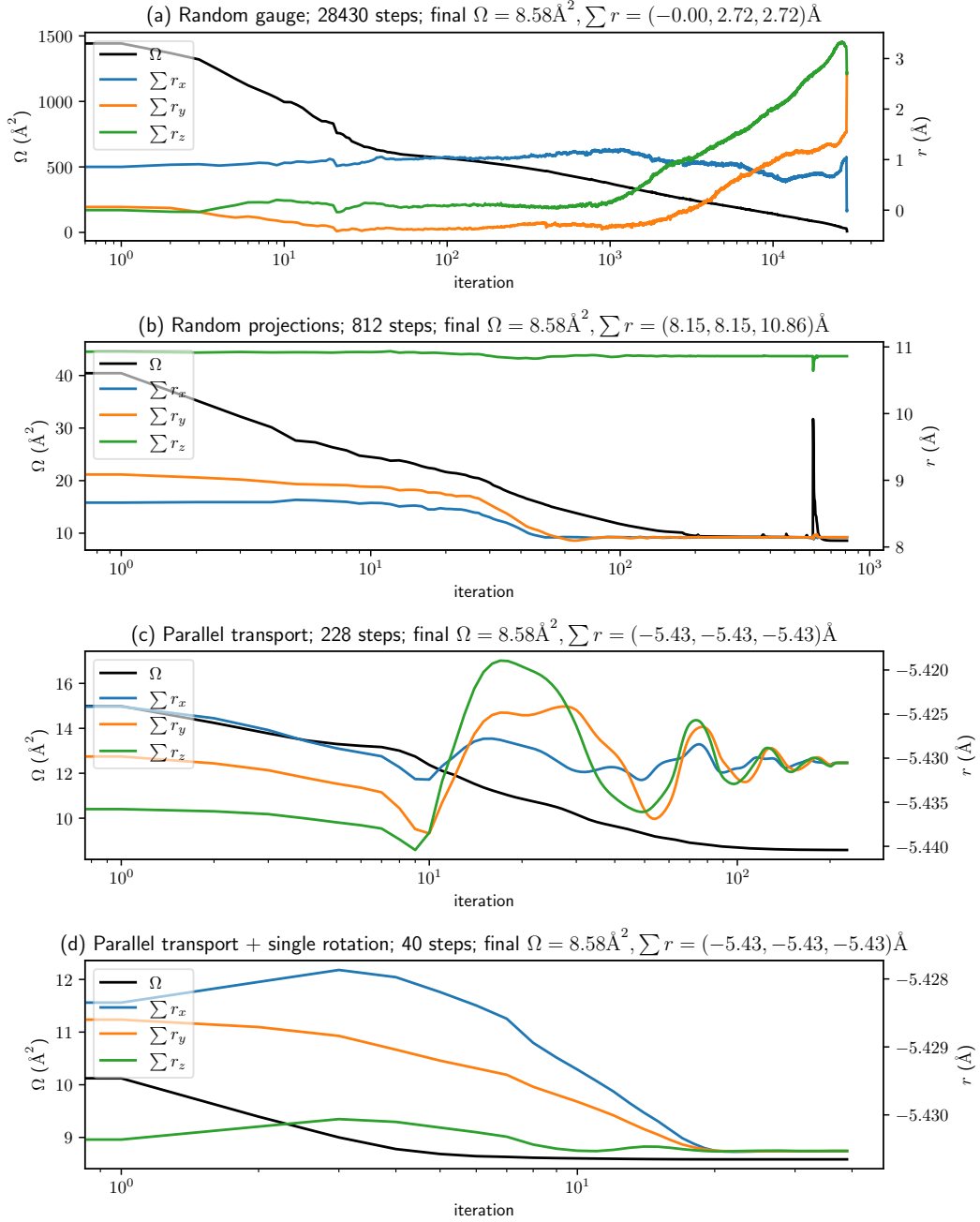


Figure S1: **Evolution of MLWF spreads and centers for the valence manifold of silicon.** The black, blue, orange, and green lines show the evolution of WF spreads, x , y , and z components of the sum of WF centers during maximal localization, respectively. (a) shows the calculation starting from random gauge, i.e., after the Wannier Hamiltonian diagonalization, the gauge at each k -point are randomized. (b) shows the calculation starting from random projection of Gaussian functions. (c) shows the calculation starting from parallel transport gauge. (d) shows the calculation starting from parallel transport + single rotation gauge. The convergence tolerance of spread is set to $2 \times 10^{-7} \text{ \AA}^2$. Note both the horizontal and vertical axes have different range for all the three subfigures. The parallel transport generates a continuous gauge, leading to much faster convergence, as well as smoother evolution of both spreads and centers during maximal localization.

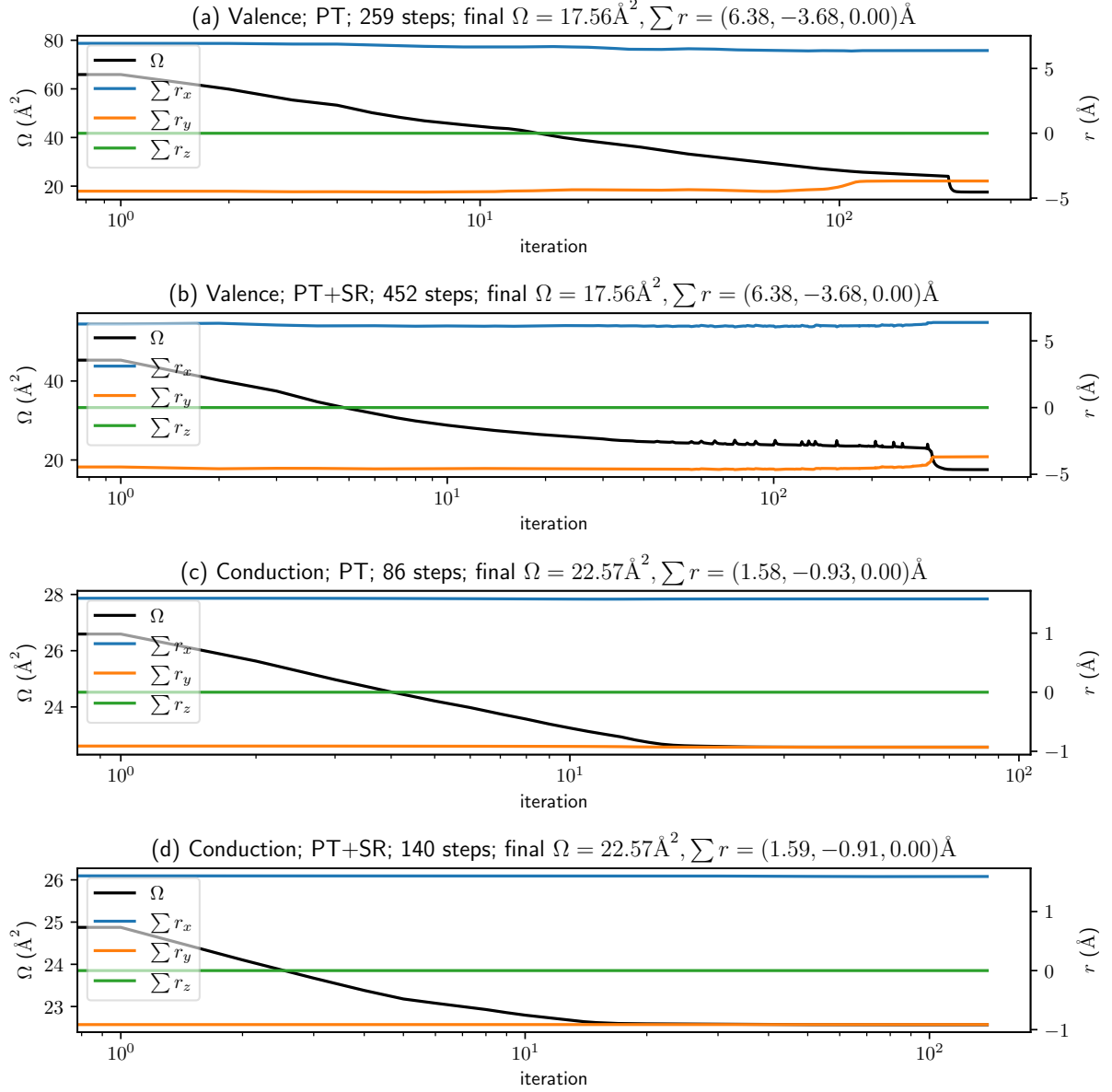
S5 Evolution of WF spreads and centers for MoS_2 

Figure S2: **Evolution of WF spreads and centers during maximal localization for MoS_2 .** (a) shows the calculation for the valence manifold starting from parallel transport gauge. (b) shows the calculation for the valence manifold starting from parallel transport + single rotation gauge. (c) shows the calculation for the conduction manifold starting from parallel transport gauge. (d) shows the calculation for the conduction manifold starting from parallel transport + single rotation gauge. The notations are the same as Fig. S1.

S6 WF shapes and spreads of SrVO_3

	VCB	3d			others		
	DIS+ML	PT	PT+SR	PT(+SR)+ML	PT	PT+SR	PT(+SR)+ML
$\Omega_{\text{WF}}(\text{\AA}^2)$	2.267 (2)	1.943	1.923	1.877 (3)	12.748 (3)*	9.164 (2)*	1.251 (3)
$\Omega_{\text{WF}}(\text{\AA}^2)$	2.215 (4)	1.917	1.919	2.000	8.343 (5)*	6.723 (6)*	1.044 (6)
$\Omega_{\text{WF}}(\text{\AA}^2)$	2.249 (2)	1.903	1.913	2.000	15.703 (2)*	19.621 (3)*	2.386 (4)
$\Omega_{\text{WF}}(\text{\AA}^2)$	2.043 (1)	2.034	2.027		19.866 (2)*	17.169 (4)*	2.409 (2)
$\Omega_{\text{WF}}(\text{\AA}^2)$	3.098 (1)	2.018	2.022		17.972	13.740	2.228
$\Omega_{\text{WF}}(\text{\AA}^2)$	0.559 (1)				24.514 (2)*	23.208 (2)*	2.417 (2)
$\Omega_{\text{WF}}(\text{\AA}^2)$	0.559 (1)				27.173 (3)*	28.083	3.520
$\Omega_{\text{WF}}(\text{\AA}^2)$	0.648 (3)				37.398		
$\Omega_{\text{WF}}(\text{\AA}^2)$	0.586 (6)						
$\Omega_{\text{WF}}(\text{\AA}^2)$	0.632 (3)						
$\Sigma\Omega_{\text{WF}}(\text{\AA}^2)$	31.510	9.815	9.804	9.629	337.013	274.445	34.956

Figure S3: **WF shape of various Wannierization methods for SrVO_3 .** The notations are the same as Fig. 1a and Fig. 2a in the main text. The green, orange, and red spheres are Sr, V and O atoms, respectively.

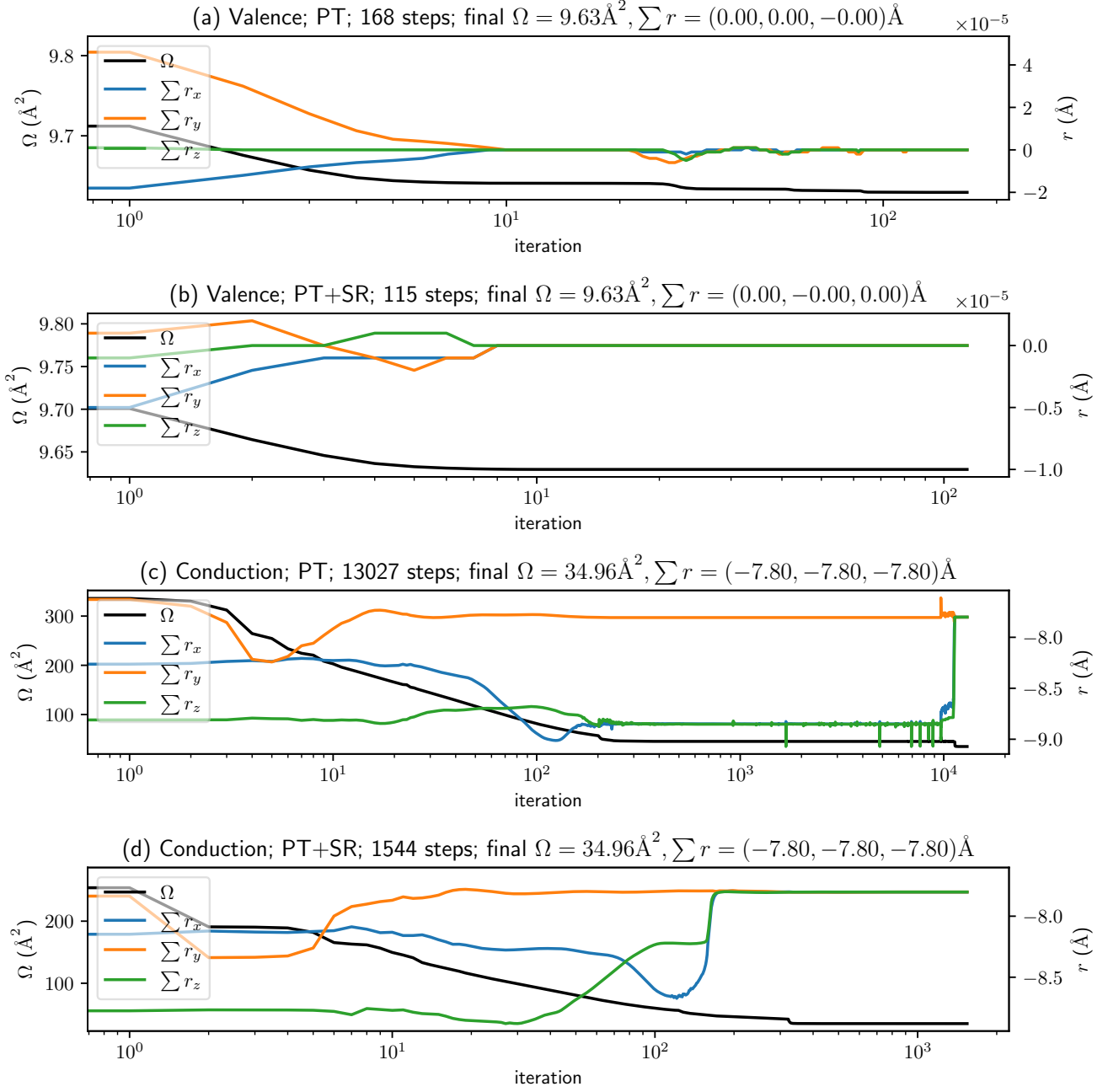


Figure S4: **Evolution of WF spreads and centers during maximal localization for SrVO_3 .** (a) shows the calculation for the $3d$ manifold starting from parallel transport gauge. (b) shows the calculation for the $3d$ manifold starting from parallel transport + single rotation gauge. (c) shows the calculation for the remaining manifold starting from parallel transport gauge. (d) shows the calculation for the remaining manifold starting from parallel transport + single rotation gauge. The notations are the same as Fig. S1.

S7 Max band distance for 77 insulators

For completeness, we also compute the max band distance $\eta_{\max}$, which is a stricter measure of band interpolation quality: for entangled bands,

$$\eta_{2,\max}^{\text{A-B}} = \max_{n\mathbf{k}} \left(\tilde{f}_{n\mathbf{k}} \left| \epsilon_{n\mathbf{k}}^{\text{A}} - \epsilon_{n\mathbf{k}}^{\text{B}} \right| \right), \quad (26)$$

and for isolated bands,

$$\eta_{\text{isolated},\max}^{\text{A-B}} = \max_{n\mathbf{k}} \left(\left| \epsilon_{n\mathbf{k}}^{\text{A}} - \epsilon_{n\mathbf{k}}^{\text{B}} \right| \right). \quad (27)$$

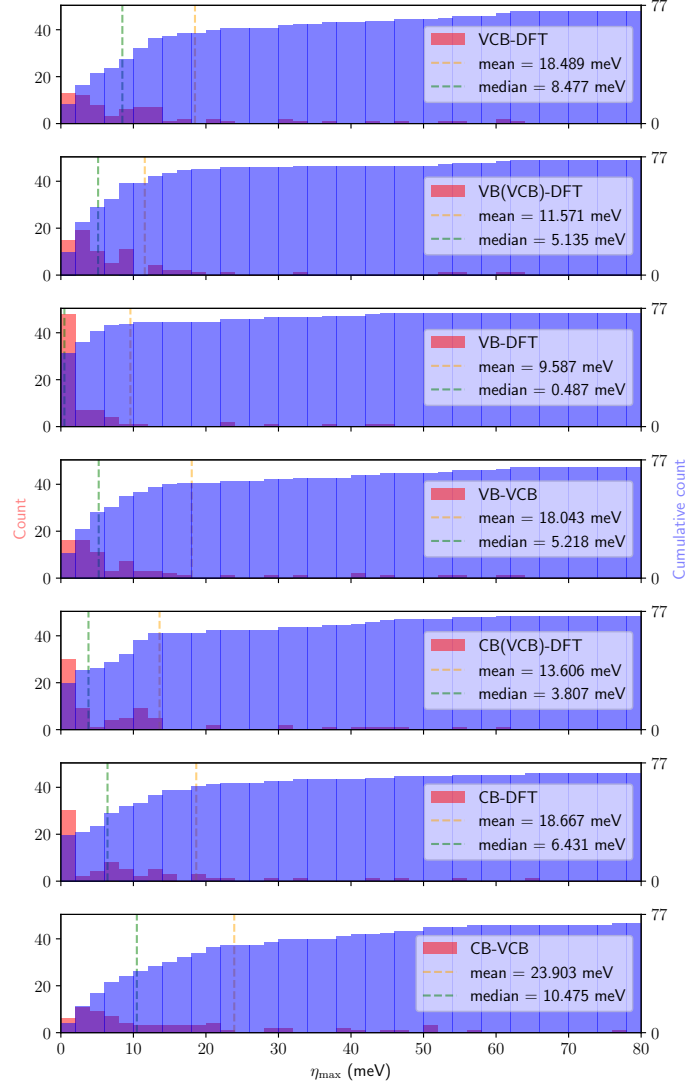


Figure S5: **Max band distances of 77 insulators.** From top to bottom: histograms of max band distances for valence plus conduction bands (VCB) w.r.t. DFT, valence bands (VB) of VCB Wannierization w.r.t. DFT, VB Wannierization w.r.t. DFT, VB Wannierization w.r.t. VCB Wannierization, conduction bands (CB) of VCB Wannierization w.r.t. DFT, CB Wannierization w.r.t. DFT, and CB Wannierization w.r.t. VCB Wannierization. The red and blue bars are the histograms and cumulative histograms, respectively. The vertical lines indicate the mean and median values.

S8 Band structures for 77 insulators

Here we show in each page the band structures, band distances, and evolution of spread and Wannier function centers during the minimization procedure, for each of the 77 structures discussed in the main text.

In each page, the left column shows the band structure comparison between **Quantum ESPRESSO** (QE), Wannier-interpolated bands obtained from valence plus conduction (VC) Wannierization, Wannier-interpolated bands corresponding to separate valence (V) Wannierization, and Wannier-interpolated bands corresponding to separate conduction (C) Wannierization. The zero of energy is set at the Fermi level. The title shows the structure formula, and a comment (enclosed in parentheses) on the calculation (see later), and the UUID of the corresponding **AiiDA** calculations for the QE band structure (PW) and Wannier interpolated bands (W90). In general, there are three types of comment: (a) “exclude semicore”: the semicore states are excluded from the Wannierization, this is the default setting; (b) “include semicore”: the semicore states are included in Wannierization, since the semicore states overlap with valence states, and the Wannierization quality would be worse if the semicore states were excluded; (c) “hydrogenic projection, energy disentanglement”: in few cases we find that the standard hydrogenic projection with energy window disentanglement results in better VC Wannierization, while all the other cases are using the projectability-disentangled Wannier functions (PDWF) method.

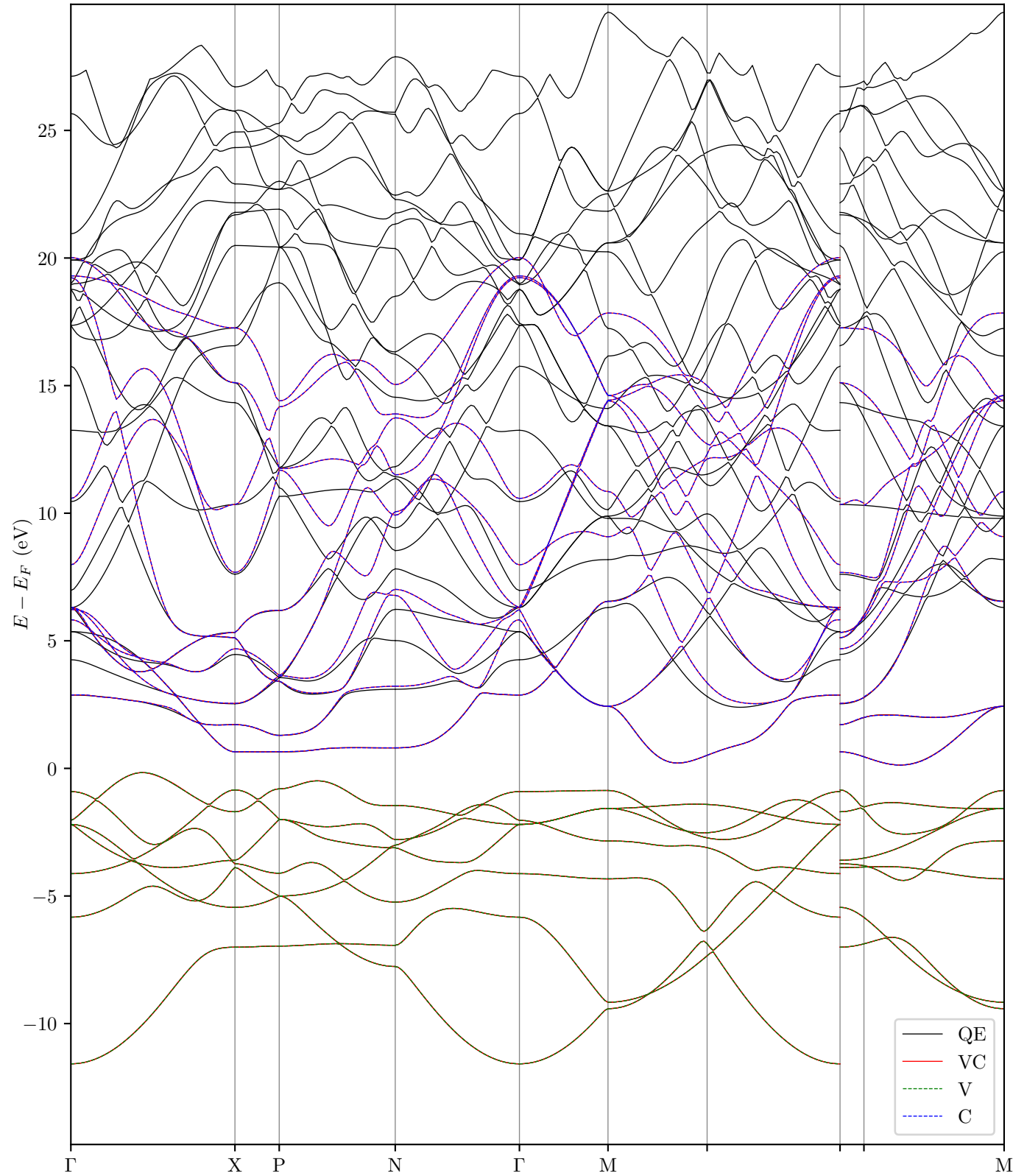
The table at the bottom left shows the band distances (in meV) between the pairs of band structures. Specifically, η_2 is used to compare the bands below Fermi energy + 2 eV with a smearing of 0.1 eV; η_{isolated} is used to compare isolated bands, for which there is no need of Fermi-Dirac smearing as in η_2 . In the header of the table, VC-QE means comparing the Wannier-interpolated VC bands of a VC Wannierization w.r.t. QE bands; similarly, V-QE, C-QE, V-VC, and C-VC, indicate comparisons of Wannier-interpolated valence bands of a separate valence Wannierization w.r.t. QE bands, Wannier-interpolated conduction bands of a separate conduction Wannierization w.r.t. QE bands, Wannier-interpolated valence bands of a separate valence Wannierization w.r.t. Wannier-interpolated VC bands of a VC Wannierization, and Wannier-interpolated conduction bands of a separate conduction Wannierization w.r.t. Wannier-interpolated VC bands of a VC Wannierization, respectively.

On the right column, the evolution of total spread and of the sum of the x, y, z components of the Wannier function centers are shown. In the title of each subfigure, the Ω and the $\sum r$ are the final total spread and sum of Wannier function centers, respectively. The convergence criteria of spread functional are set as number of atoms times 1×10^{-7} for VC Wannierizations (i.e., for both `dis_conv_tol` and `conv_tol` in the `wannier90` input parameters), , and 1×10^{-9} for separate V and C Wannierizations. The separate V and C Wannierizations are stricter since no disentanglement is performed and they are thus easier to converge.

List of structures (Hill formula, in alphabetic order)

1. Al ₂ Os	15	40. Cu ₄ P ₈	54
2. Al ₄ O ₈ Zn ₂	16	41. Cu ₈ O ₈ Sr ₄	55
3. As ₄ O ₁₆ Pb ₆	17	42. F ₂ Xe	56
4. As ₄ O ₁₆ Y ₄	18	43. F ₄ H ₂ K ₂	57
5. As ₈ Si ₄ Zn ₄	19	44. F ₄ Sn	58
6. AsB	20	45. FLi	59
7. B ₁₆ Mg ₄	21	46. FNa	60
8. B ₆ Si	22	47. Ge ₄ Ru ₄	61
9. B ₈ H ₁₆ O ₁₆	23	48. H ₈ O ₁₆ W ₄	62
10. BaS	24	49. HK	63
11. BaTe	25	50. HLi	64
12. BeO ₄ S	26	51. Hg ₃ O ₃	65
13. Bi ₄ Cl ₁₂	27	52. INa	66
14. Br ₁₈ W ₃	28	53. InP	67
15. Br ₂ Fe	29	54. K ₂ O	68
16. Br ₄ Ca ₂	30	55. K ₄ O ₆ S ₂	69
17. BrLi	31	56. K ₄ Sb ₈	70
18. BrNa	32	57. Li ₂ Te	71
19. C ₂ Cd ₂ O ₆	33	58. Li ₄ O ₆ Si ₂	72
20. C ₂ N ₂ Na ₂	34	59. Mg ₂ O ₁₀ Ti ₄	73
21. C ₃ Ag ₃ N ₃	35	60. Mg ₄ O ₁₂ Se ₄	74
22. C ₄ Mg ₂	36	61. N ₂ Na ₂ O ₆	75
23. C ₄ O ₁₂ Sr ₄	37	62. Na ₂ O	76
24. C ₆ Mg ₄	38	63. Na ₂ Se	77
25. C ₆ O ₁₈ Zn ₆	39	64. Na ₂ Te	78
26. C ₉ B ₃₆	40	65. Na ₆ O ₆	79
27. CBe ₂	41	66. Na ₈ Sb ₈	80
28. Ca ₄ O ₁₄ V ₄	42	67. O ₁₆ Ti ₄ Zn ₈	81
29. Ca ₆ O ₁₄ Ti ₄	43	68. O ₂ Pb ₂	82
30. Ca ₆ O ₁₆ V ₄	44	69. O ₂ Sr	83
31. CaI ₂	45	70. O ₄ Rb ₄	84
32. CaO	46	71. Pd ₄ S ₈	85
33. CdCl ₂	47	72. PtS ₂	86
34. Cl ₄ Li ₄ O ₁₆	48	73. Ru ₄ S ₈	87
35. Cl ₆ Rh ₂	49	74. S ₂ Zr	88
36. Cl ₈ Hf ₂	50	75. Se ₂ Sn	89
37. Cl ₈ Sr ₄	51	76. Se ₄ Tl ₄	90
38. Cs ₄ O ₄	52	77. SeSr	91
39. CsH	53		

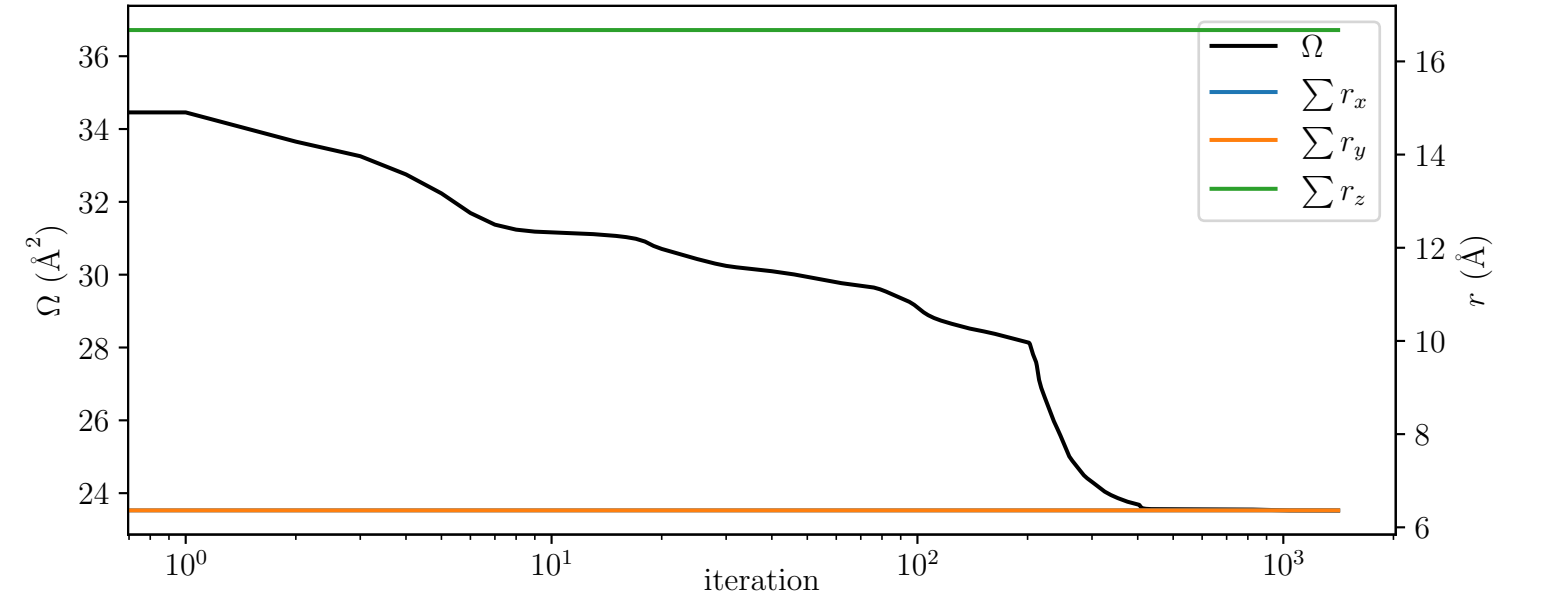
Al₂O₃ (exclude semicore)
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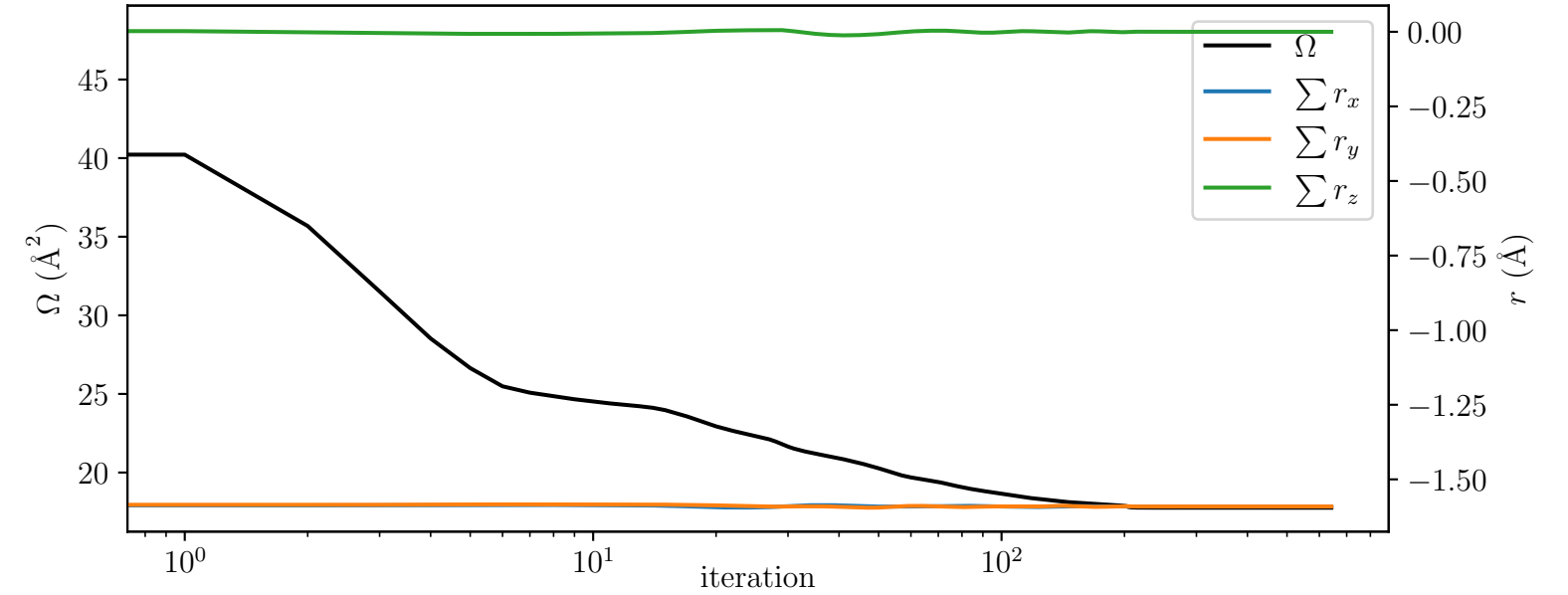
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	3.5	3.0	0.4	3.1	6.2	8.0	4.3
η_{max}	16.9	16.9	6.0	15.8	13.1	18.0	21.9

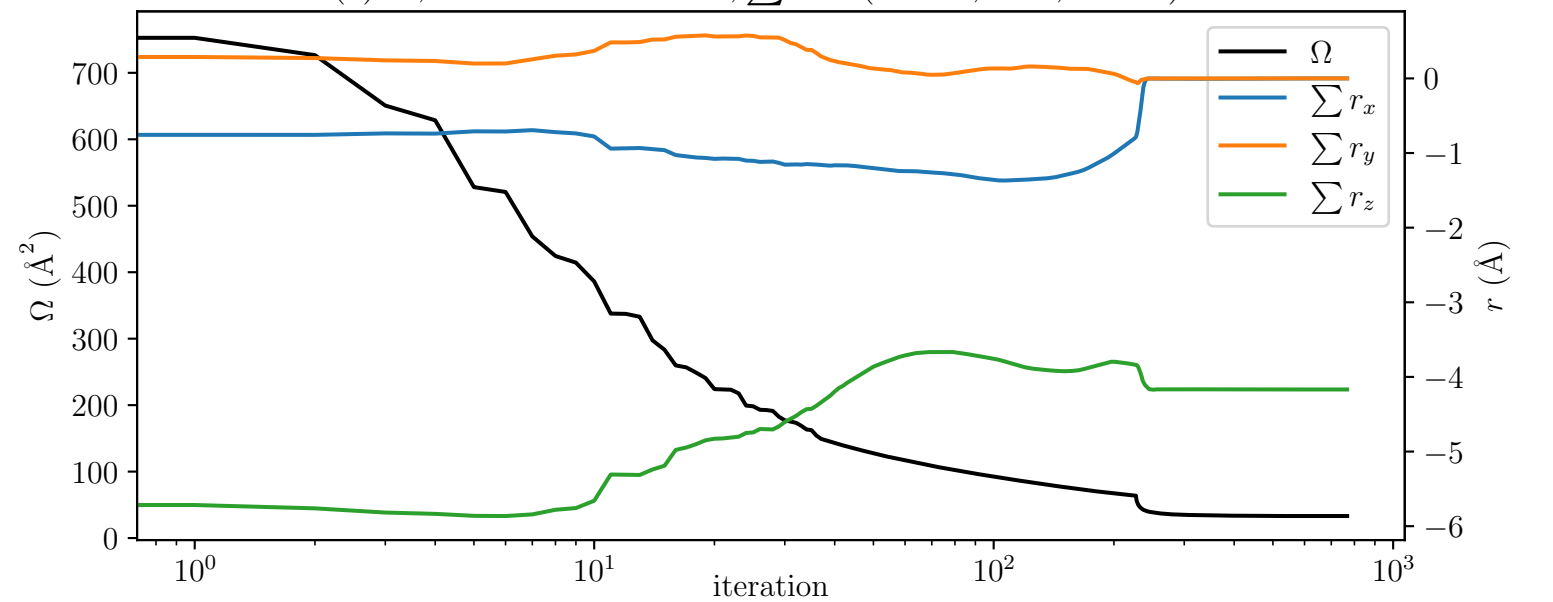
(a) VC; final $\Omega = 23.52 \text{ \AA}^2$, $\sum r = (6.36, 6.36, 16.67) \text{ \AA}$



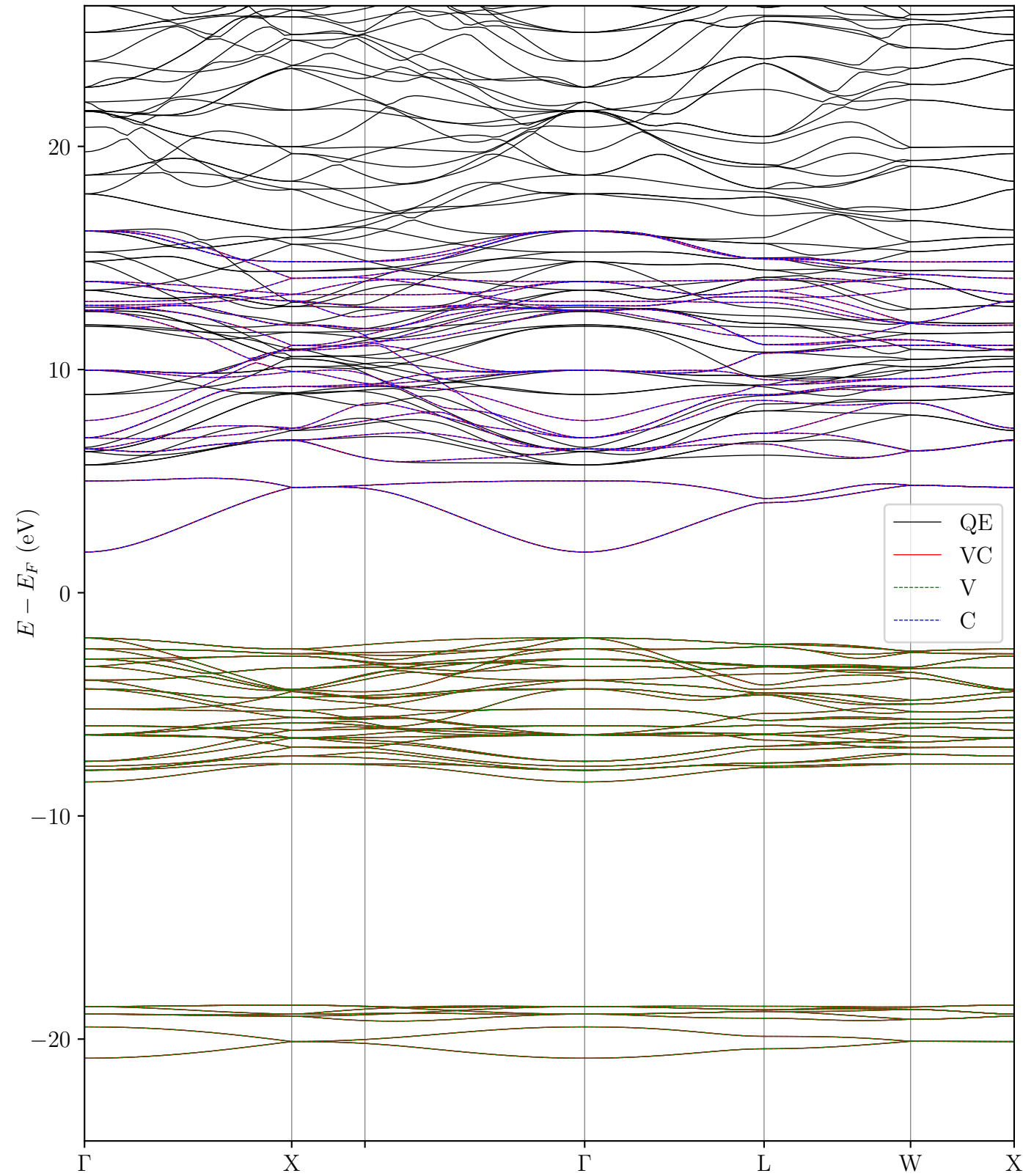
(b) V; final $\Omega = 17.76 \text{ \AA}^2$, $\sum r = (-1.59, -1.59, 0.00) \text{ \AA}$



(c) C; final $\Omega = 33.13 \text{ \AA}^2$, $\sum r = (-0.00, 0.00, -4.17) \text{ \AA}$



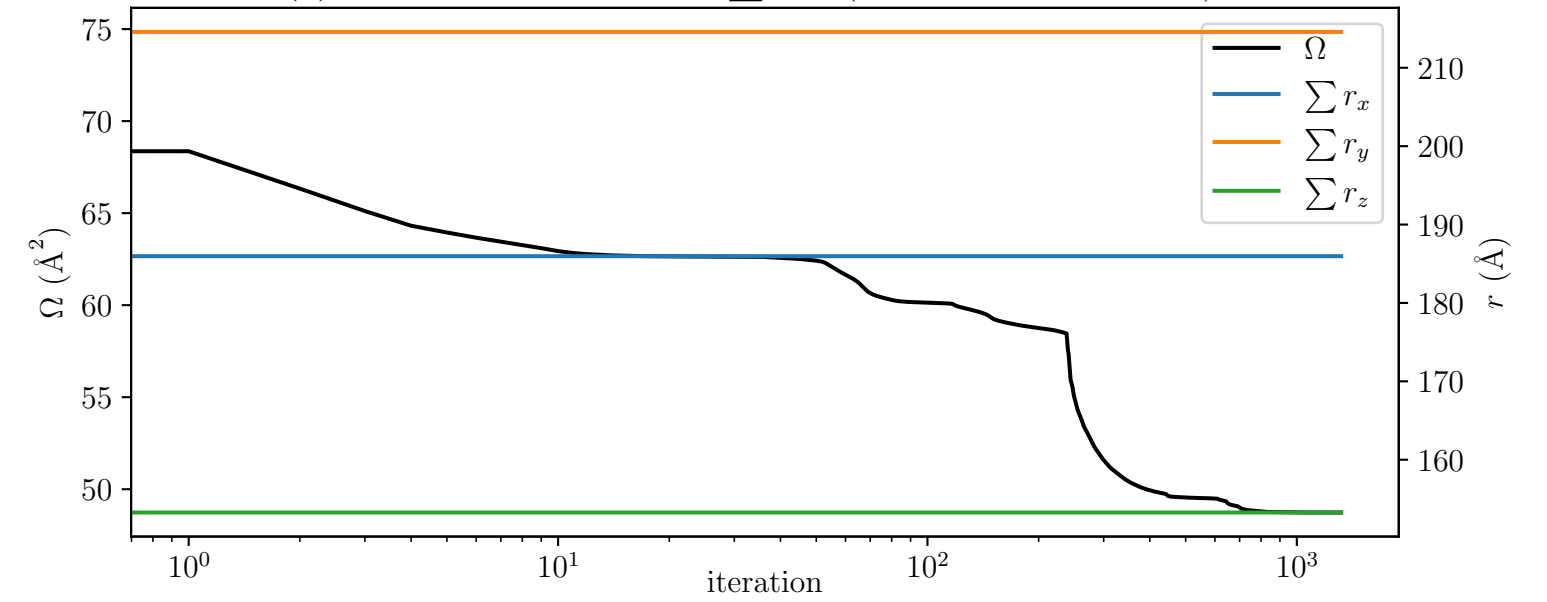
Al₄O₈Zn₂ (exclude semicore)
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W90 AiiDA UUID: d9bc3505-eeda-4ed2-9d73-6668ab38b5cc



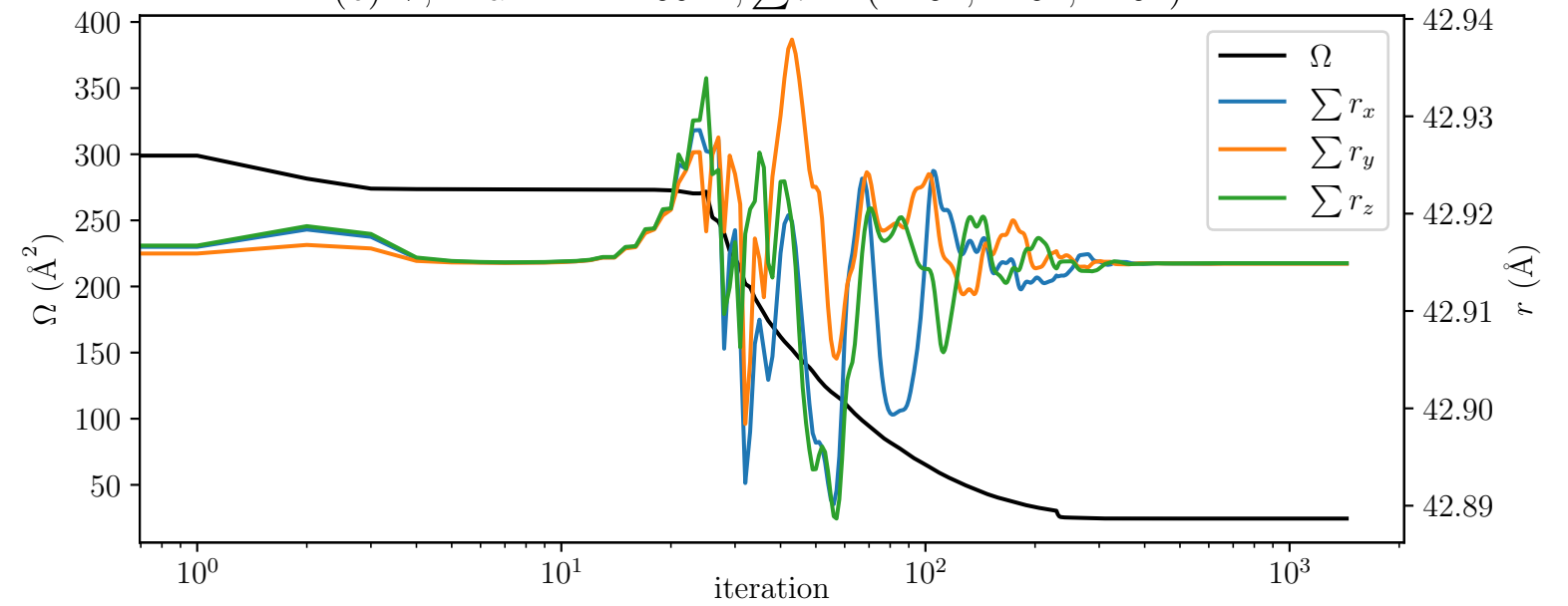
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.6	0.6	0.0	0.6	0.7	0.2	1.3
η_{max}	5.8	5.8	0.5	5.8	0.7	0.4	7.1

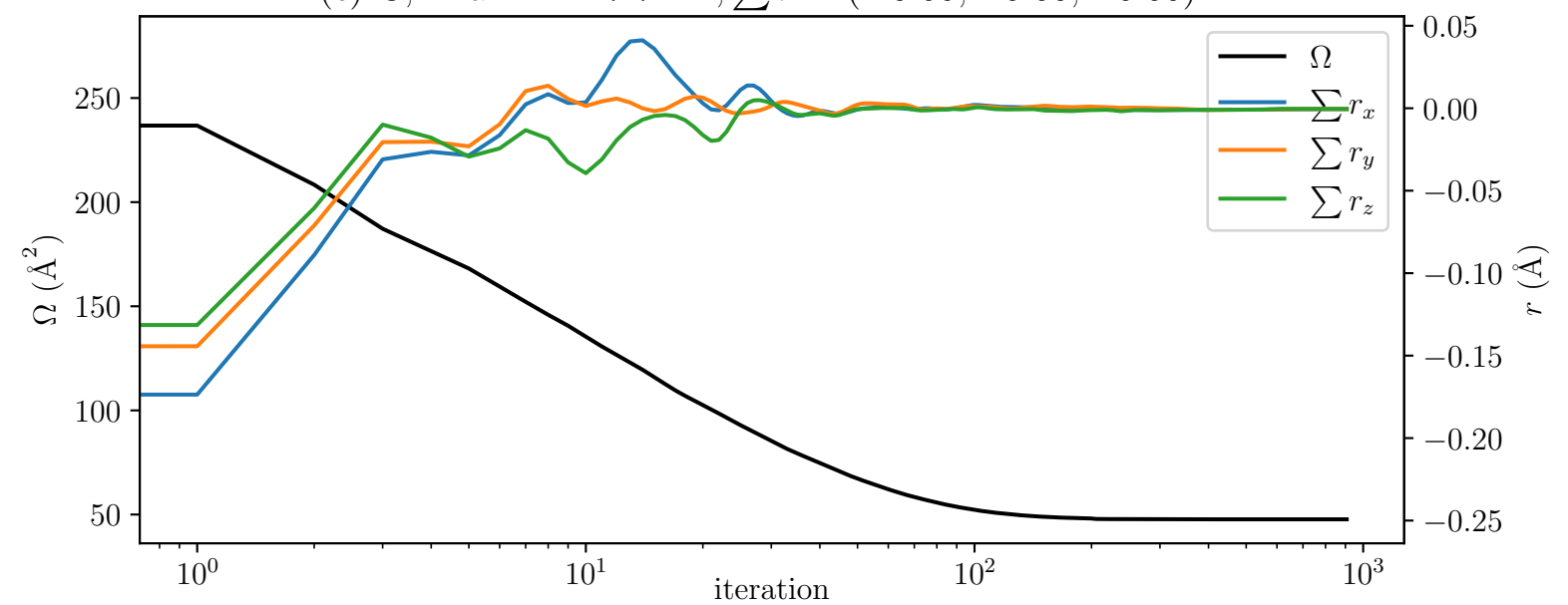
(a) VC; final $\Omega = 48.73 \text{ \AA}^2$, $\sum r = (185.96, 214.57, 153.27) \text{ \AA}$



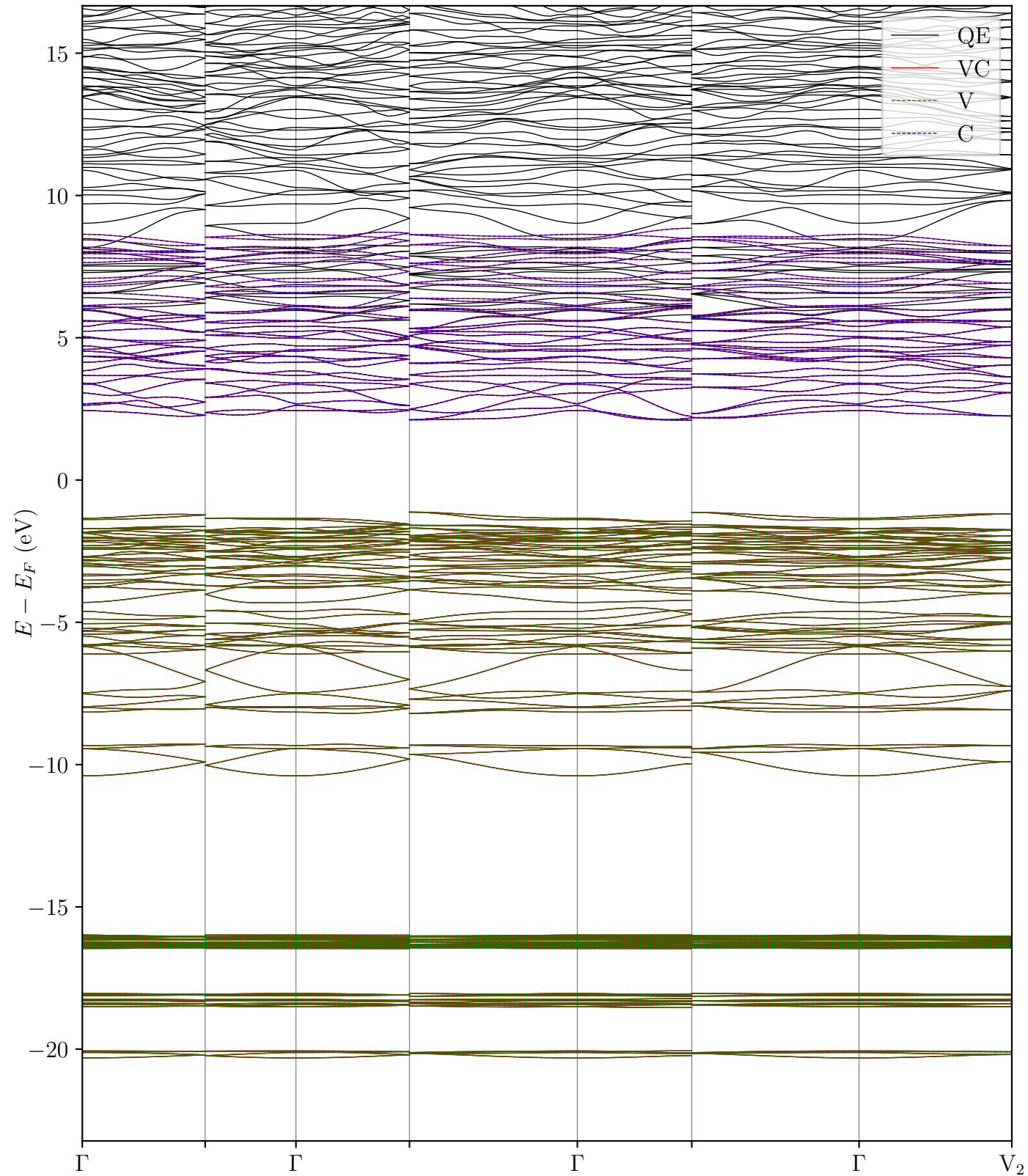
(b) V; final $\Omega = 24.50 \text{ \AA}^2$, $\sum r = (42.91, 42.91, 42.91) \text{ \AA}$



(c) C; final $\Omega = 47.71 \text{ \AA}^2$, $\sum r = (-0.00, -0.00, -0.00) \text{ \AA}$



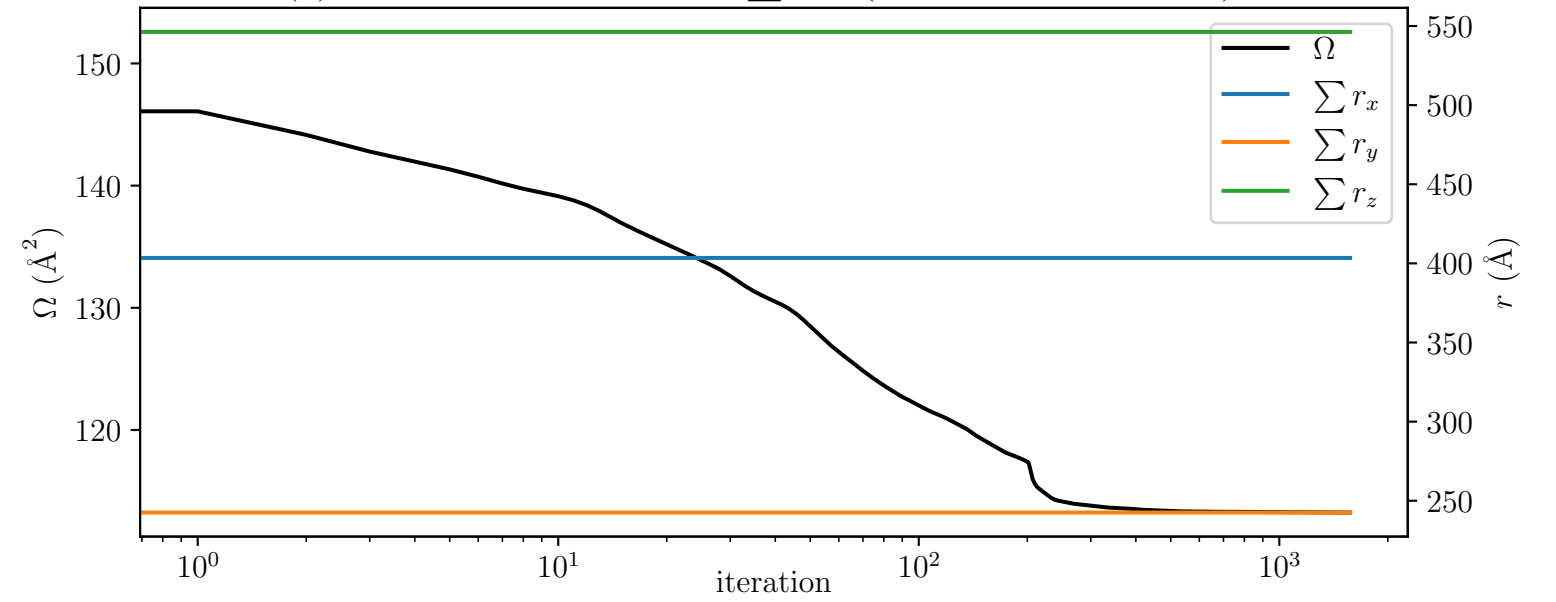
As₄O₁₆Pb₆ (**include** semicore)
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W90 AiiDA UUID: 809d5b3b-9471-4dcb-bf1f-a67443ca5dbc



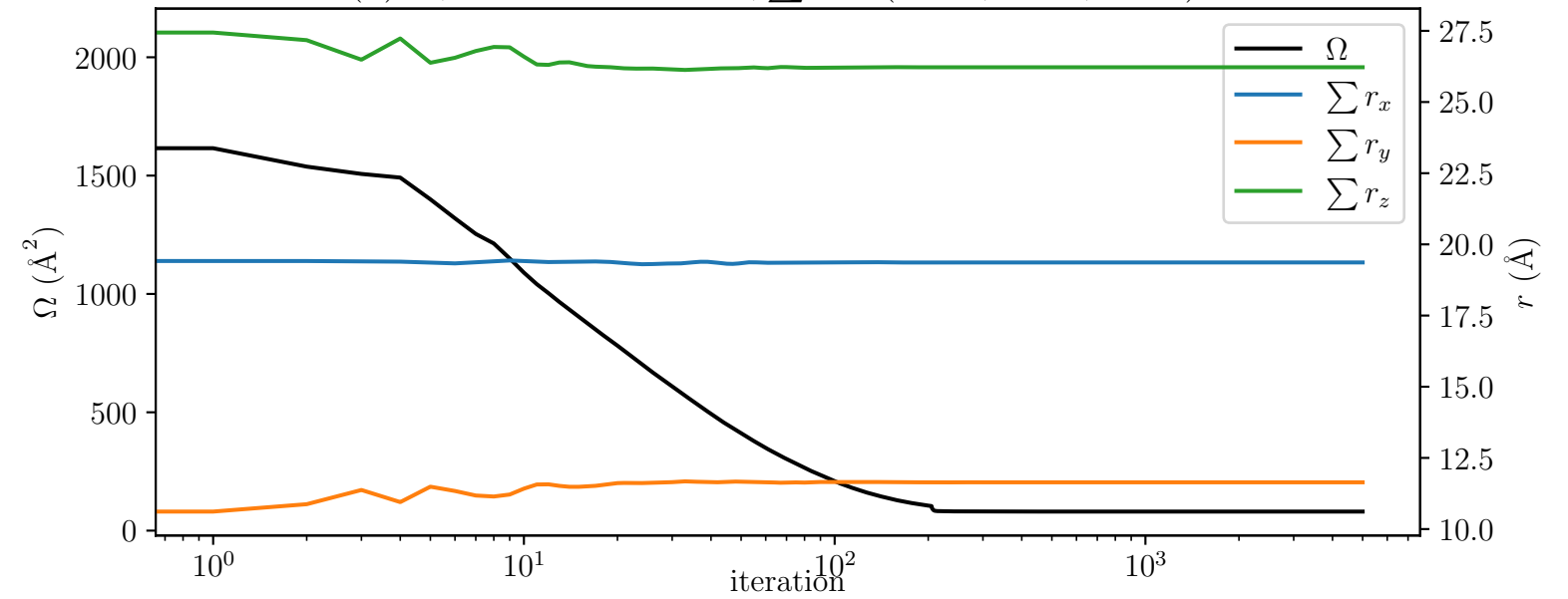
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.1	0.1	0.0	0.1	0.7	1.4	0.5
η_{max}	0.9	0.9	0.6	1.0	0.5	1.0	3.9

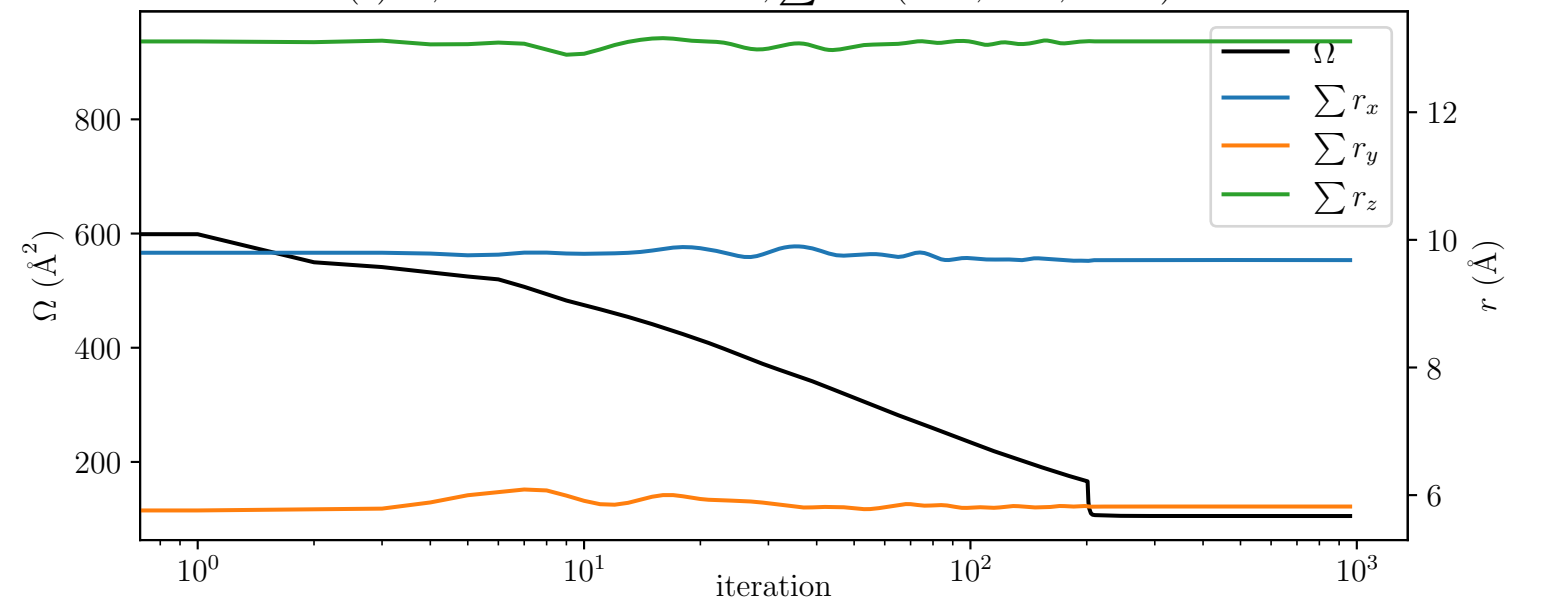
(a) VC; final $\Omega = 113.24 \text{\AA}^2$, $\sum r = (403.44, 242.55, 546.28) \text{\AA}$



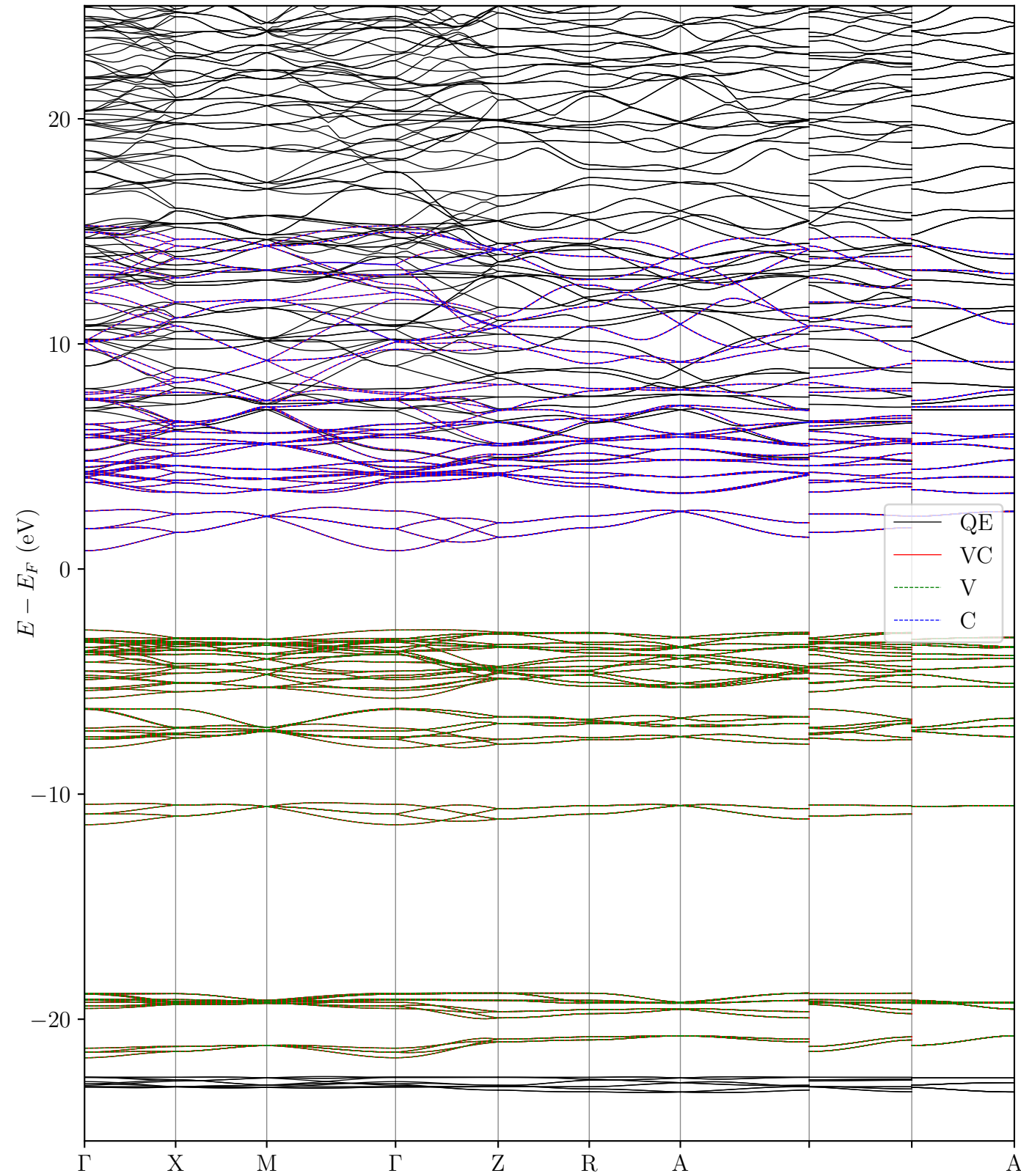
(b) V; final $\Omega = 80.51 \text{\AA}^2$, $\sum r = (19.37, 11.64, 26.22) \text{\AA}$



(c) C; final $\Omega = 105.28 \text{\AA}^2$, $\sum r = (9.68, 5.82, 13.11) \text{\AA}$



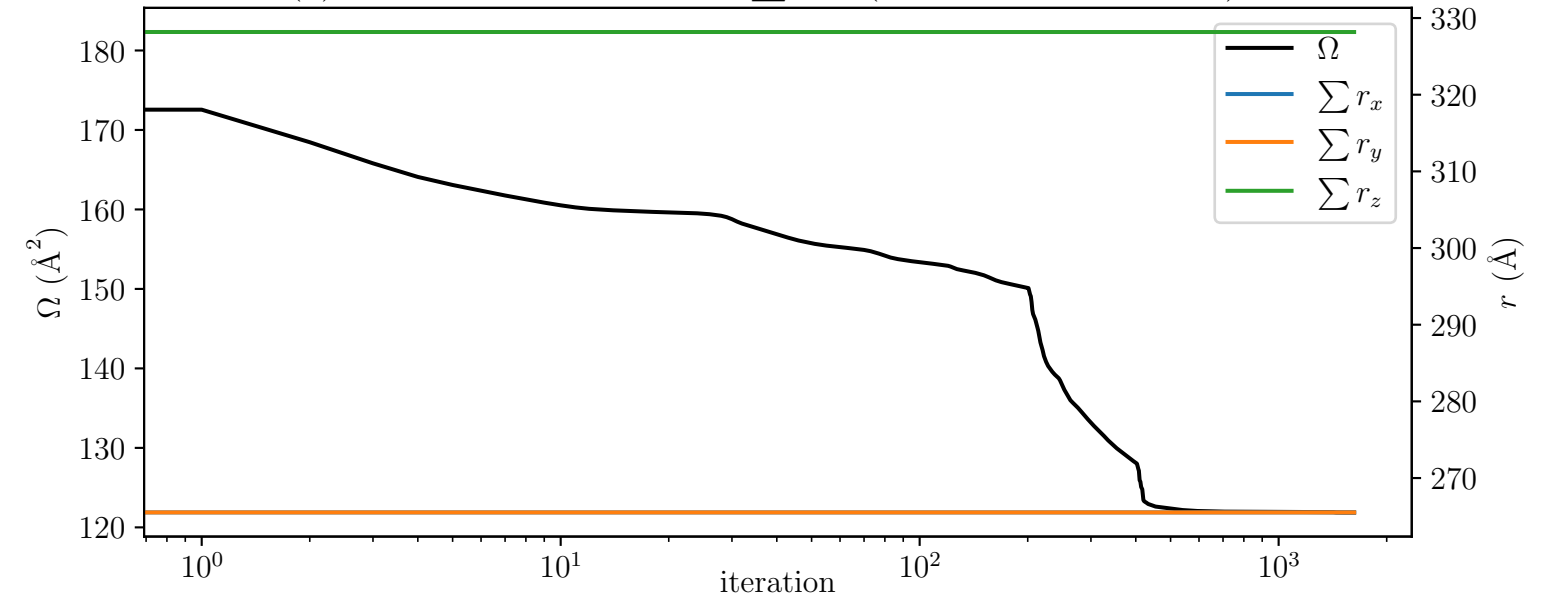
As₄O₁₆Y₄ (exclude semicore)
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W90 AiiDA UUID: 041a7b8e-f5d3-4611-8b4b-61800266d687



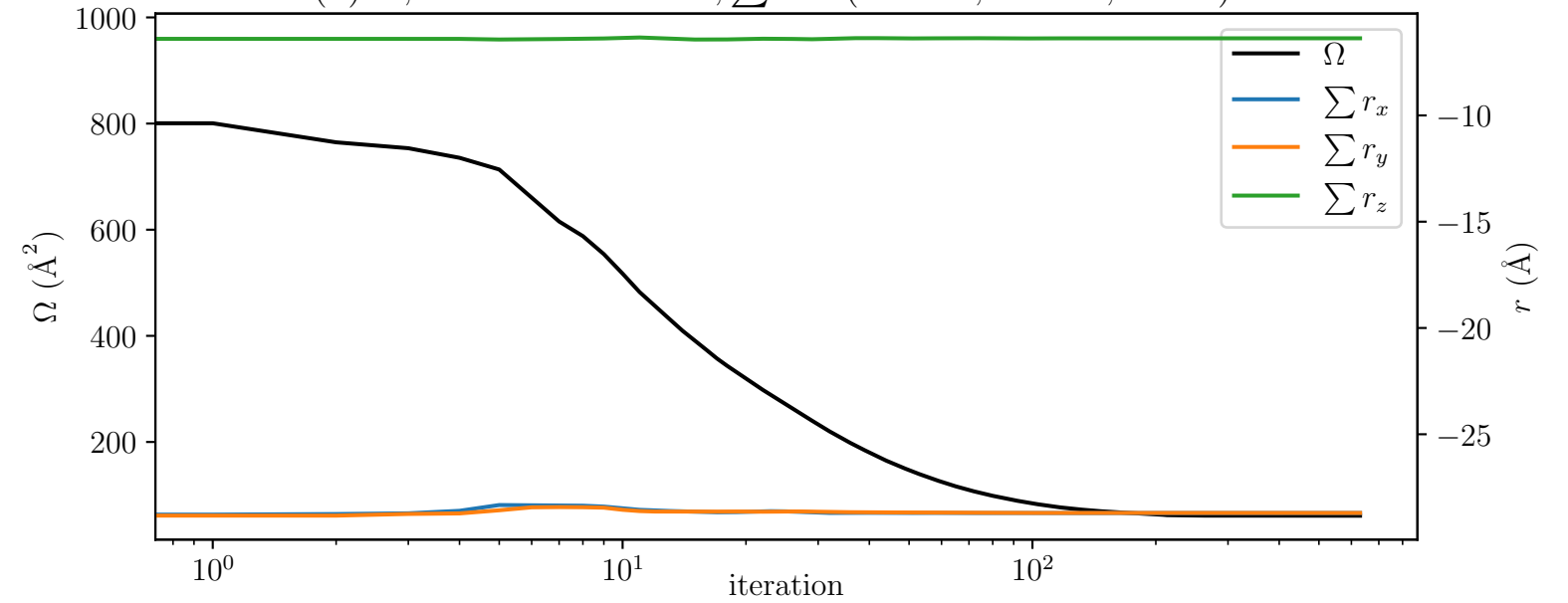
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.5	0.5	0.1	0.5	0.7	1.1	1.5
η_{max}	4.8	4.8	1.2	5.0	2.0	3.4	14.2

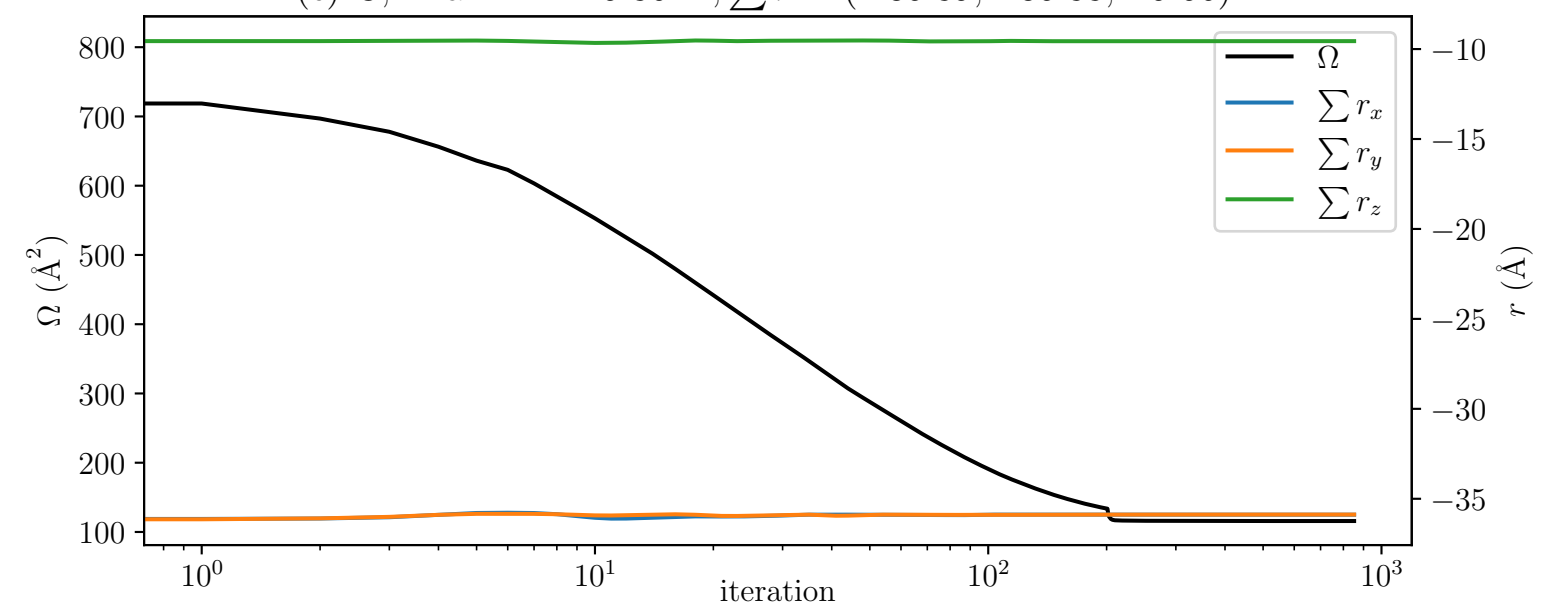
(a) VC; final $\Omega = 121.87 \text{\AA}^2$, $\sum r = (265.52, 265.52, 328.18) \text{\AA}$



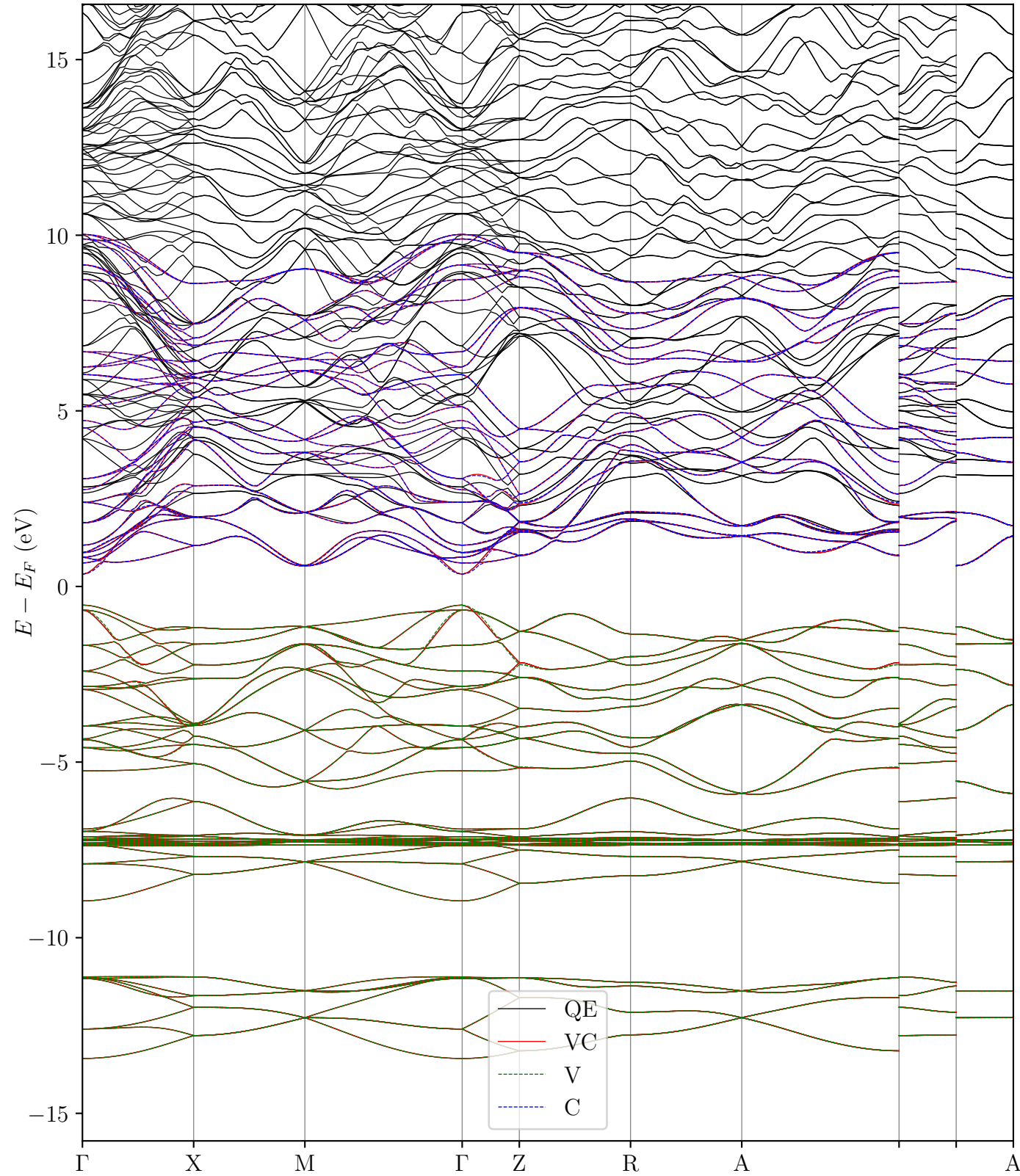
(b) V; final $\Omega = 61.07 \text{\AA}^2$, $\sum r = (-28.70, -28.70, -6.37) \text{\AA}$



(c) C; final $\Omega = 115.80 \text{\AA}^2$, $\sum r = (-35.89, -35.88, -9.56) \text{\AA}$

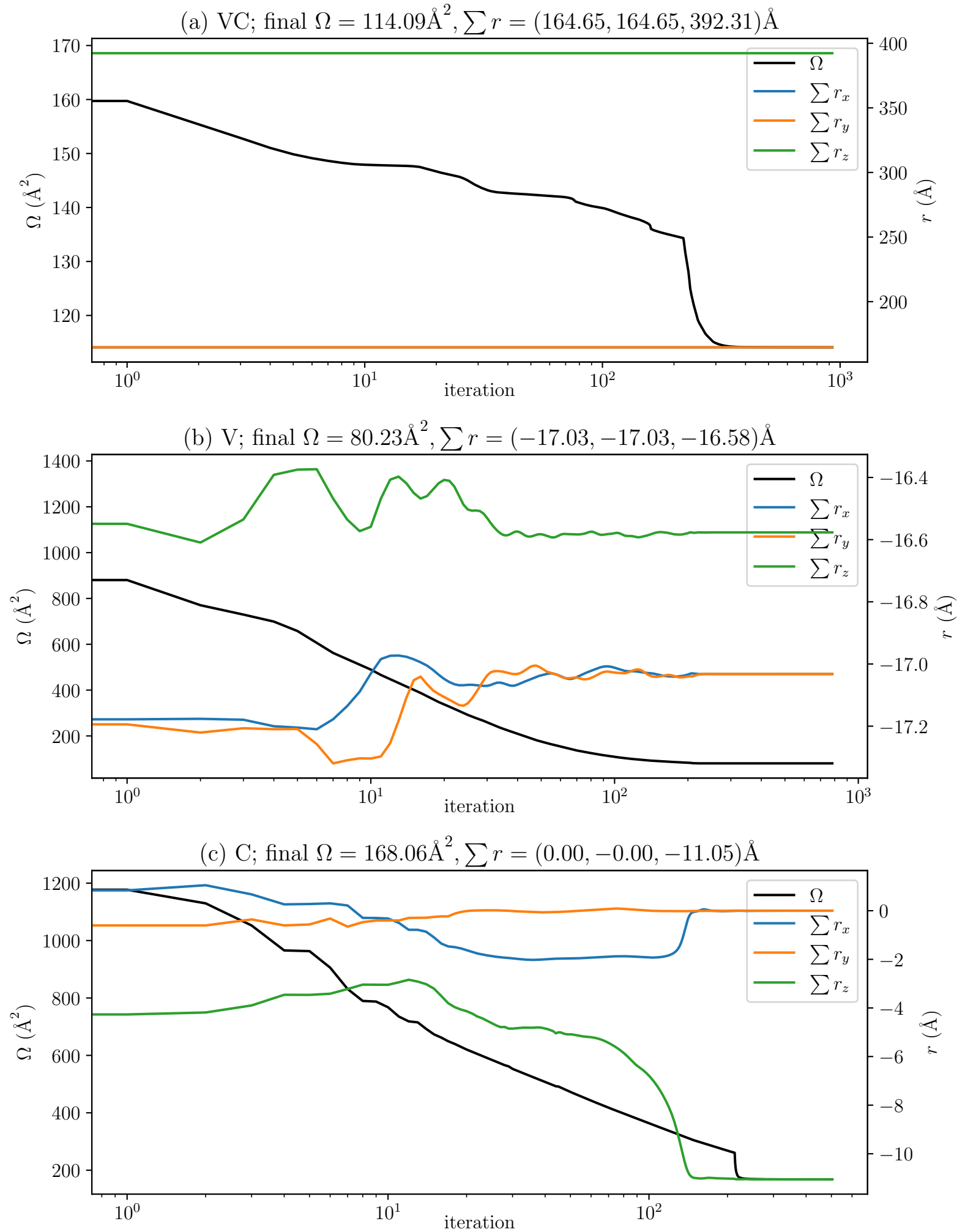


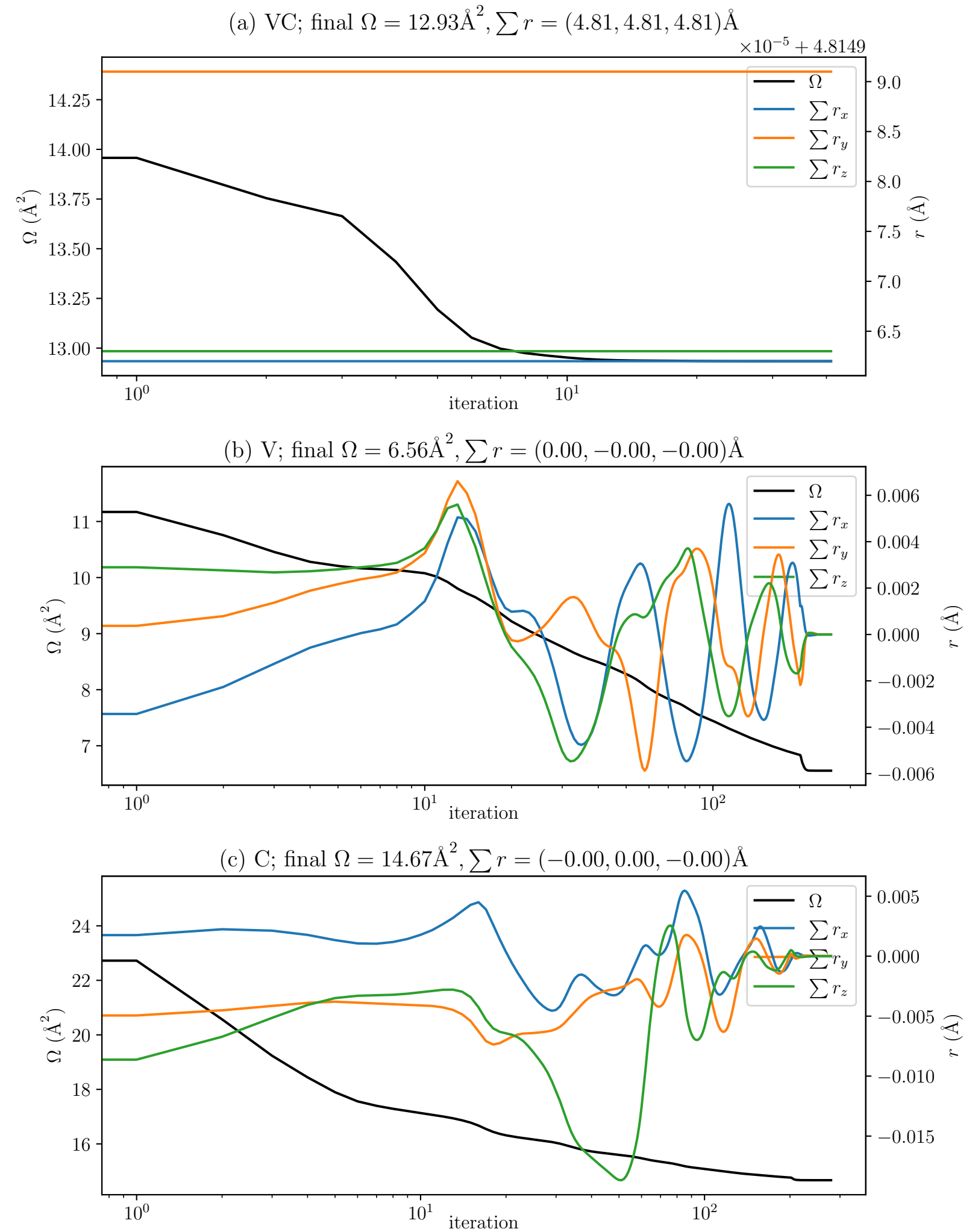
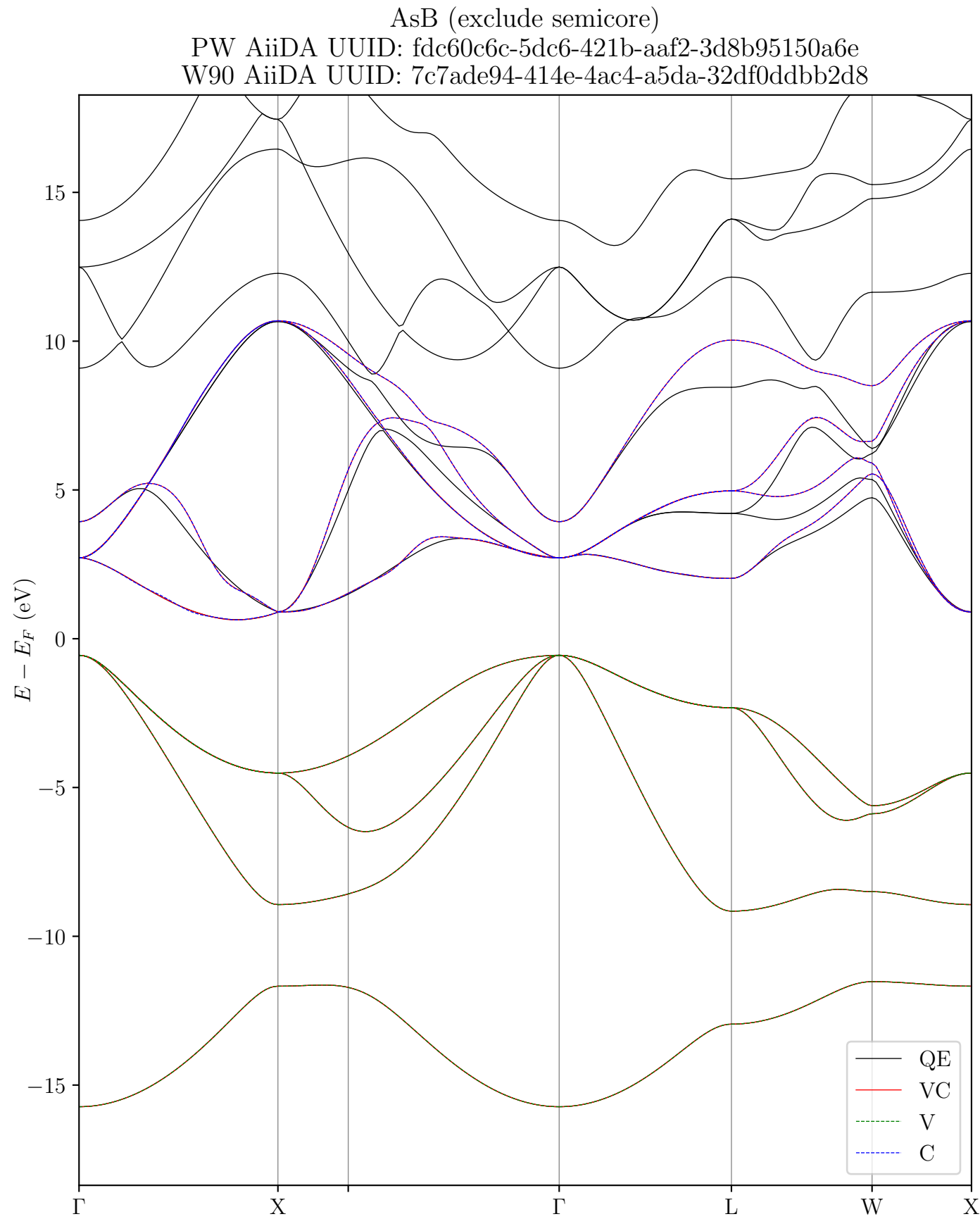
As₈Si₄Zn₄ (exclude semicore)
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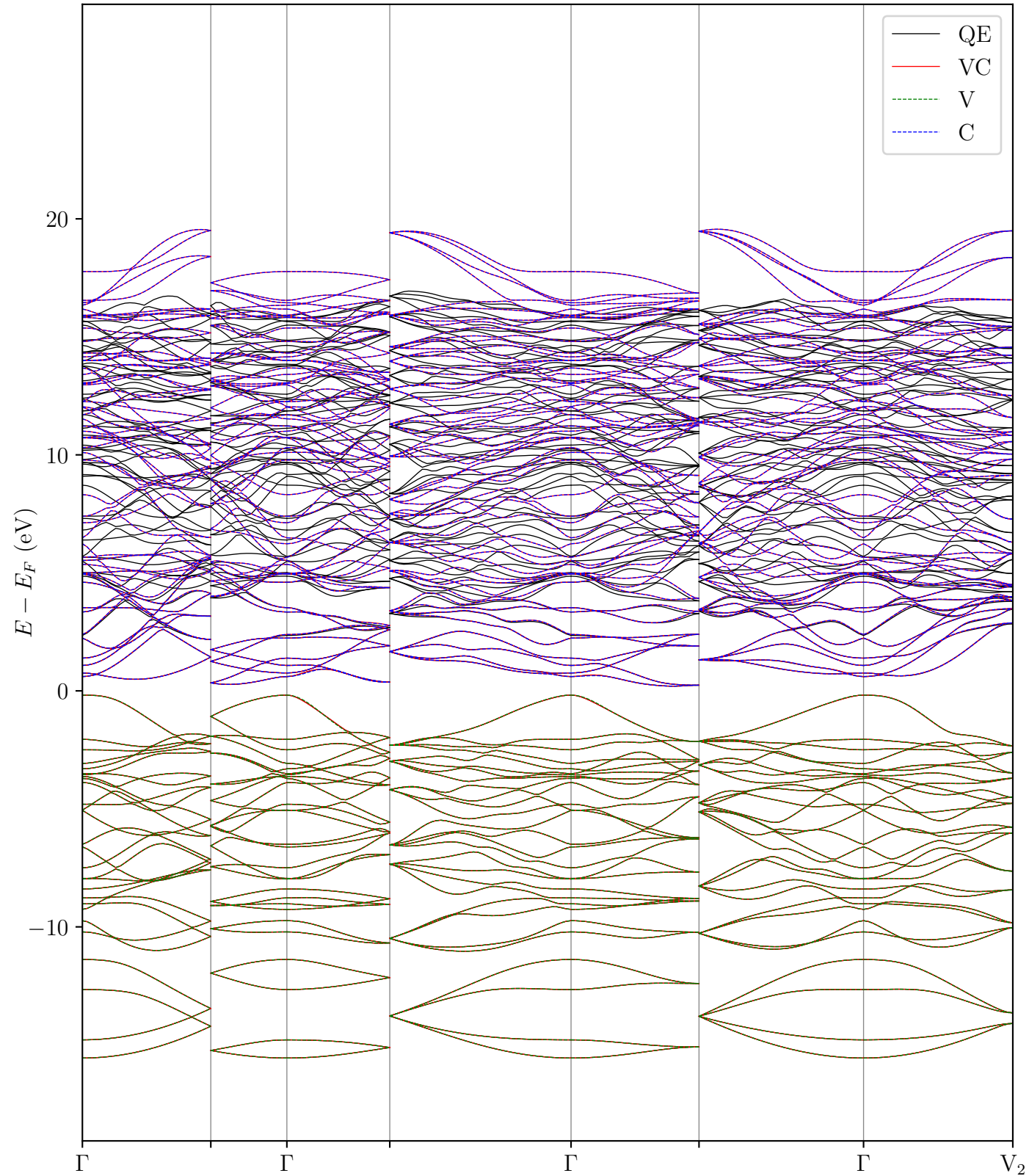
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	4.8	1.8	4.2	4.5	14.0	17.6	6.3
η_{max}	55.6	19.3	80.6	81.2	55.6	83.8	80.2





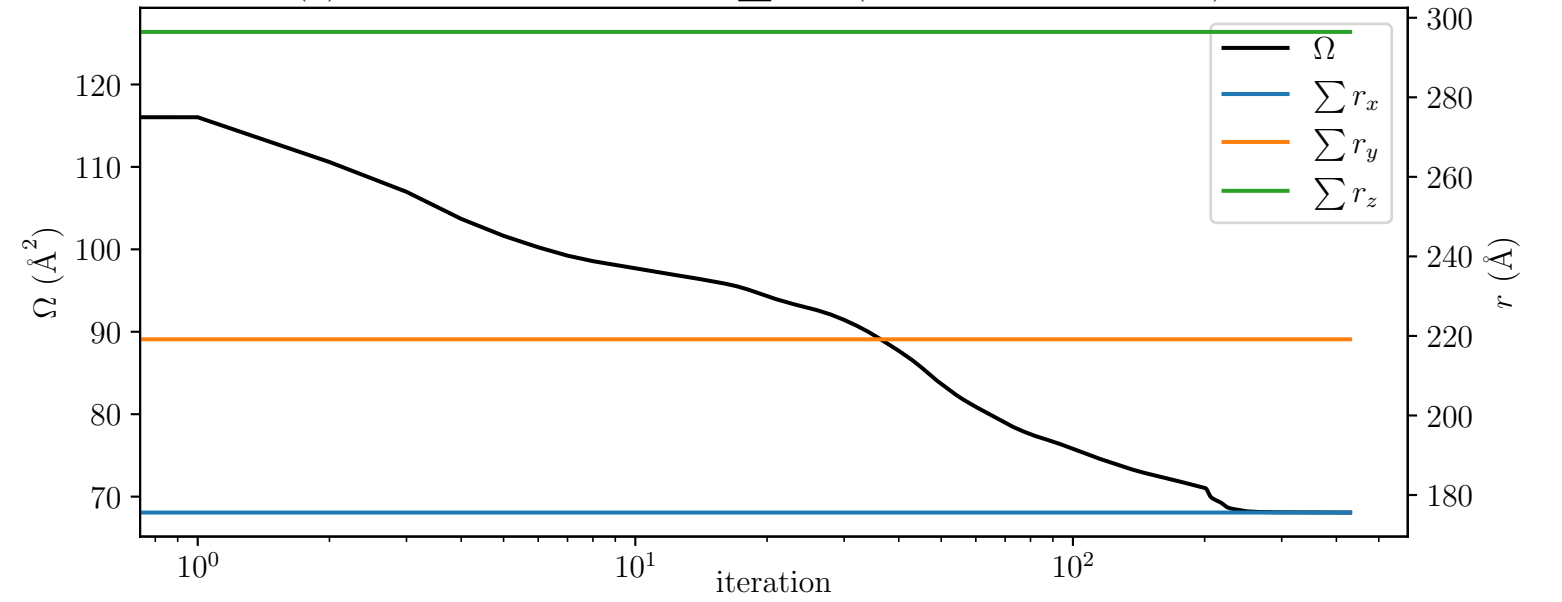
B₁₆Mg₄ (exclude semicore)
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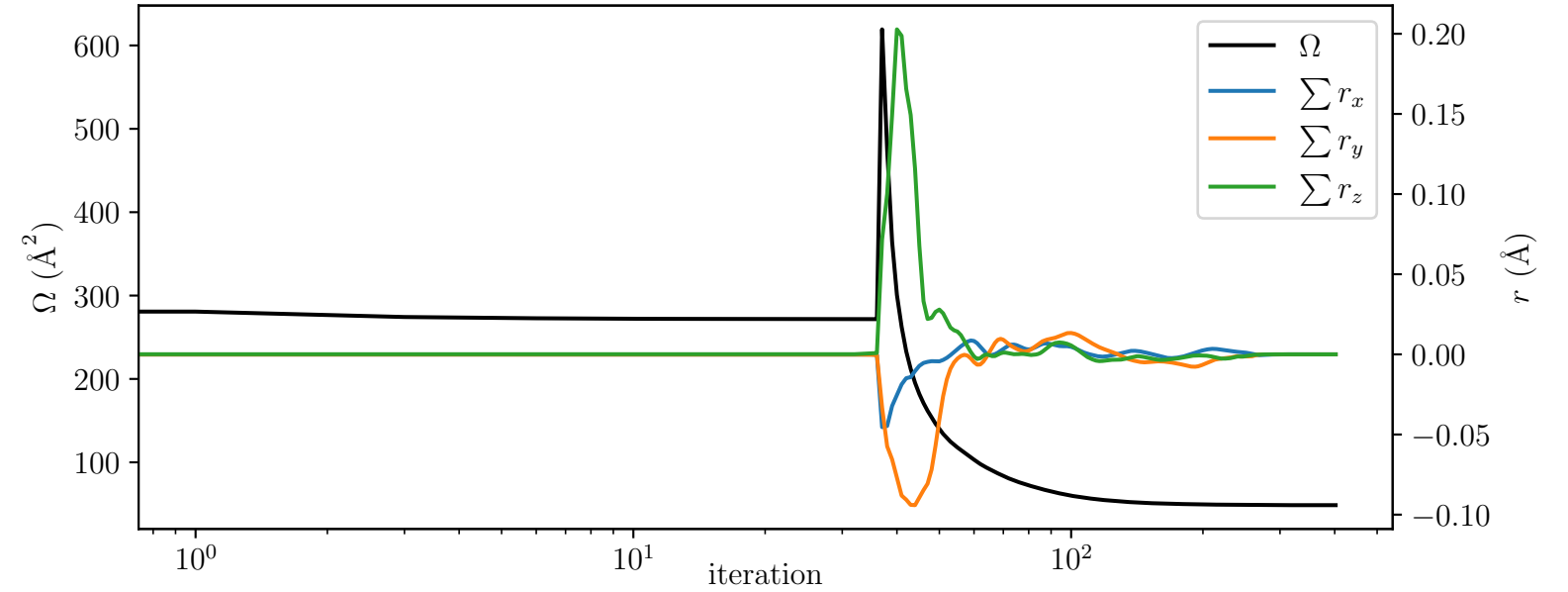
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.9	1.5	1.8	2.5	3.7	6.5	2.5
η_{max}	10.1	8.5	37.6	41.8	10.1	34.0	41.1

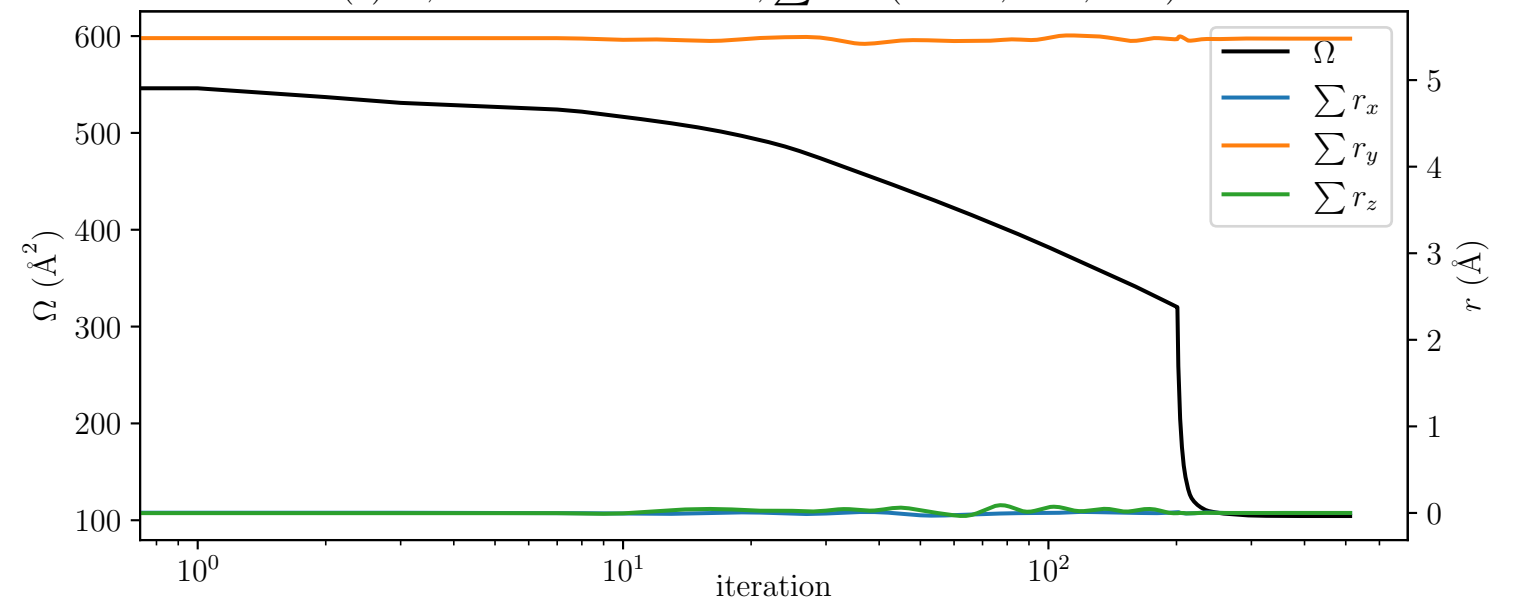
(a) VC; final $\Omega = 68.07 \text{\AA}^2$, $\sum r = (175.60, 219.15, 296.44) \text{\AA}$

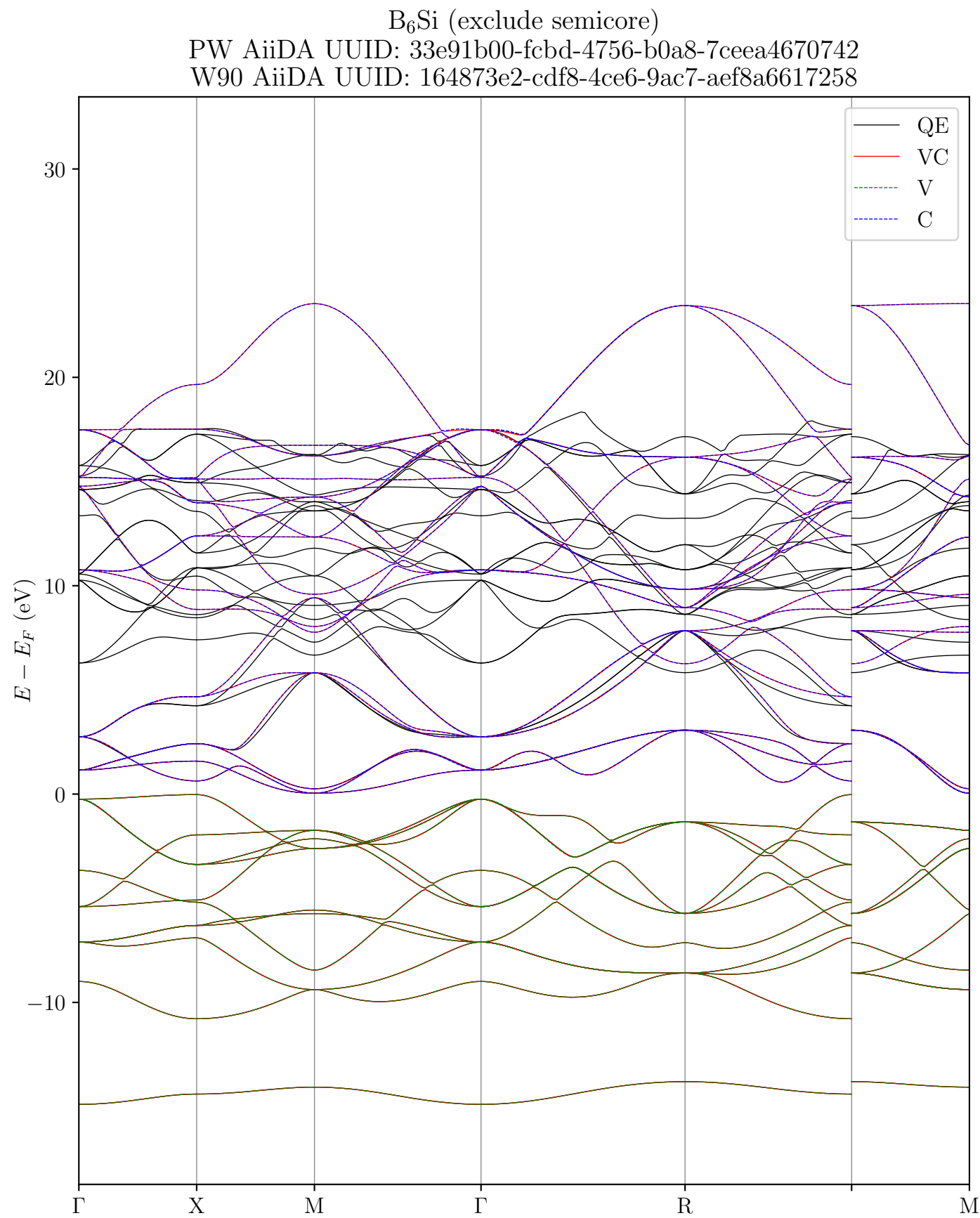


(b) V; final $\Omega = 48.60 \text{\AA}^2$, $\sum r = (0.00, -0.00, 0.00) \text{\AA}$

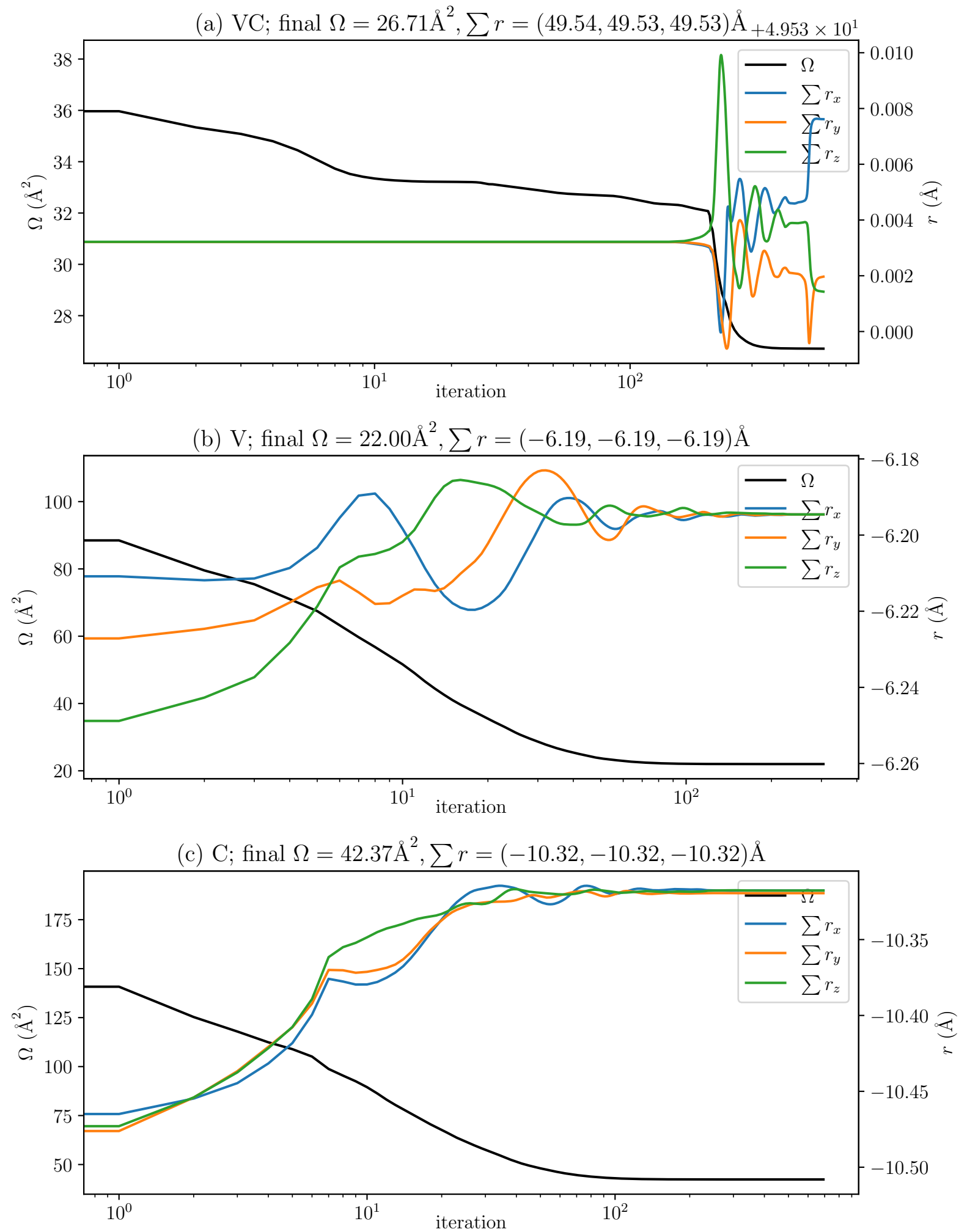


(c) C; final $\Omega = 104.35 \text{\AA}^2$, $\sum r = (-0.00, 5.48, 0.00) \text{\AA}$

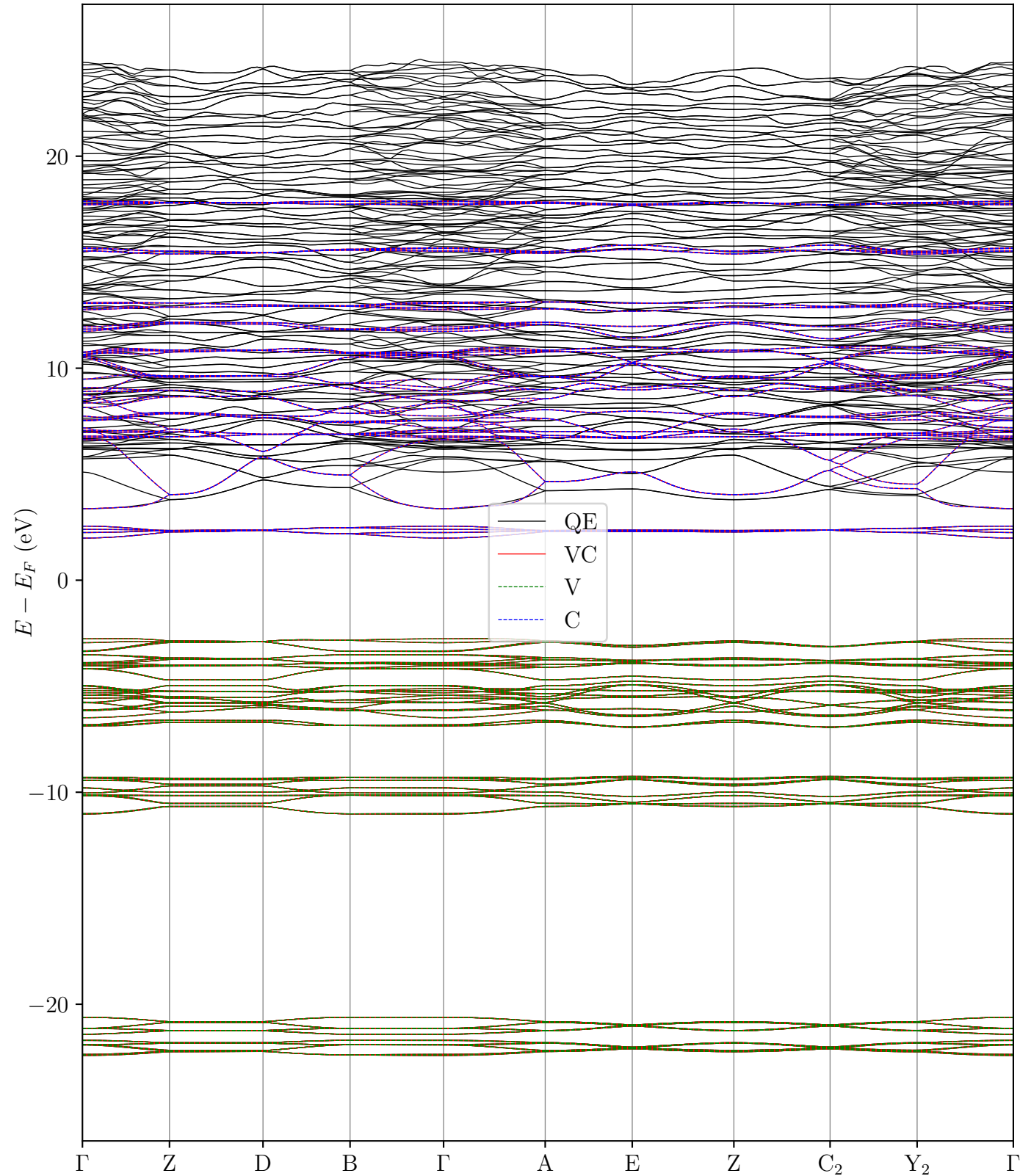




	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	2.5	2.0	4.4	4.3	4.1	7.9	5.9
η_{max}	22.0	14.6	28.4	28.7	22.0	30.0	56.6

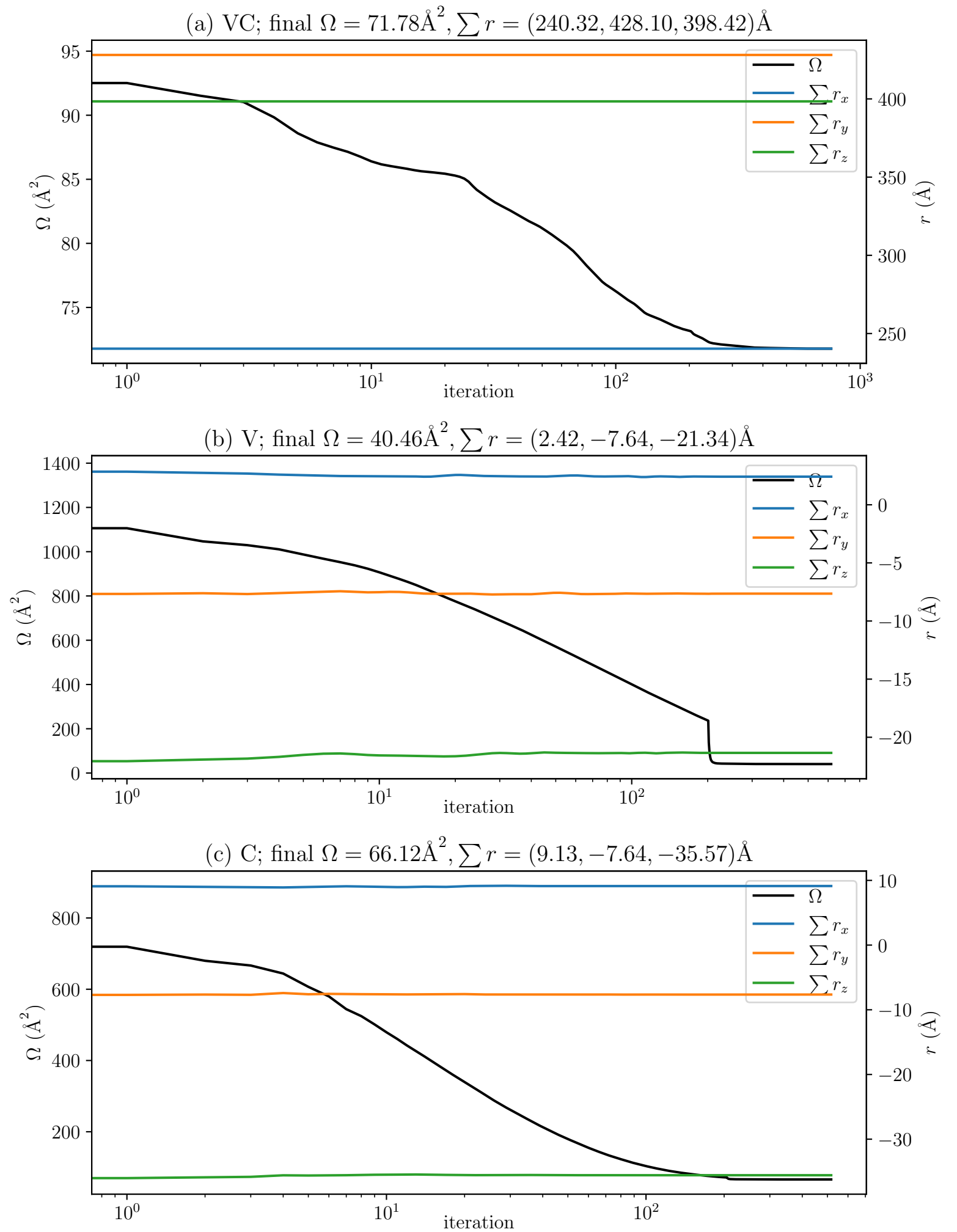


B₈H₁₆O₁₆ (exclude semicore)
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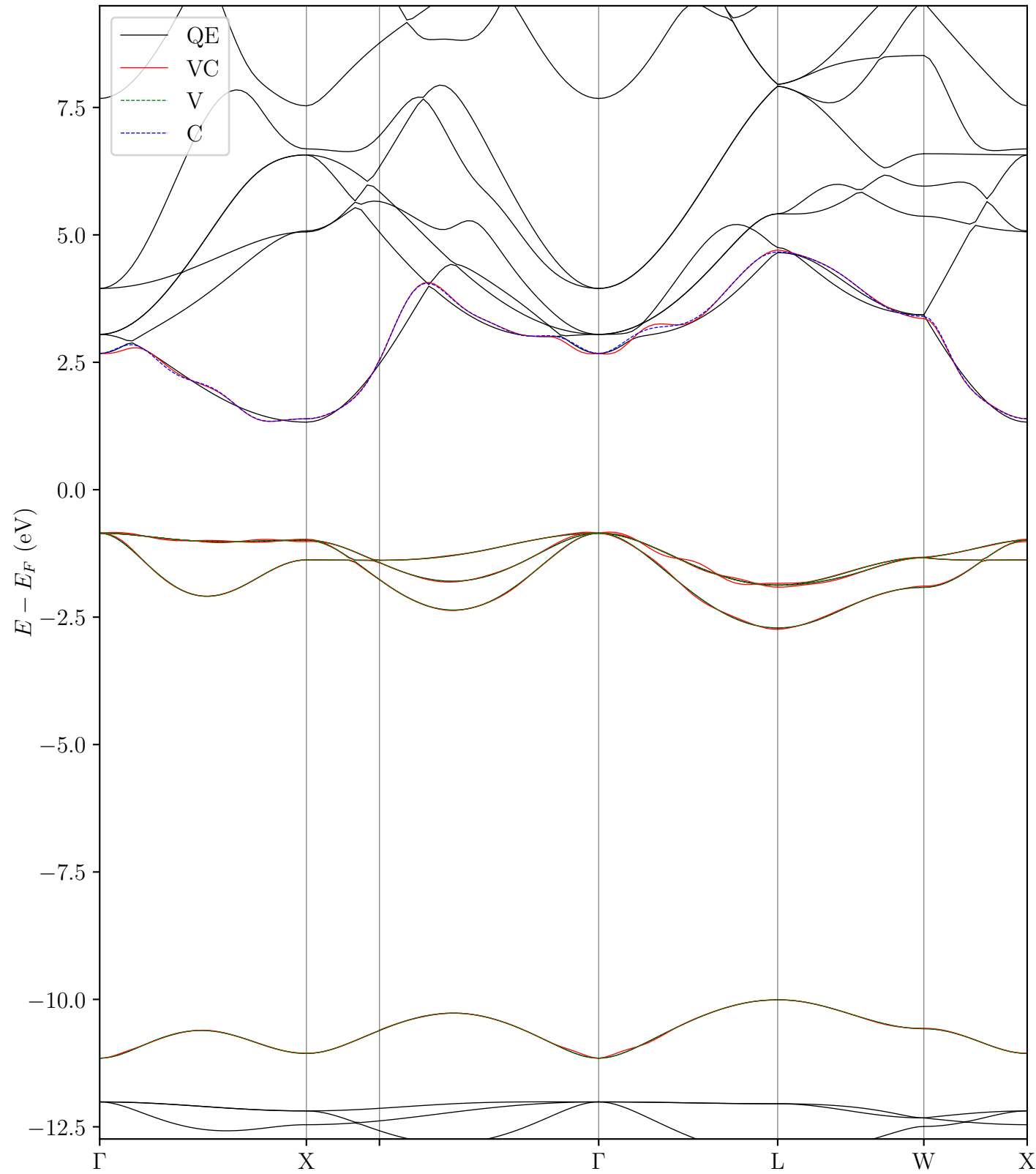


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.3	0.3	0.0	0.3	1.6	1.7	0.9
η_{max}	2.3	2.3	0.0	2.3	1.4	1.4	5.1

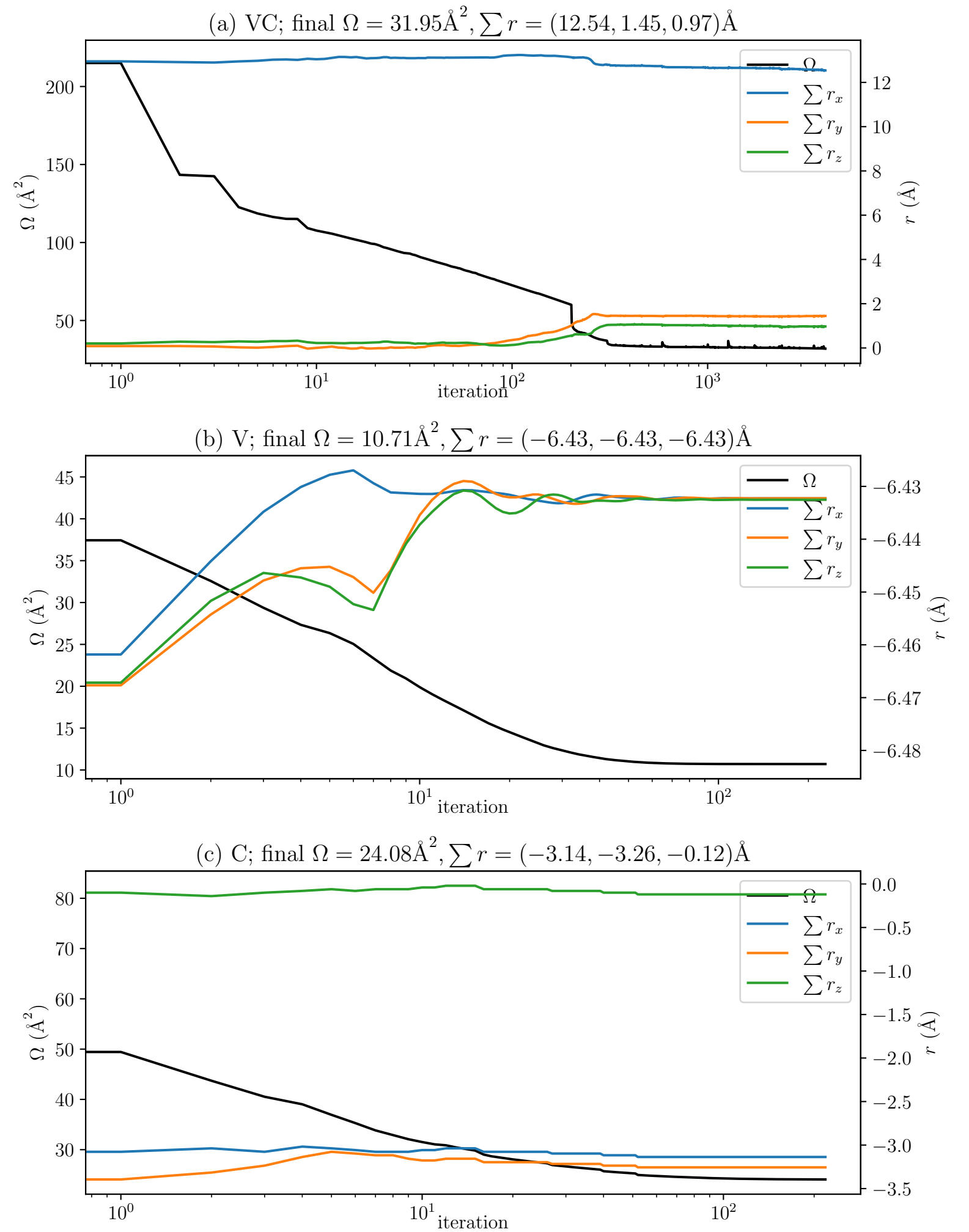


BaS (exclude semicore)
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W90 AiiDA UUID: fbe5e4d1-b9b8-4c08-8583-575a7830c403



band distance (meV)

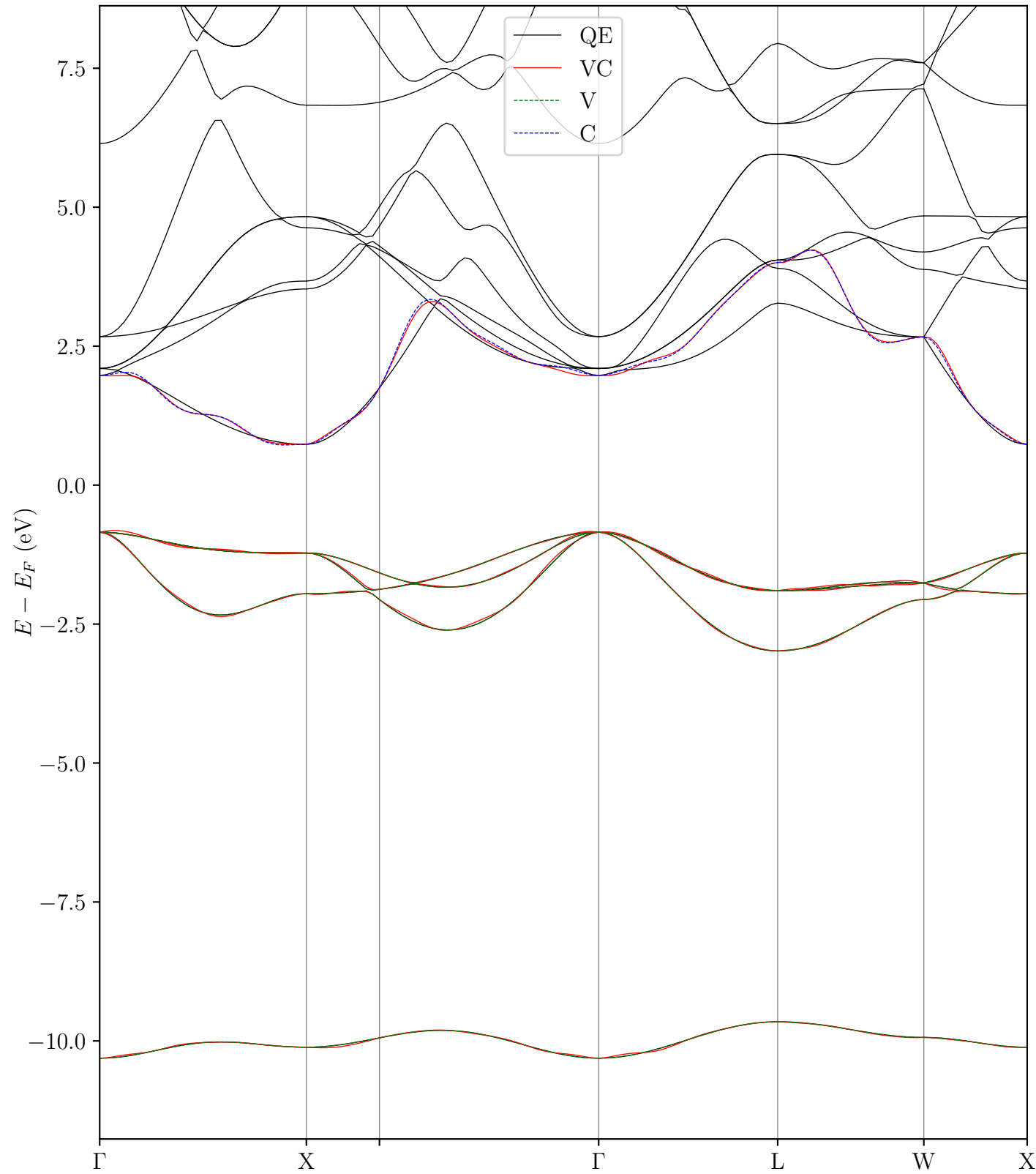
	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	20.2	15.7	0.5	15.8	57.8	58.6	28.4
η_{max}	102.0	83.0	2.6	82.8	102.0	98.6	95.8



BaTe (exclude semicore)

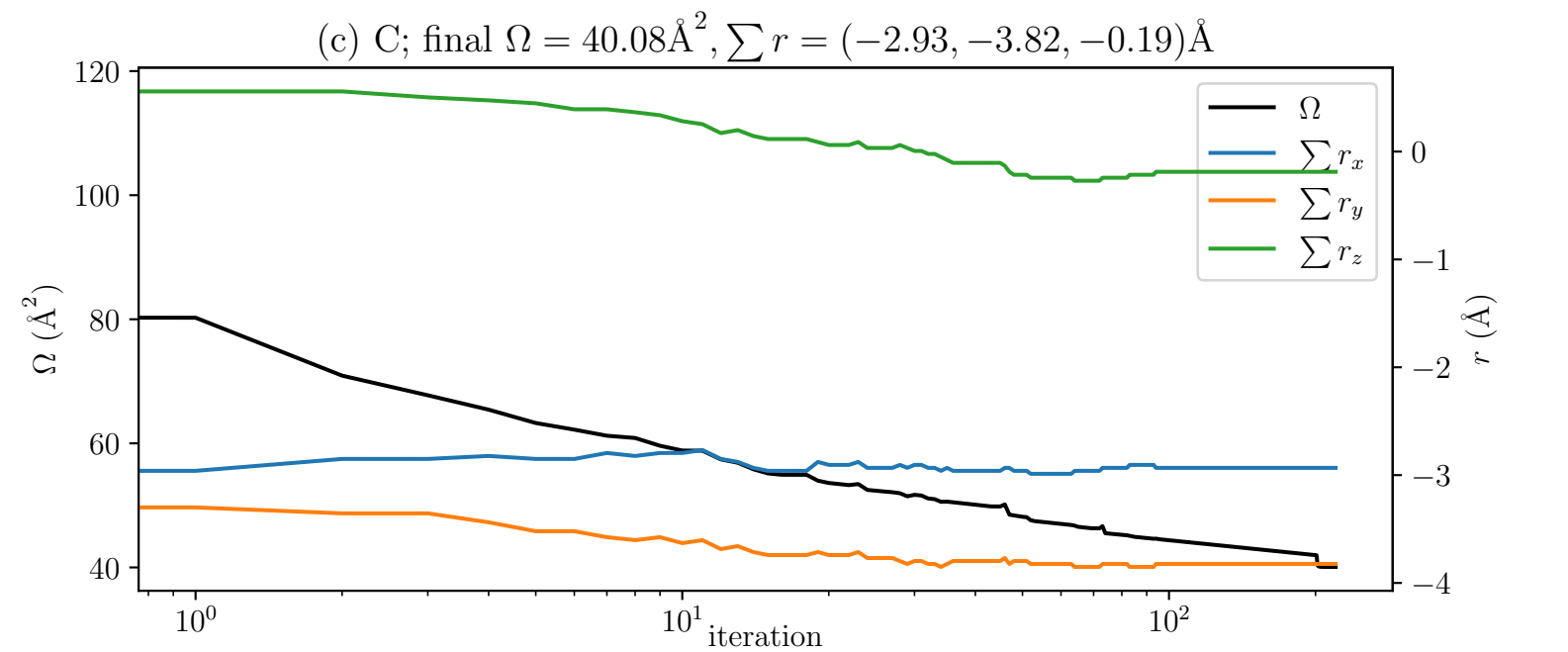
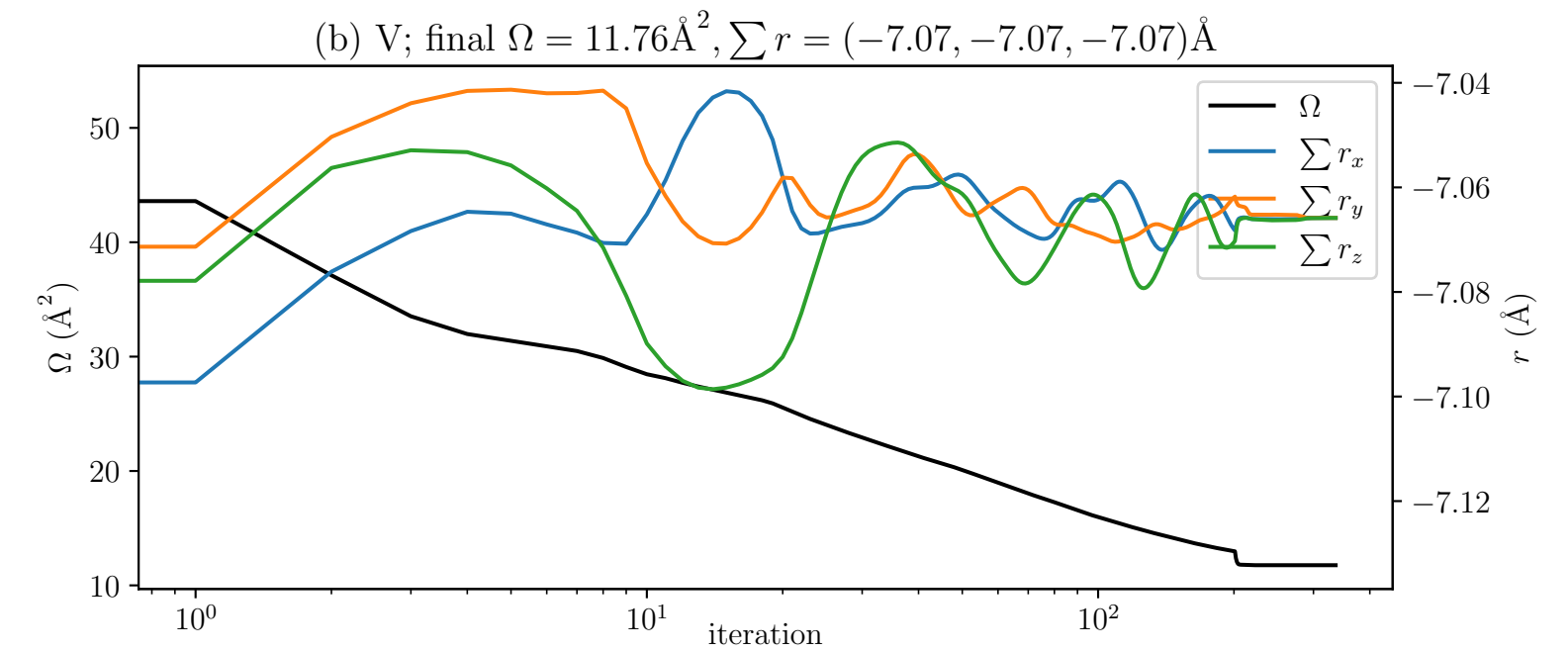
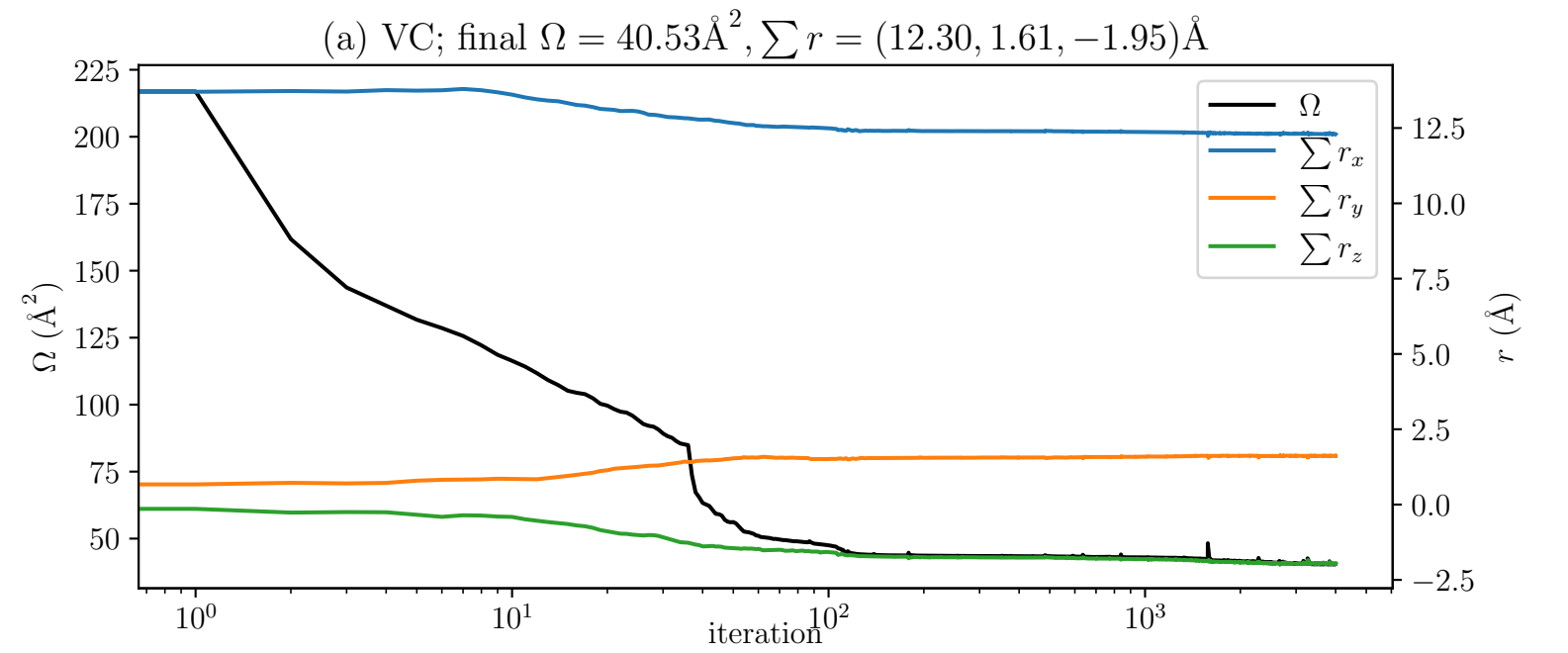
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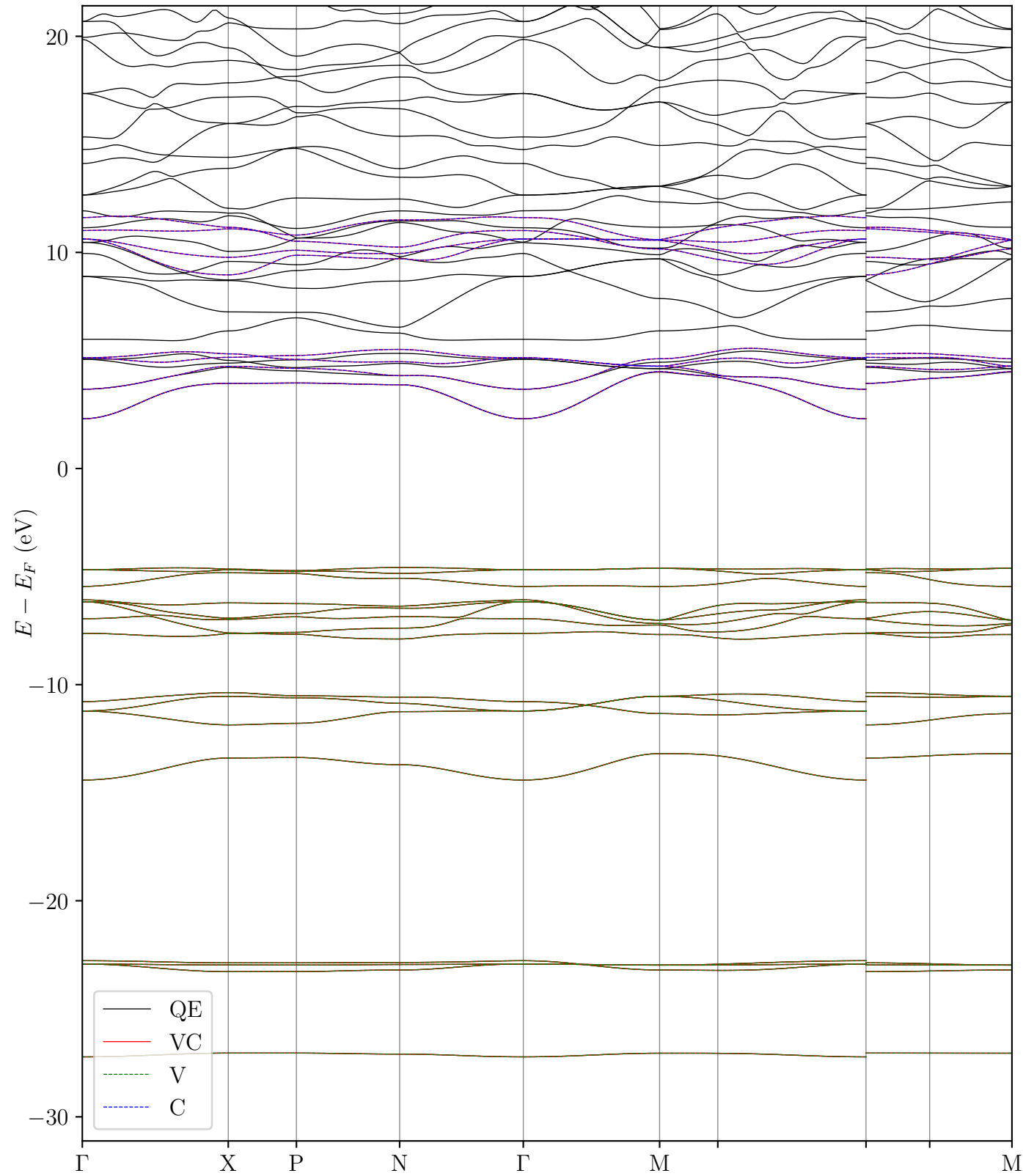


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	24.7	15.5	1.1	15.6	64.2	61.7	26.1
η_{max}	128.0	55.7	7.2	54.4	128.0	134.6	77.0



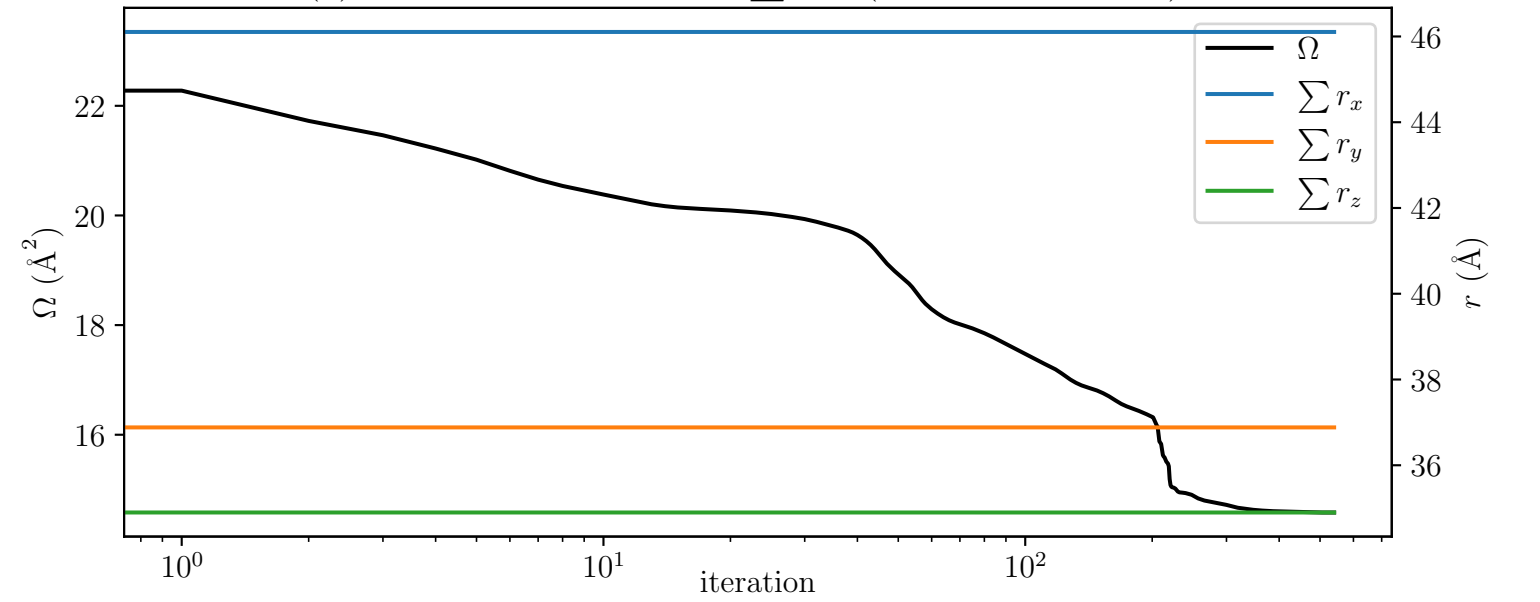
BeO₄S (exclude semicore)
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 W90 AiiDA UUID: 7b751387-5e6a-408f-adb4-87bd60918e24



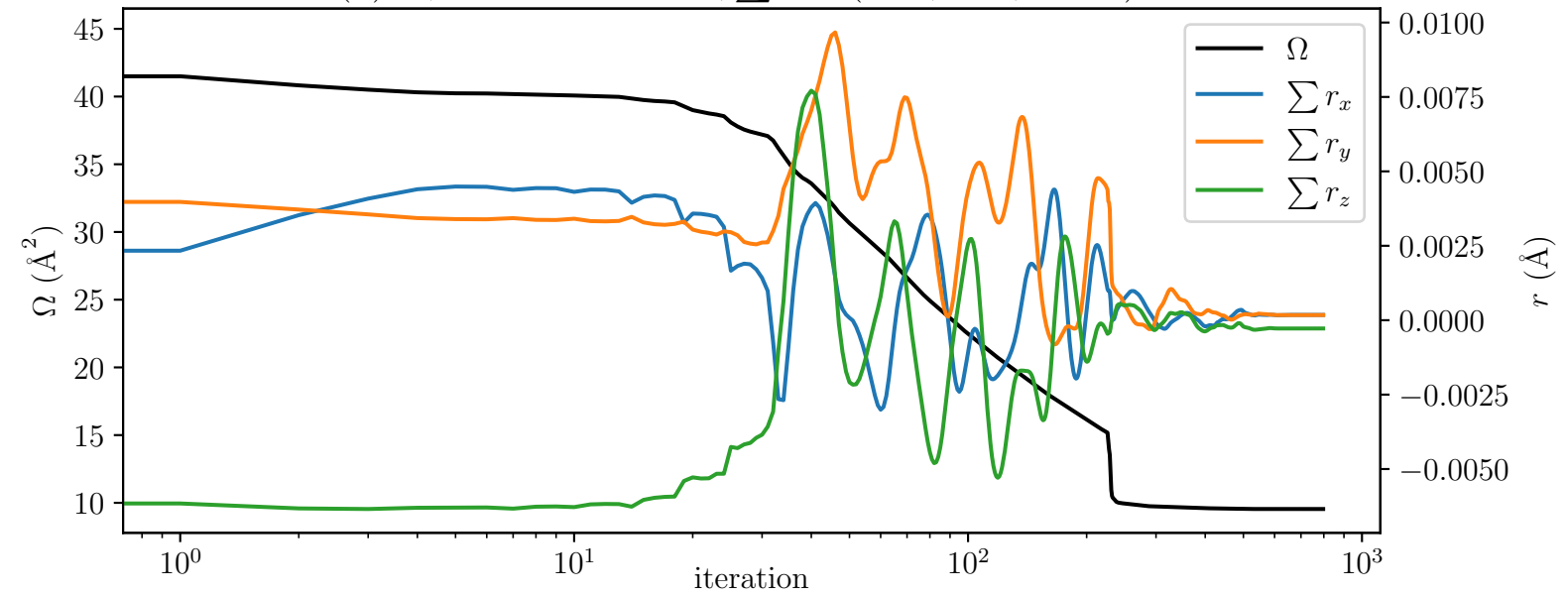
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.2	0.2	0.0	0.2	1.0	1.0	0.6
η_{max}	1.4	1.4	0.0	1.4	0.1	0.1	2.3

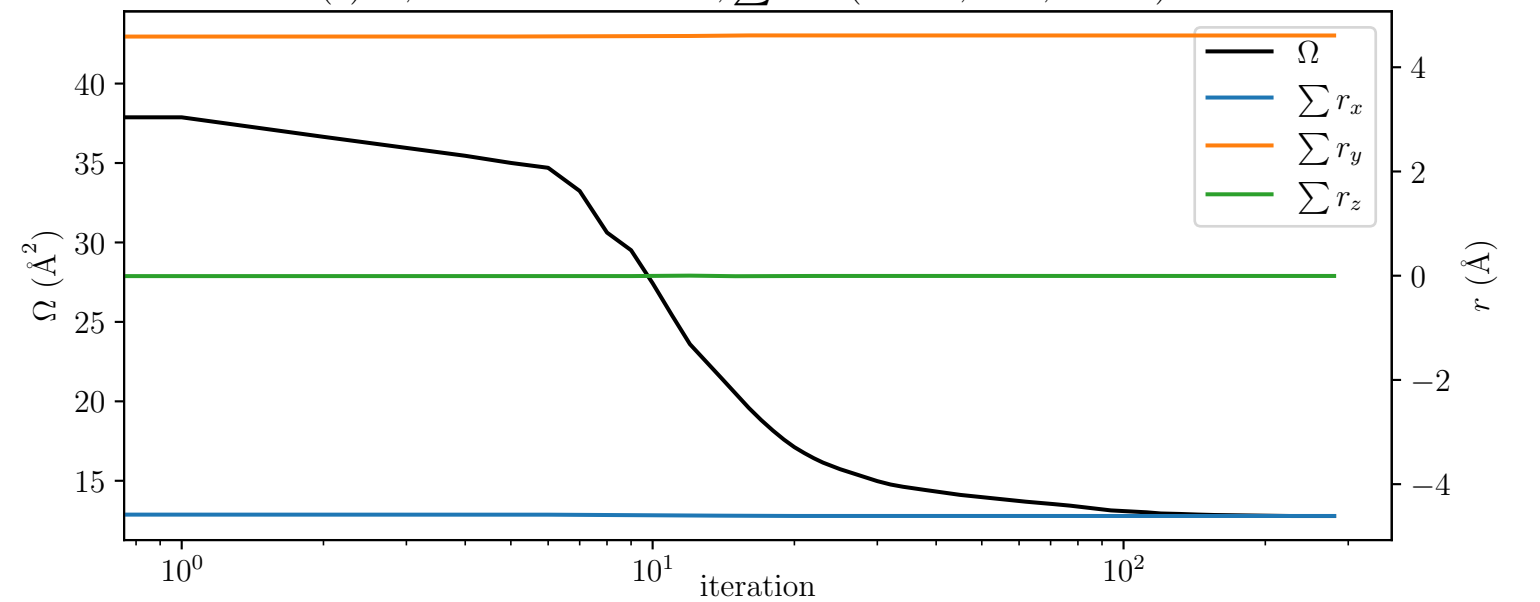
(a) VC; final $\Omega = 14.58 \text{ \AA}^2$, $\sum r = (46.11, 36.88, 34.90) \text{ \AA}$



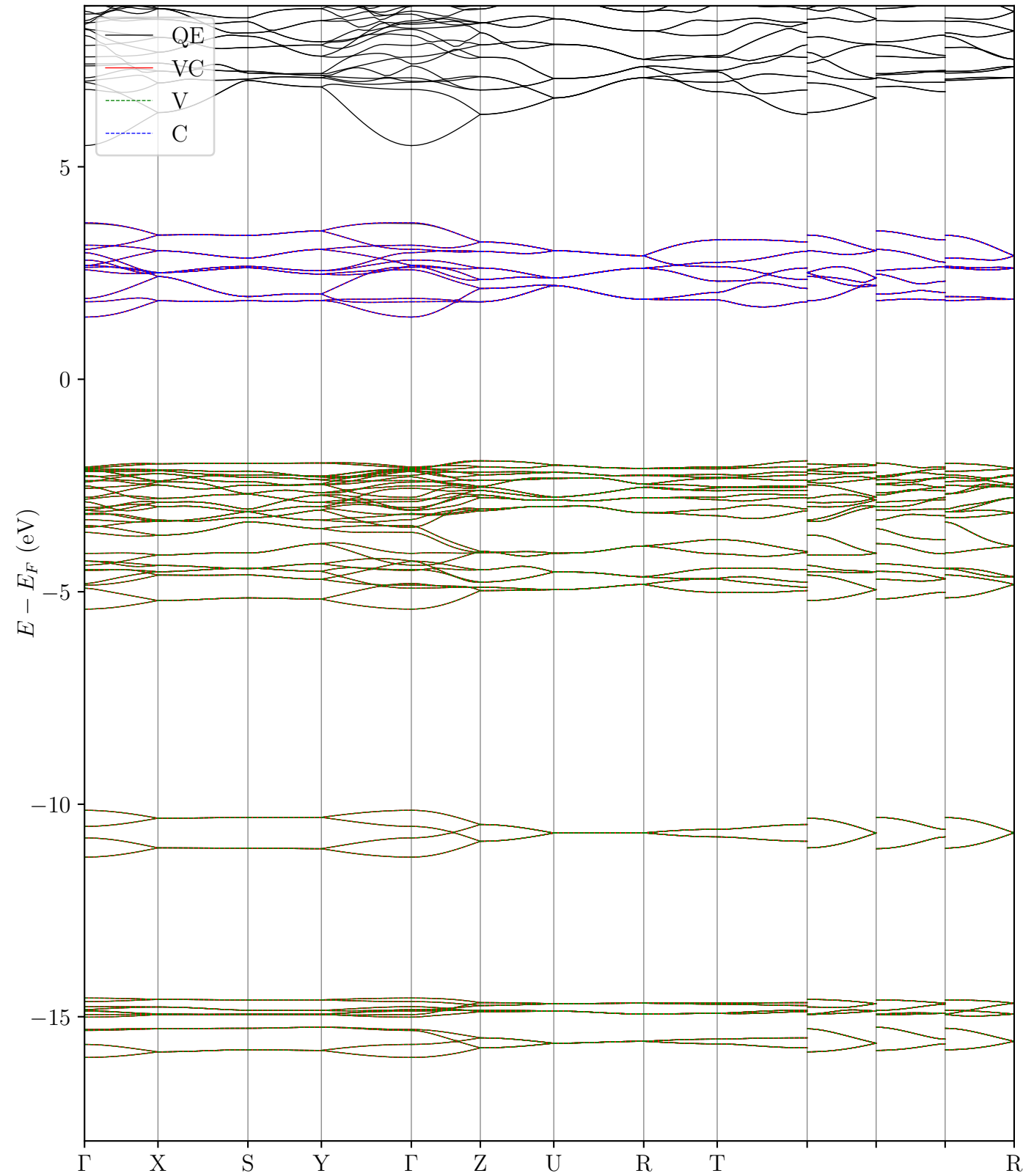
(b) V; final $\Omega = 9.54 \text{ \AA}^2$, $\sum r = (0.00, 0.00, -0.00) \text{ \AA}$



(c) C; final $\Omega = 12.78 \text{ \AA}^2$, $\sum r = (-4.61, 4.61, -0.00) \text{ \AA}$



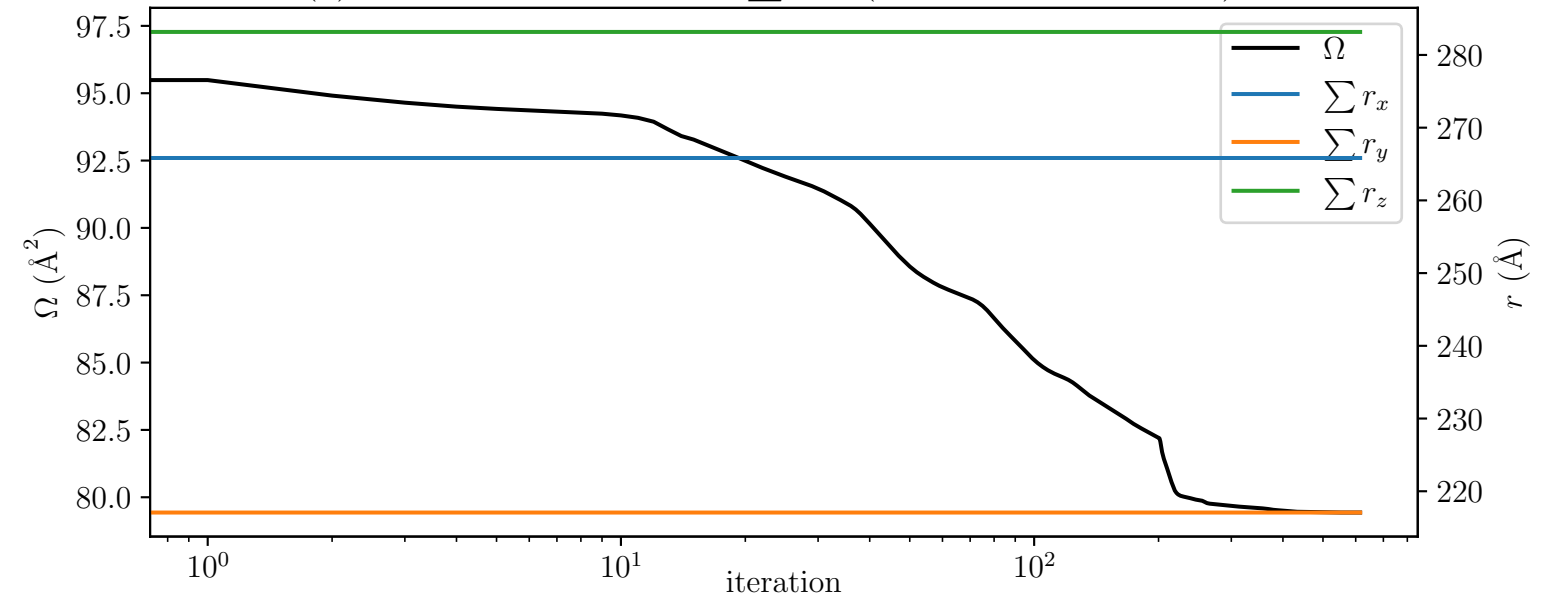
Bi₄Cl₁₂ (exclude semicore)
PW AiiDA UUID: 68744737-5ecd-4ab4-ac36-671454cef582
W90 AiiDA UUID: 58929f18-6a9d-4d4d-964c-f9c3267613e5



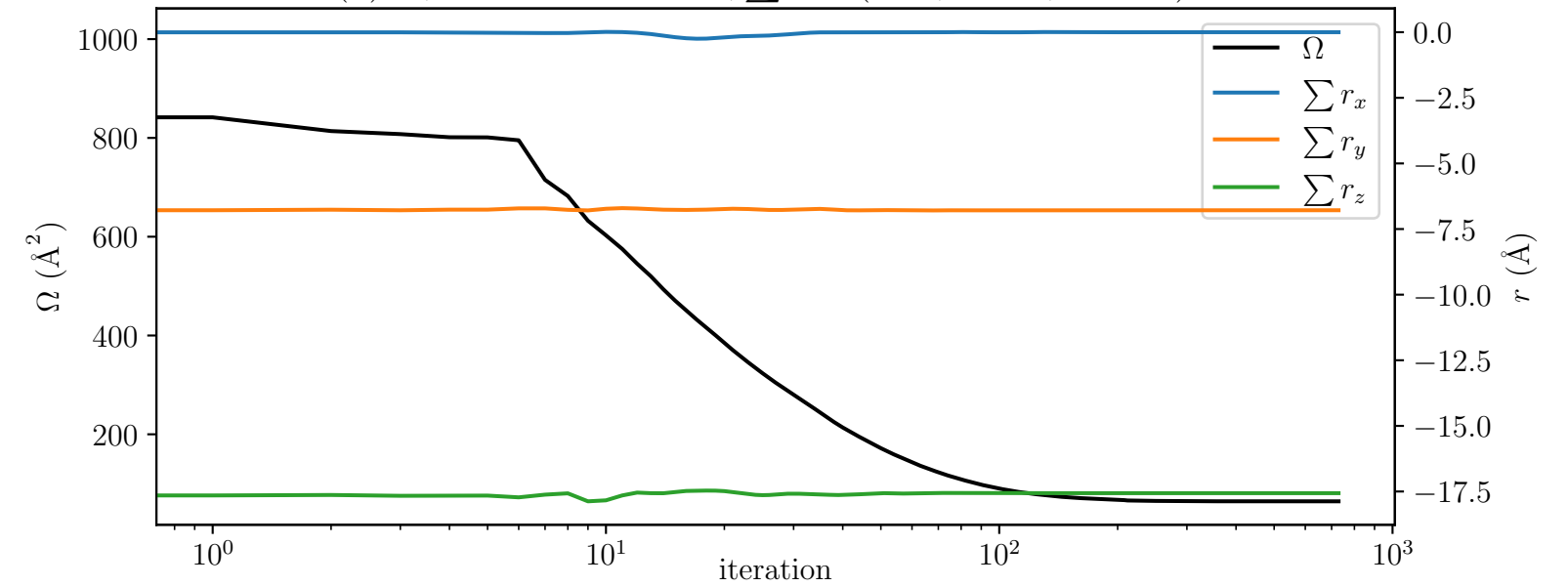
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.1	0.1	0.0	0.1	0.1	0.2	0.2
η_{max}	0.5	0.5	0.4	0.5	0.3	0.5	0.9

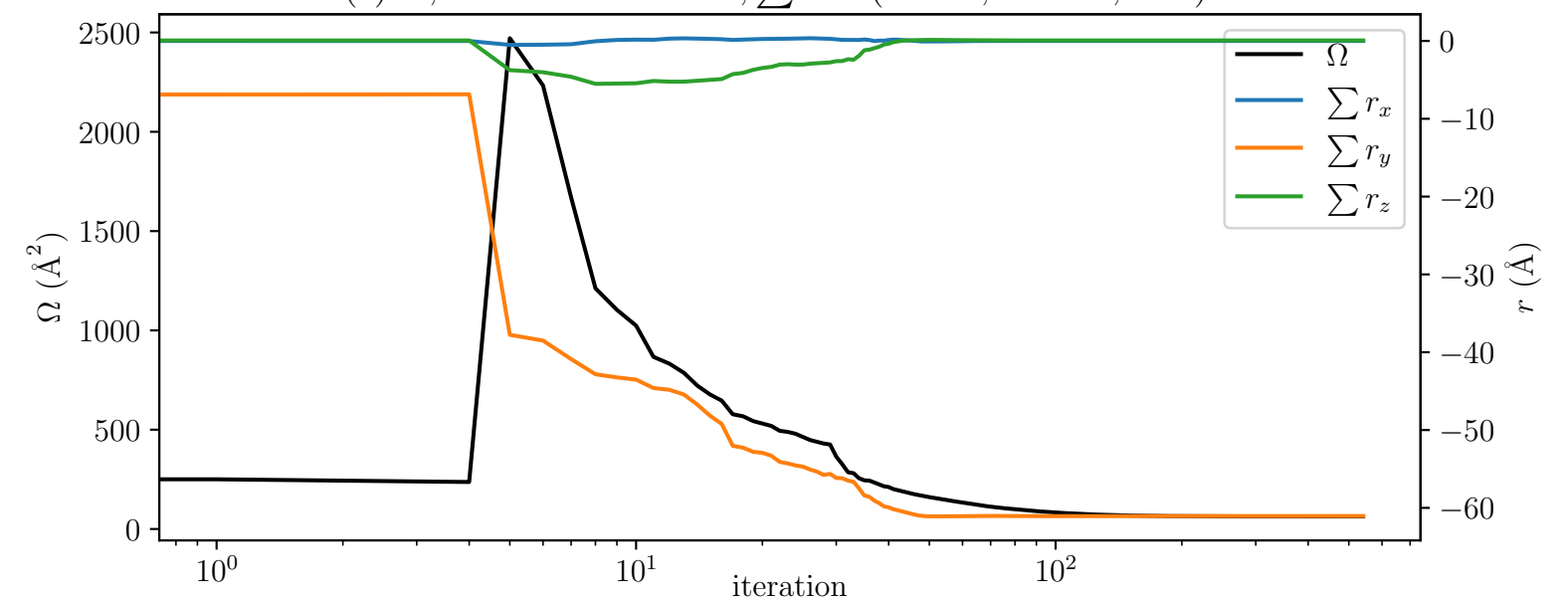
(a) VC; final $\Omega = 79.43 \text{ \AA}^2$, $\sum r = (265.83, 217.07, 283.16) \text{ \AA}$



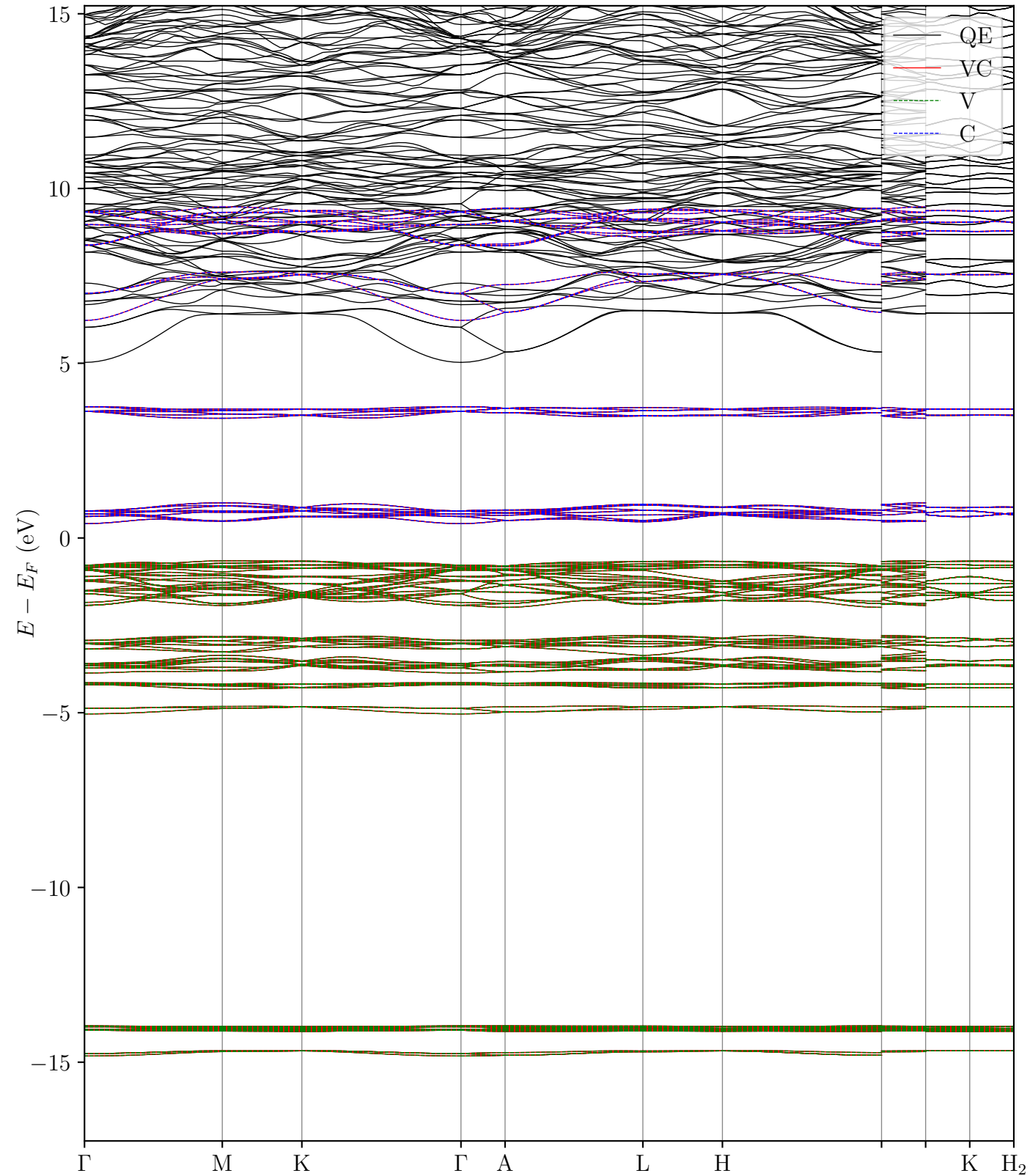
(b) V; final $\Omega = 64.29 \text{ \AA}^2$, $\sum r = (0.00, -6.78, -17.56) \text{ \AA}$



(c) C; final $\Omega = 63.16 \text{ \AA}^2$, $\sum r = (-0.00, -61.05, 0.07) \text{ \AA}$



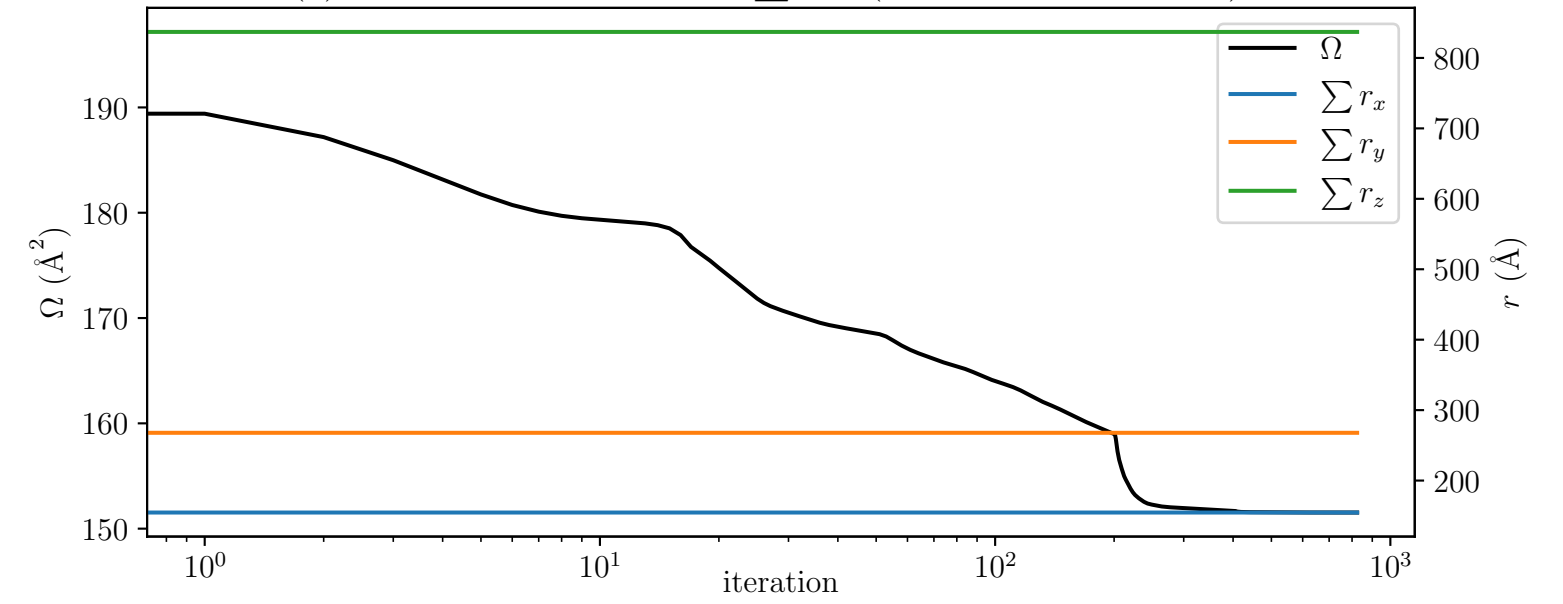
Br₁₈W₃ (exclude semicore)
PW AiiDA UUID: 7b8c7c12-cce7-4ff0-b038-8e7e9ce751cd
W90 AiiDA UUID: 848d64e5-8476-4099-942e-48681d0729a2



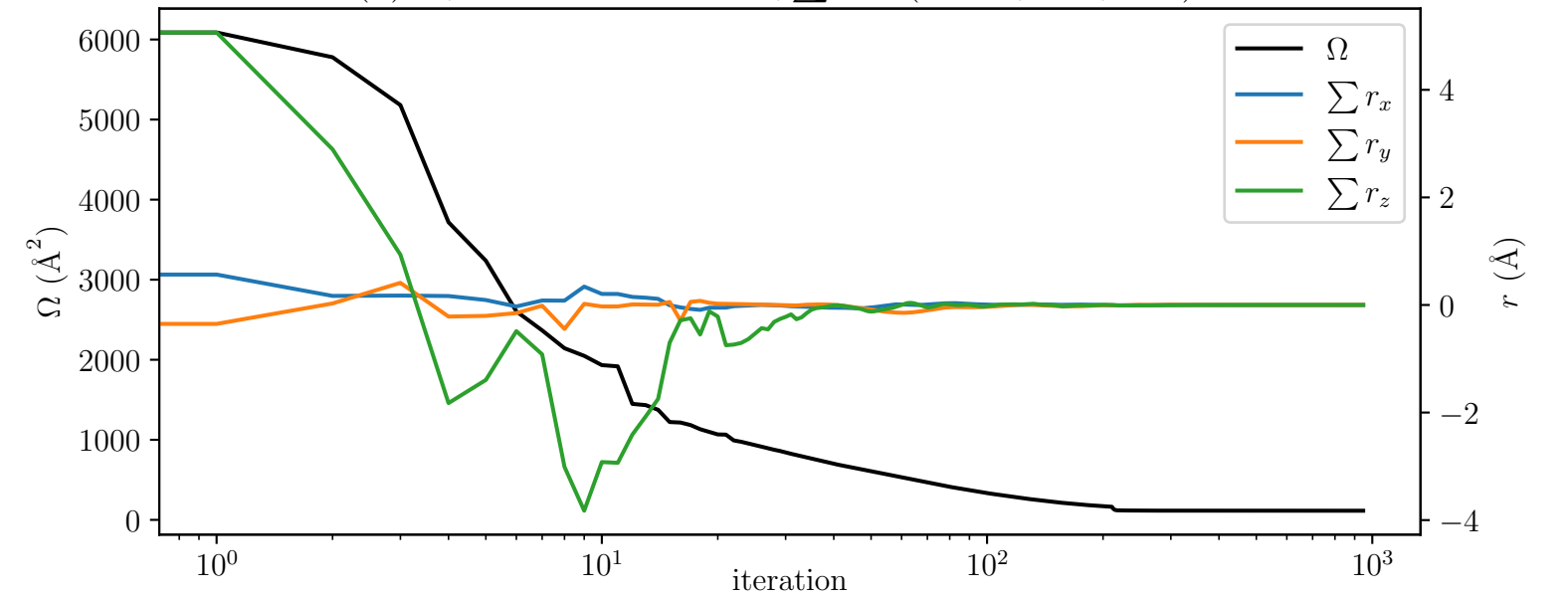
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.1	0.1	0.1	0.1	0.1	0.1	0.3
η_{max}	0.7	0.7	1.4	1.0	0.7	0.9	1.9

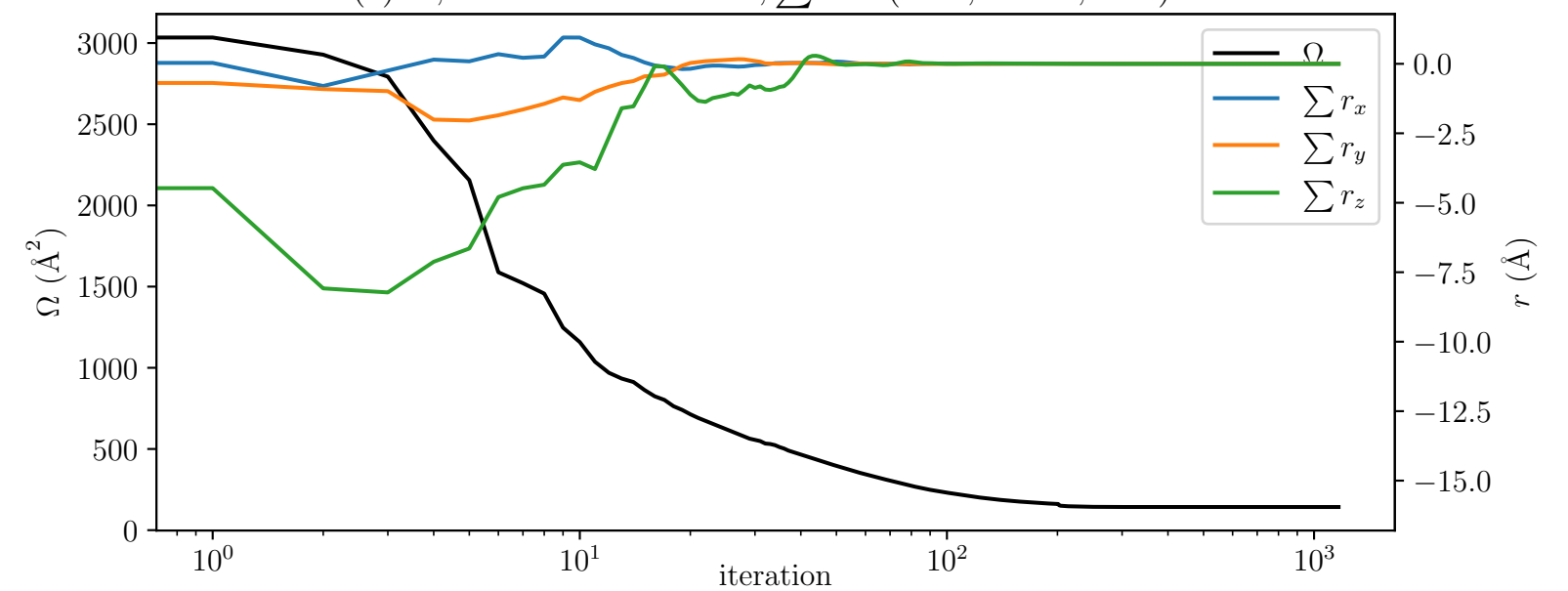
(a) VC; final $\Omega = 151.53 \text{\AA}^2$, $\sum r = (154.62, 267.81, 836.95) \text{\AA}$

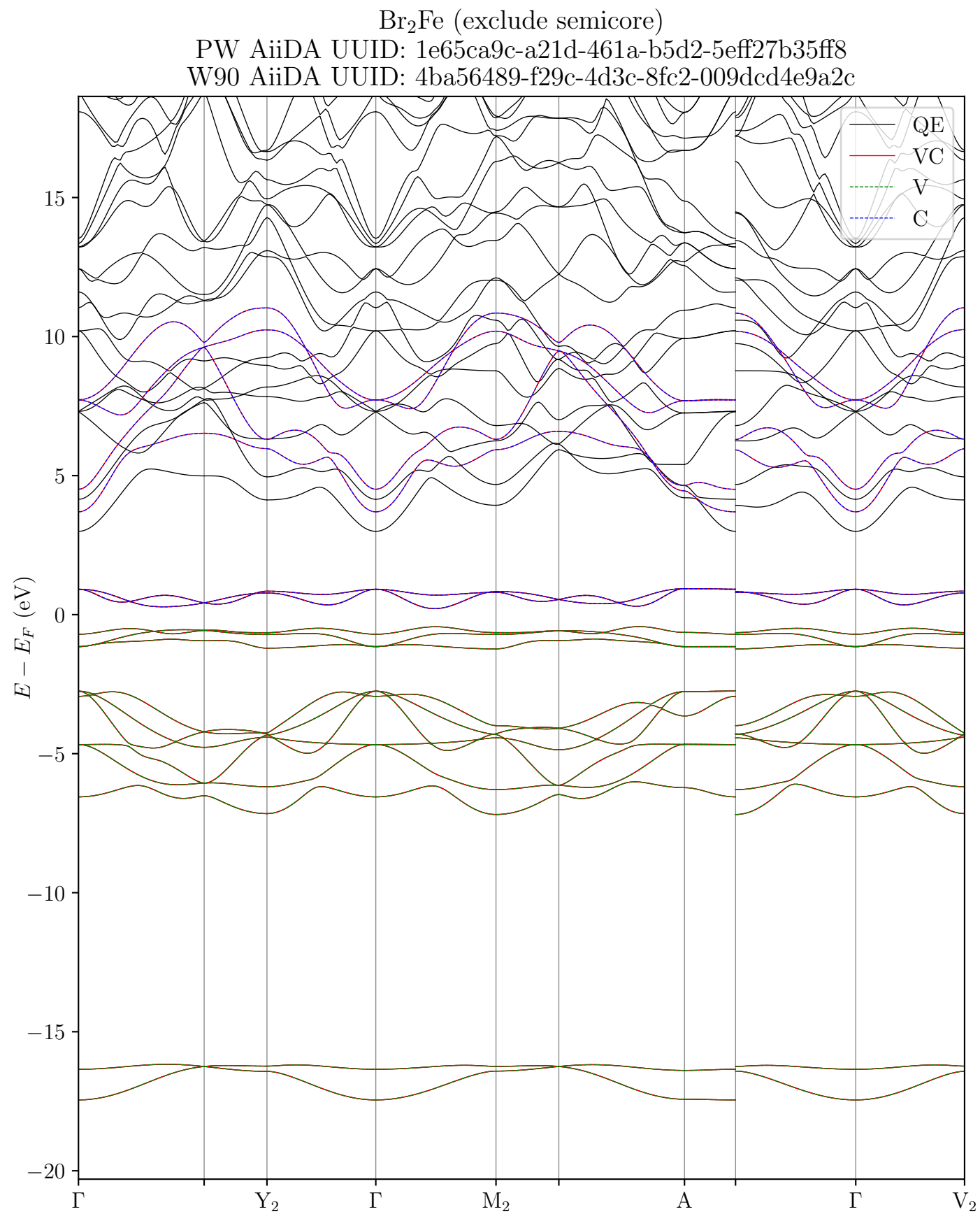


(b) V; final $\Omega = 114.35 \text{\AA}^2$, $\sum r = (-0.00, 0.00, 0.00) \text{\AA}$



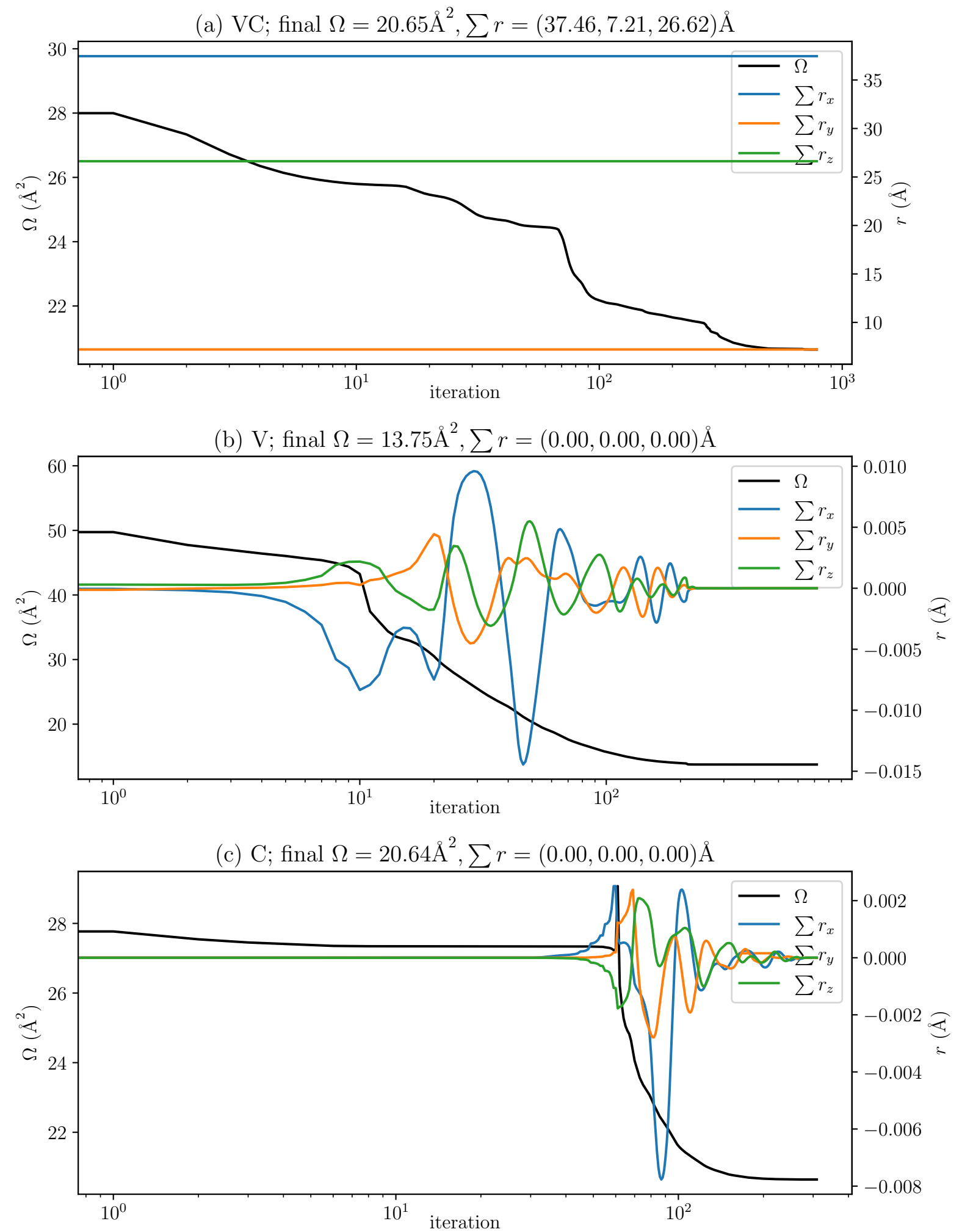
(c) C; final $\Omega = 142.54 \text{\AA}^2$, $\sum r = (0.00, -0.00, 0.00) \text{\AA}$

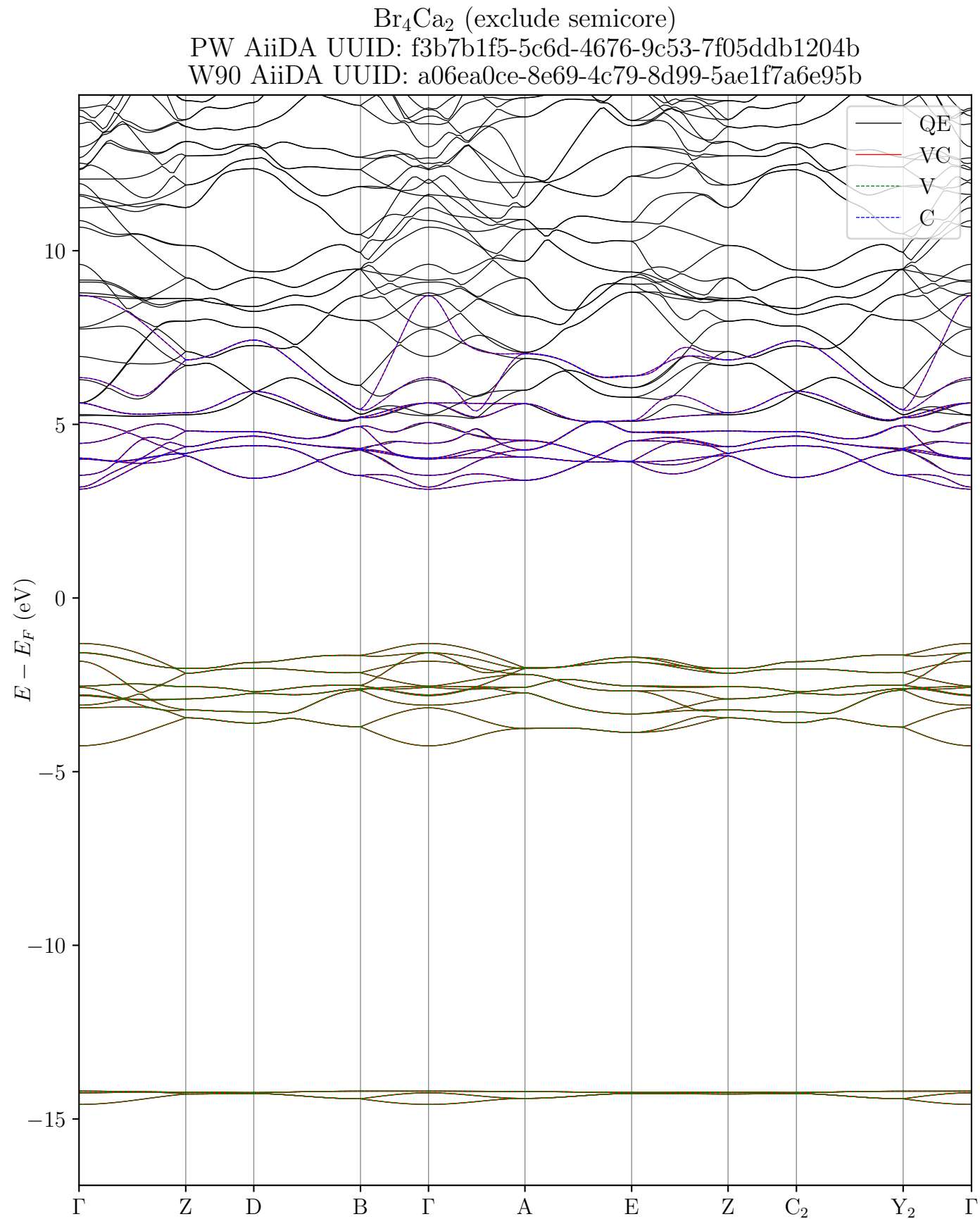




band distance (meV)

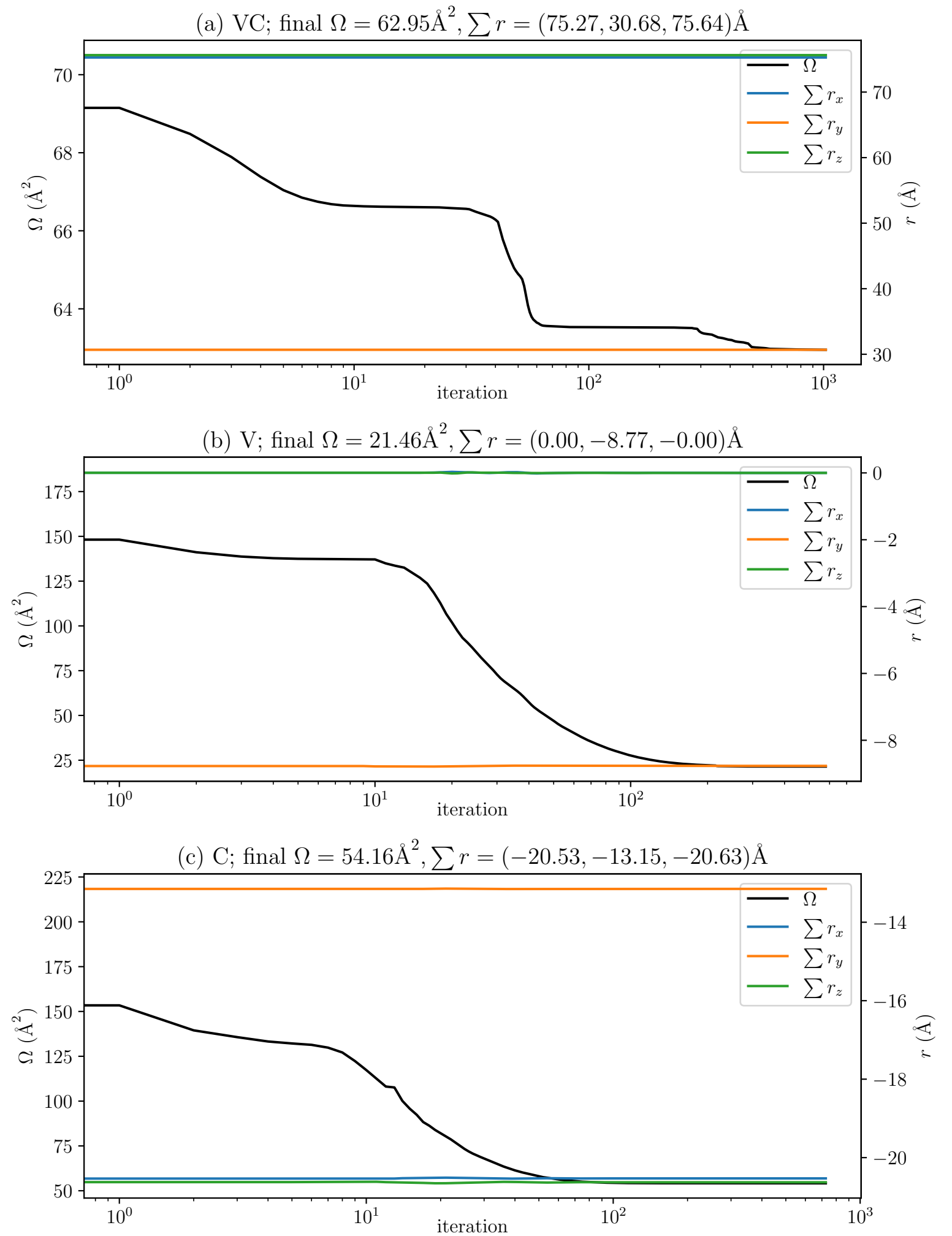
	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.7	0.7	0.1	0.7	0.4	1.7	1.5
η_{max}	4.5	4.5	0.4	4.5	1.3	6.2	8.9



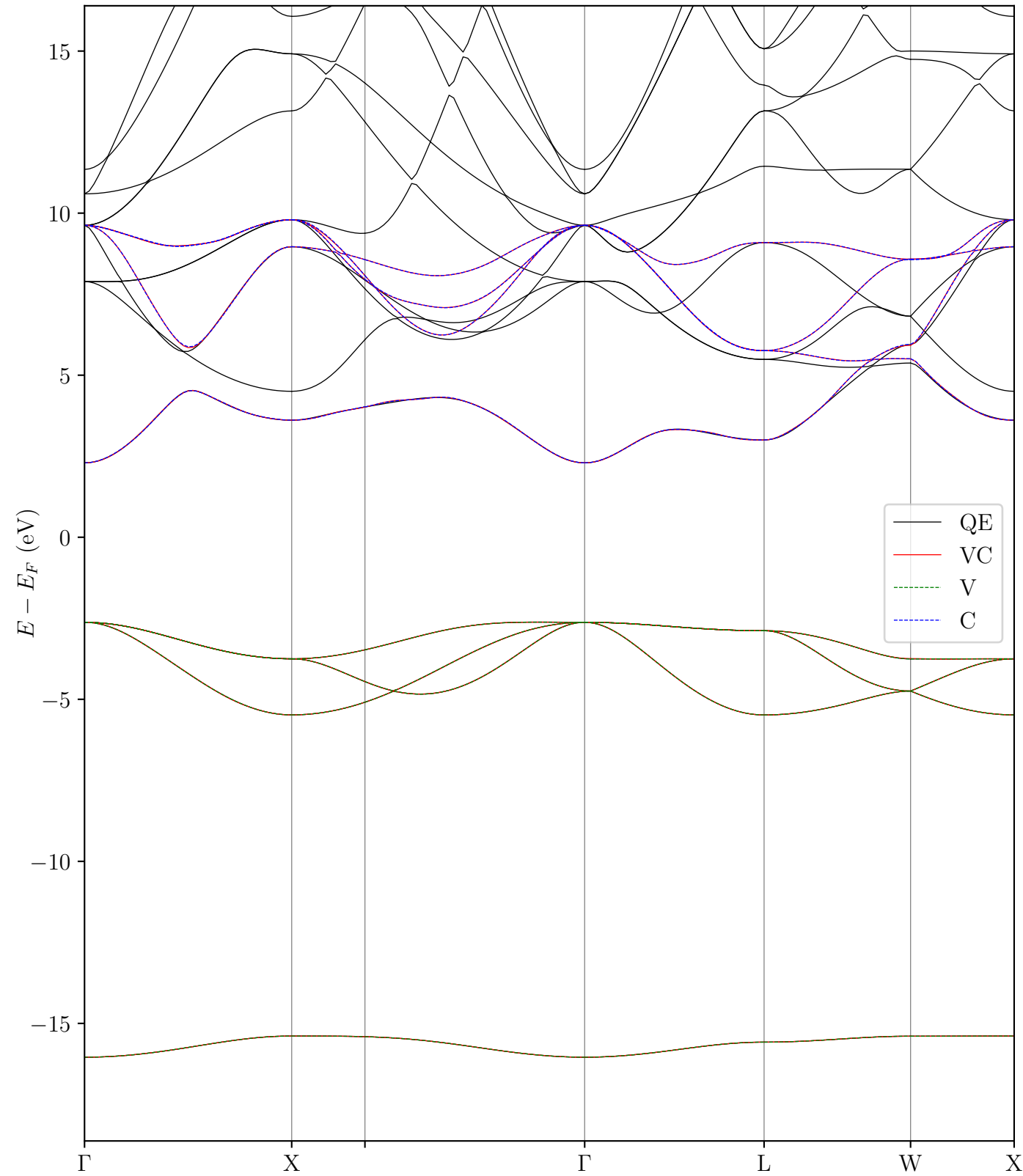


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.8	0.8	0.0	0.7	1.4	1.2	1.4
η_{max}	4.9	4.9	0.5	4.9	0.0	0.0	10.5



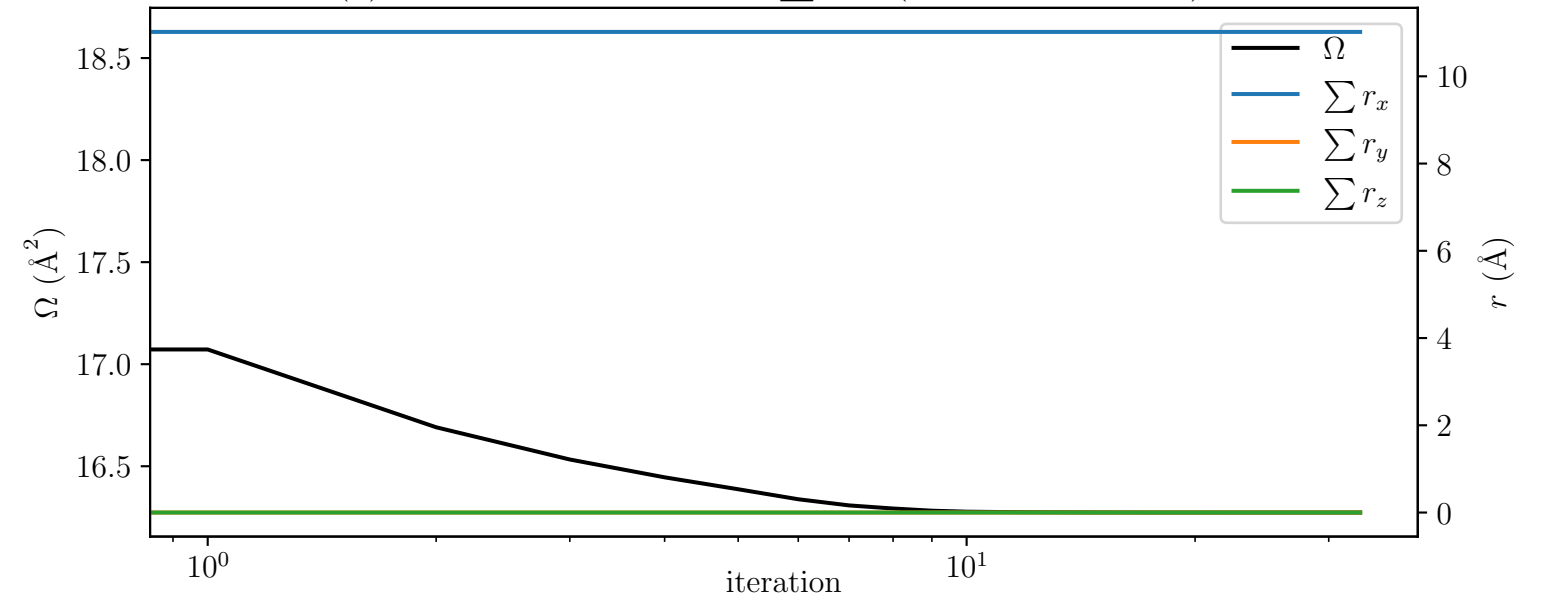
BrLi (exclude semicore)
PW AiiDA UUID: d6e387af-5960-423c-907b-386980b9faed
W90 AiiDA UUID: 536b6ca3-b4c4-45d4-98aa-e0c0aabe7266



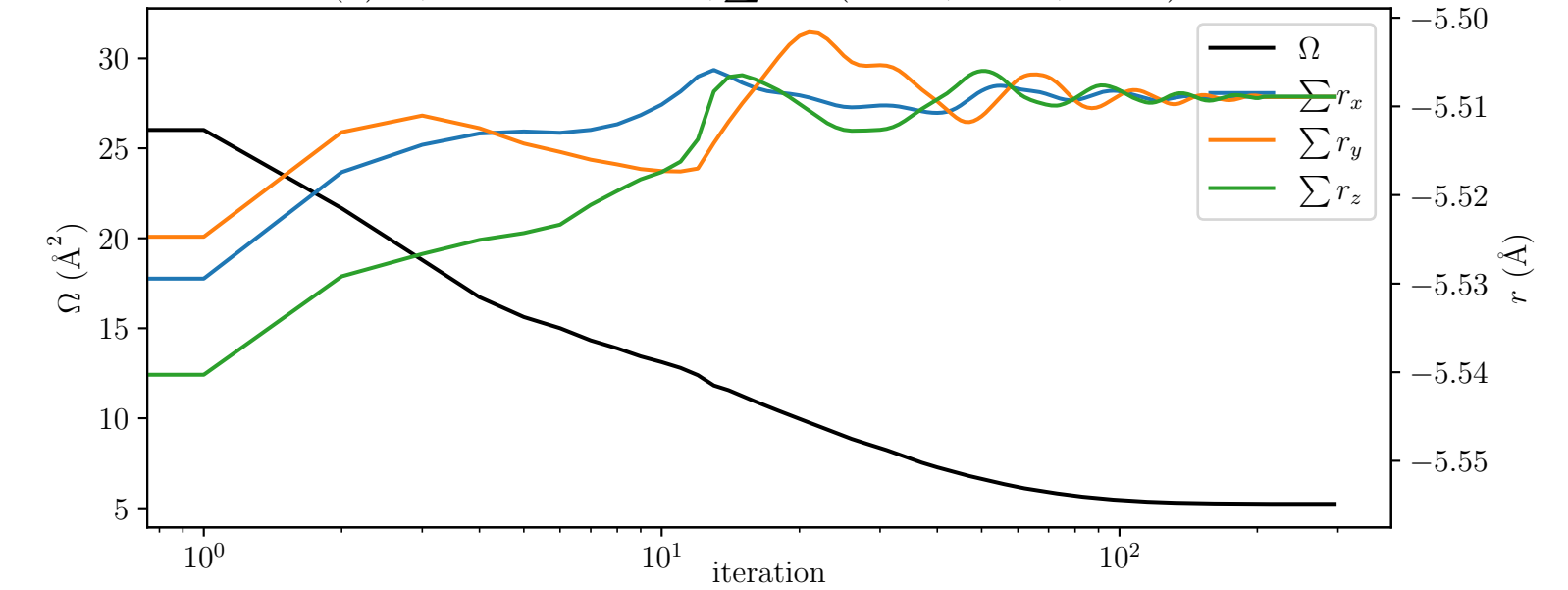
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.6	1.6	0.1	1.6	2.5	1.8	6.7
η_{max}	9.6	9.6	0.5	9.6	0.1	0.1	28.1

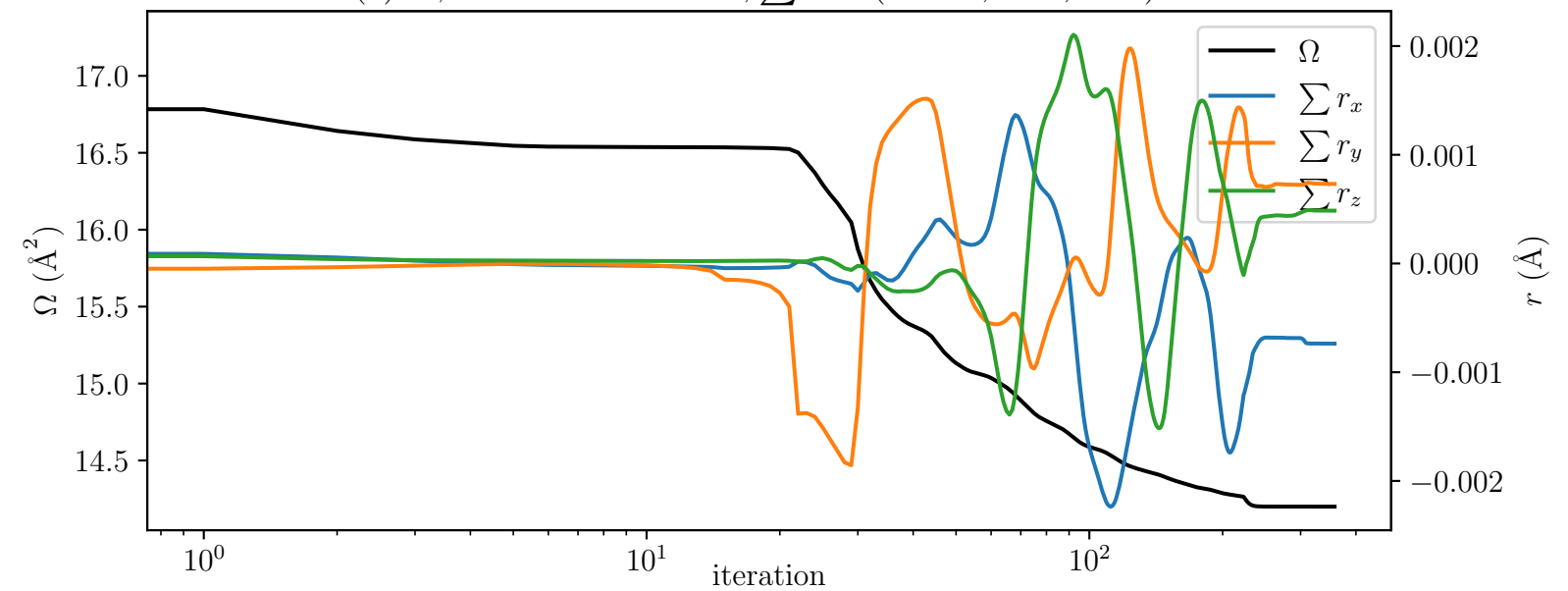
(a) VC; final $\Omega = 16.27 \text{ \AA}^2$, $\sum r = (11.02, 0.00, -0.00) \text{ \AA}$



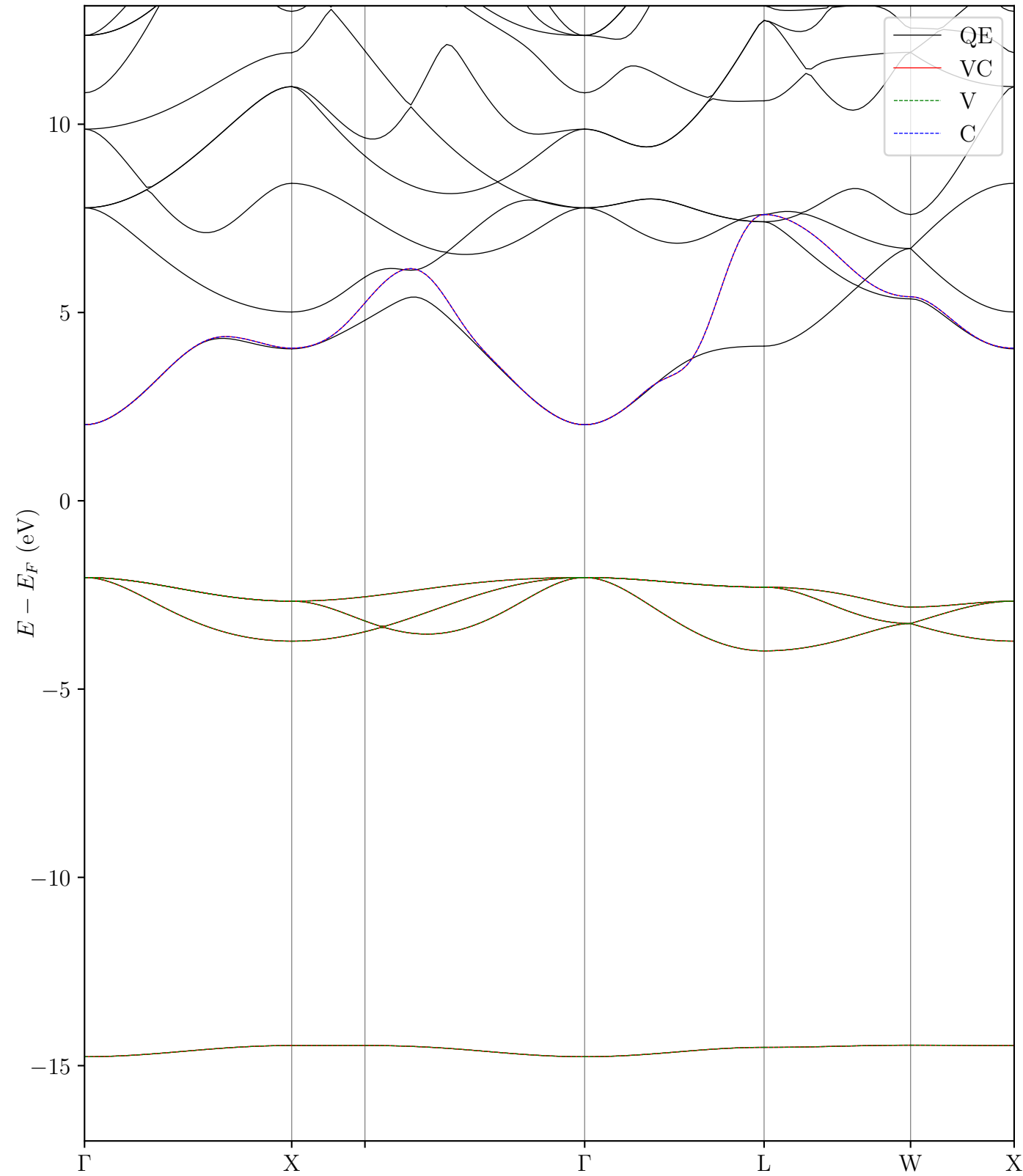
(b) V; final $\Omega = 5.24 \text{ \AA}^2$, $\sum r = (-5.51, -5.51, -5.51) \text{ \AA}$



(c) C; final $\Omega = 14.20 \text{ \AA}^2$, $\sum r = (-0.00, 0.00, 0.00) \text{ \AA}$

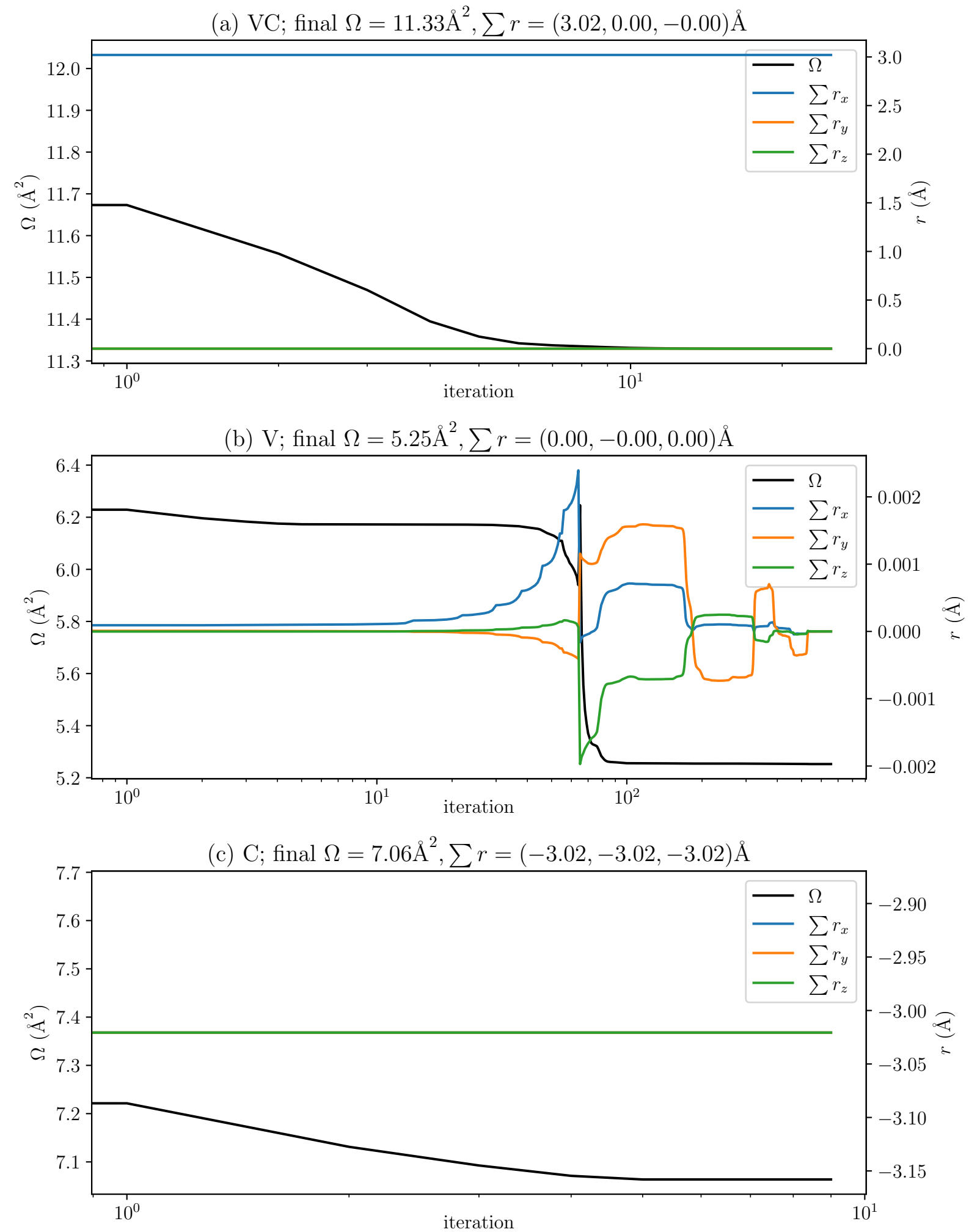


BrNa (exclude semicore)
PW AiiDA UUID: 69240d29-acf2-40d6-9e5f-034f7d73c686
W90 AiiDA UUID: 0d764e61-c9e6-4194-80f5-2118d7404b31

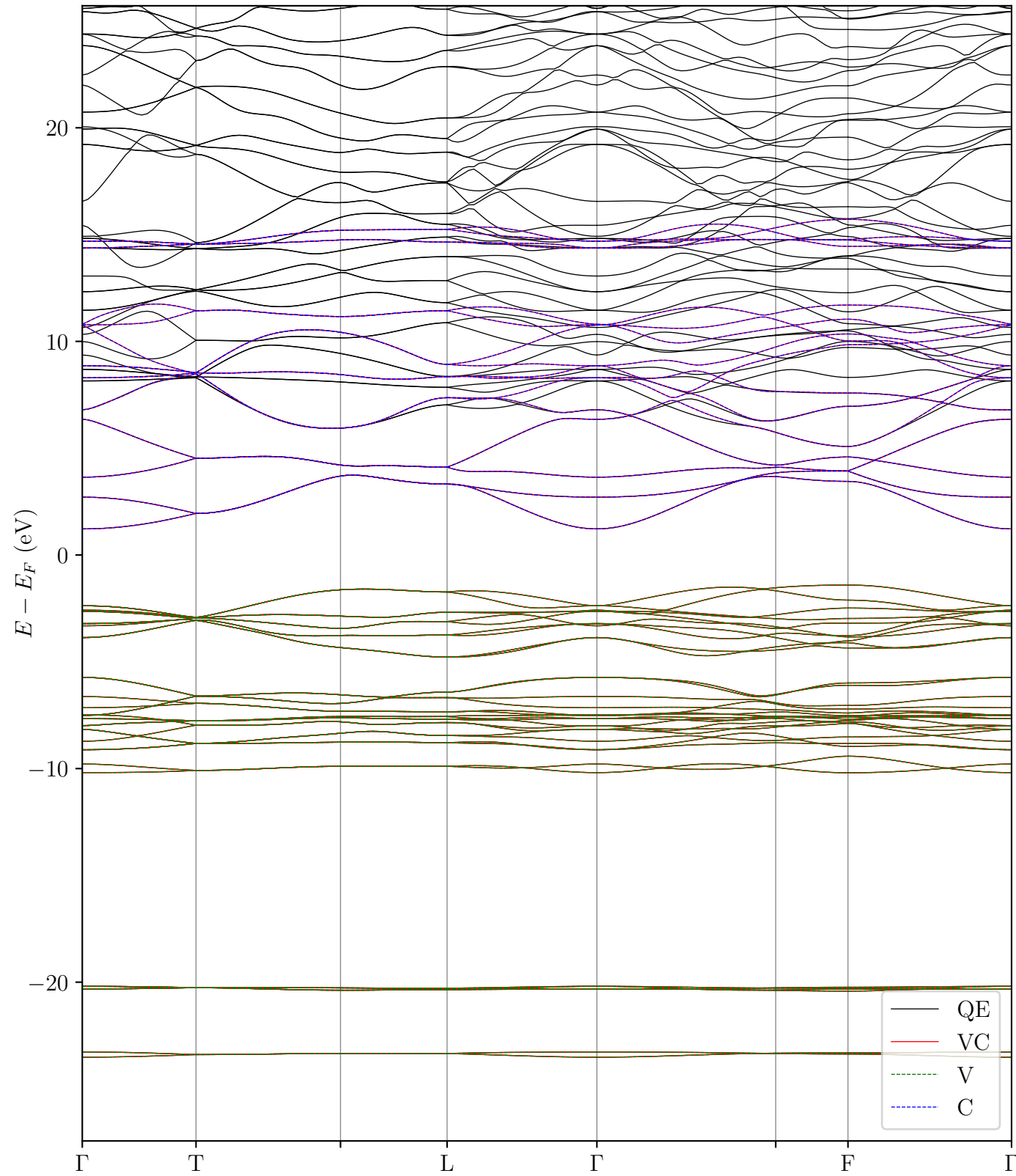


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.6	0.6	0.0	0.6	1.6	1.2	1.4
η_{max}	3.3	3.3	0.2	3.3	0.7	0.4	5.3

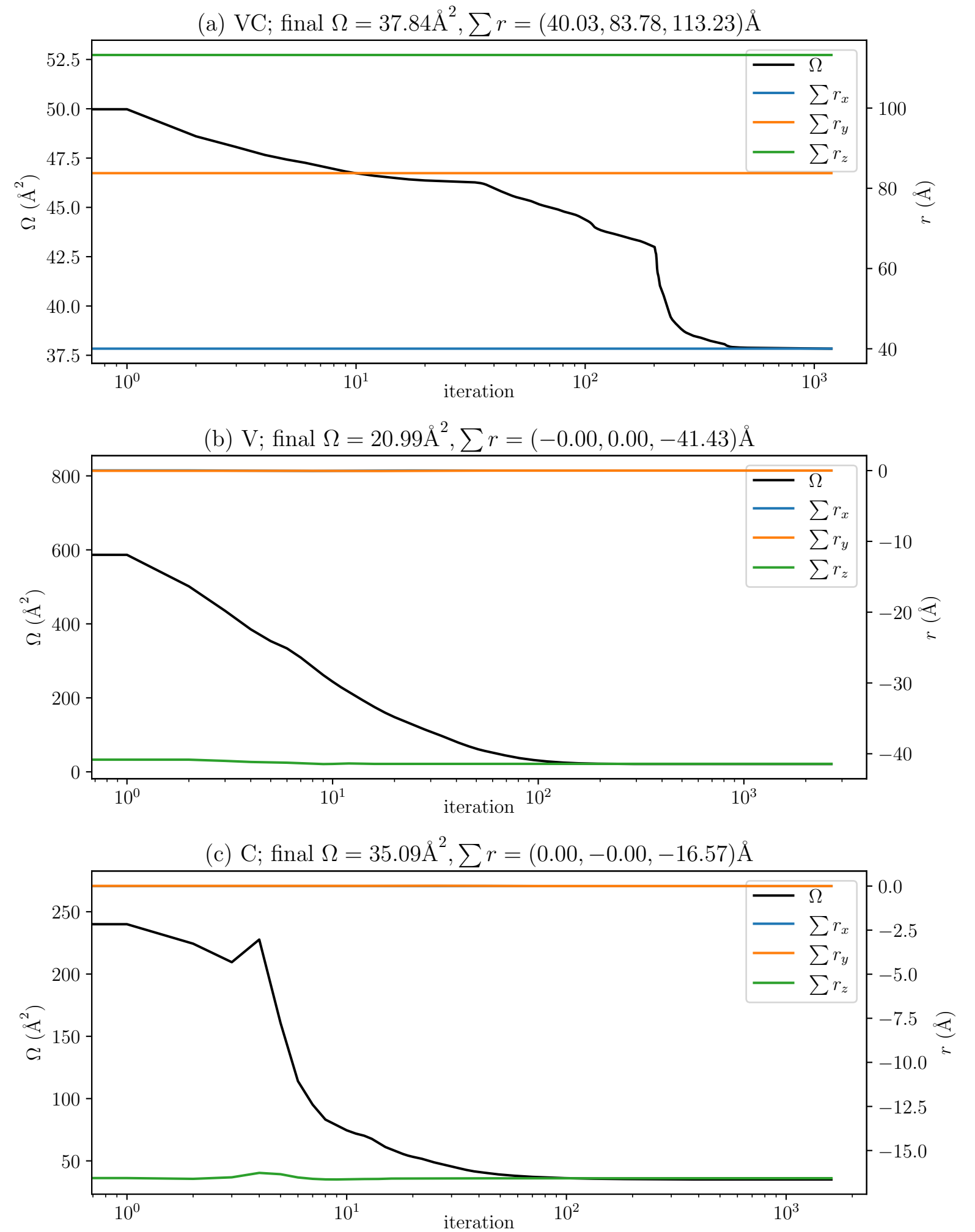


C₂Cd₂O₆ (exclude semicore)
PW AiiDA UUID: 99f65b29-d15d-4778-9c2c-41ddd0602b22
W90 AiiDA UUID: 4a54f24b-cd1b-49a3-93e6-fa48bf963870

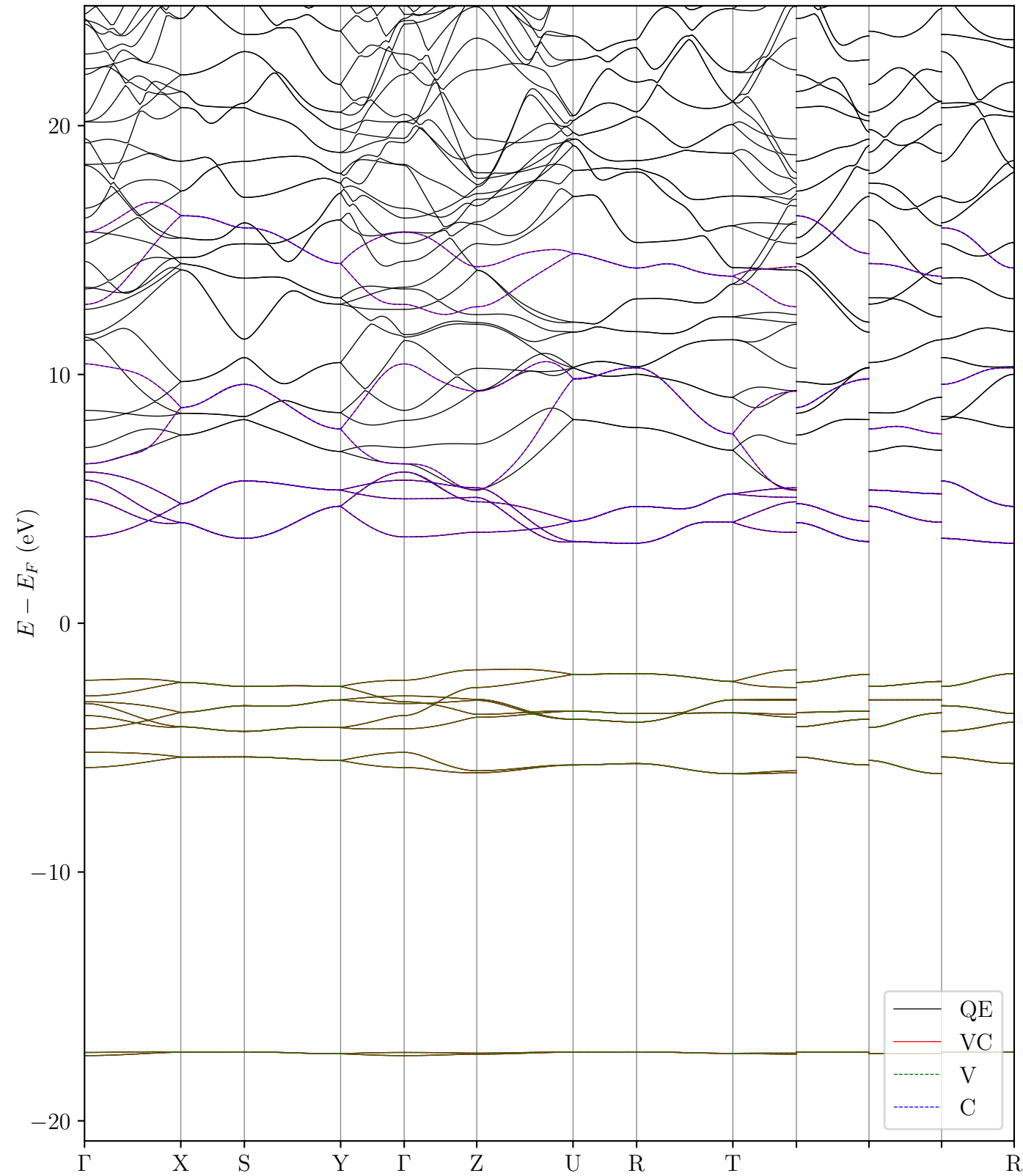


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.3	0.3	0.0	0.3	0.9	0.7	1.0
η_{max}	2.3	2.3	0.1	2.3	1.5	1.8	8.6

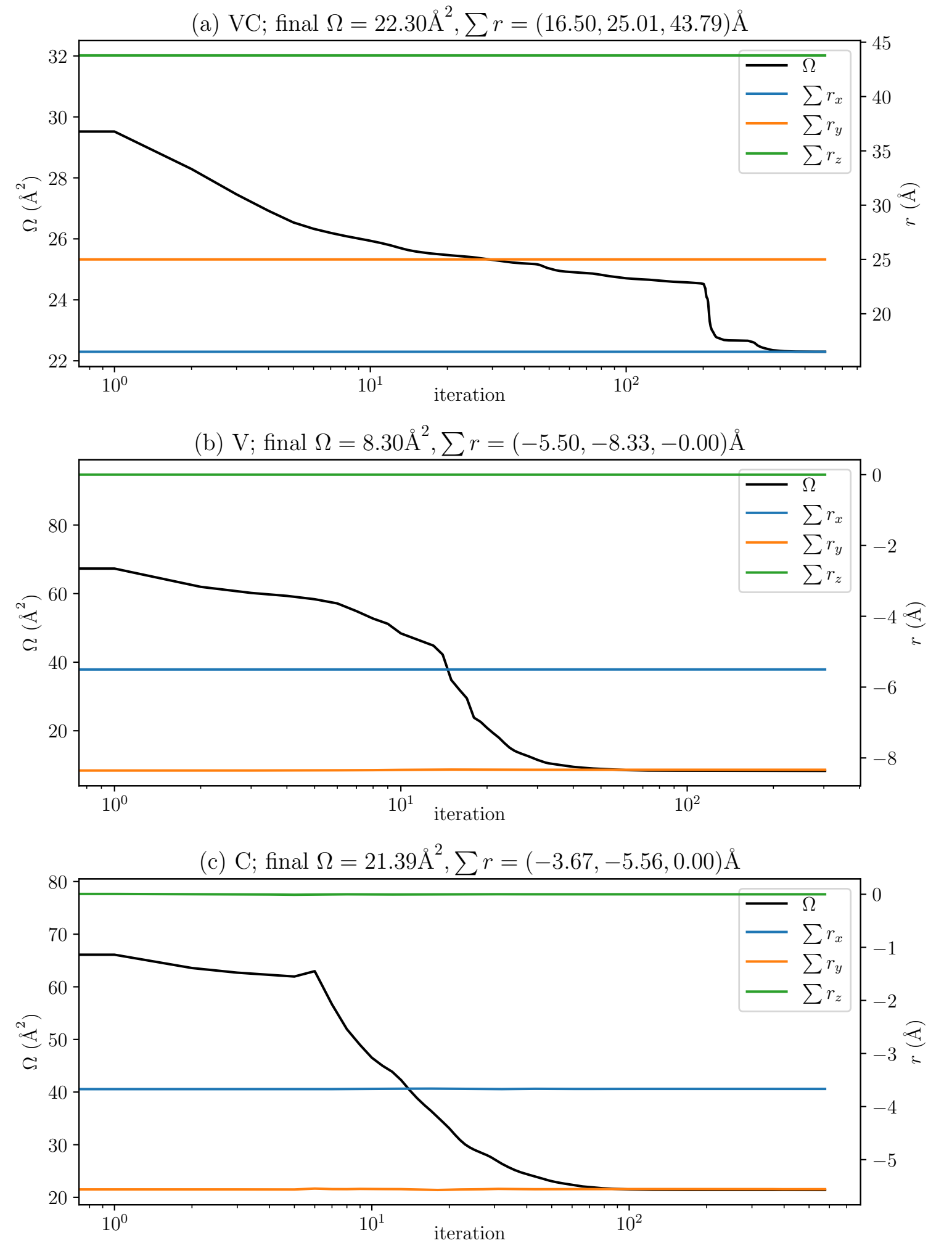


C₂N₂Na₂ (exclude semicore)
PW AiiDA UUID: c9e040dc-4239-472d-b833-746c27430709
W90 AiiDA UUID: eb074fb6-c887-4237-8fa3-3af6c45cf200

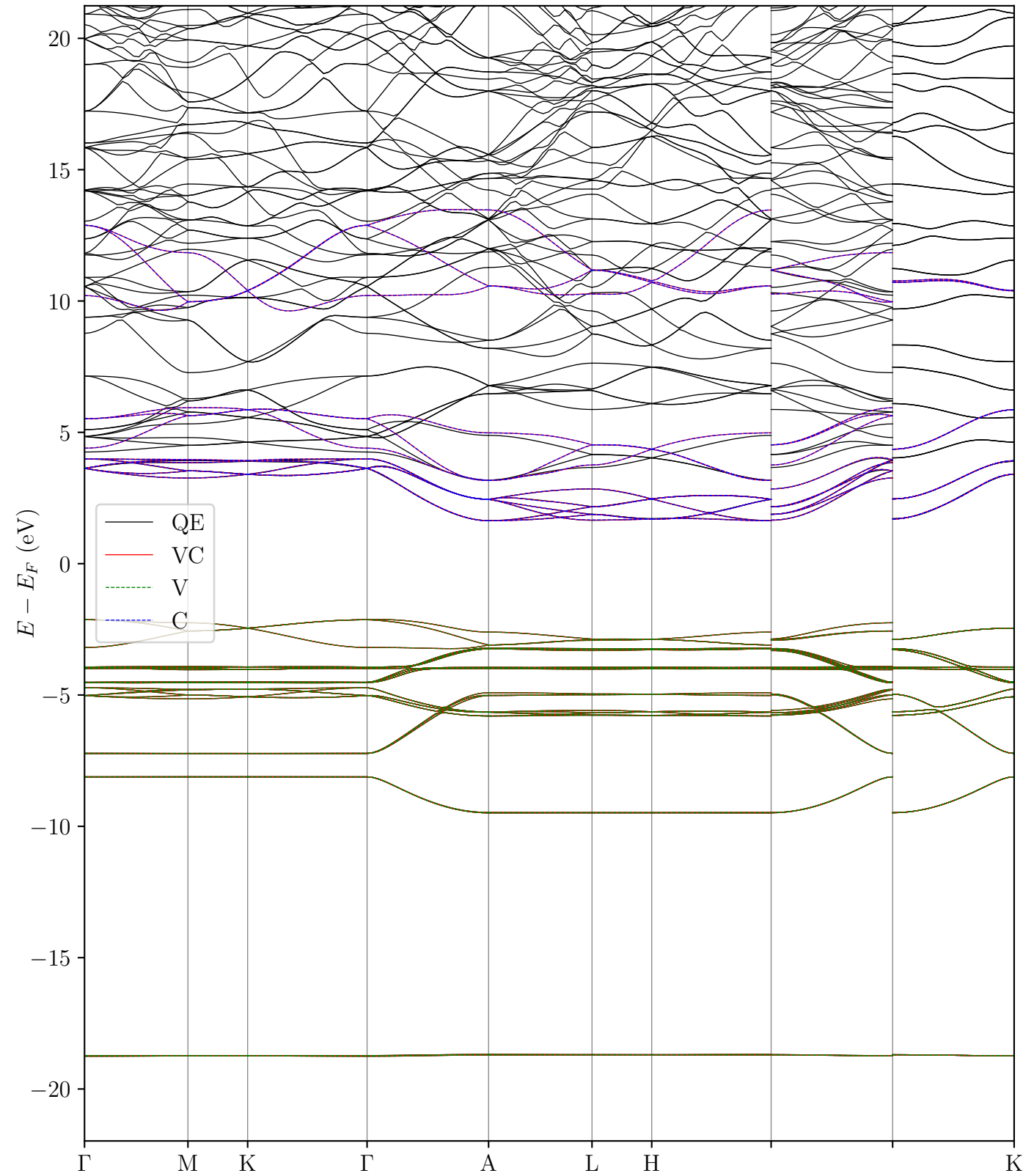


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.8	0.8	0.0	0.8	3.1	4.8	2.8
η_{max}	5.1	5.1	0.1	5.1	0.0	0.0	20.6



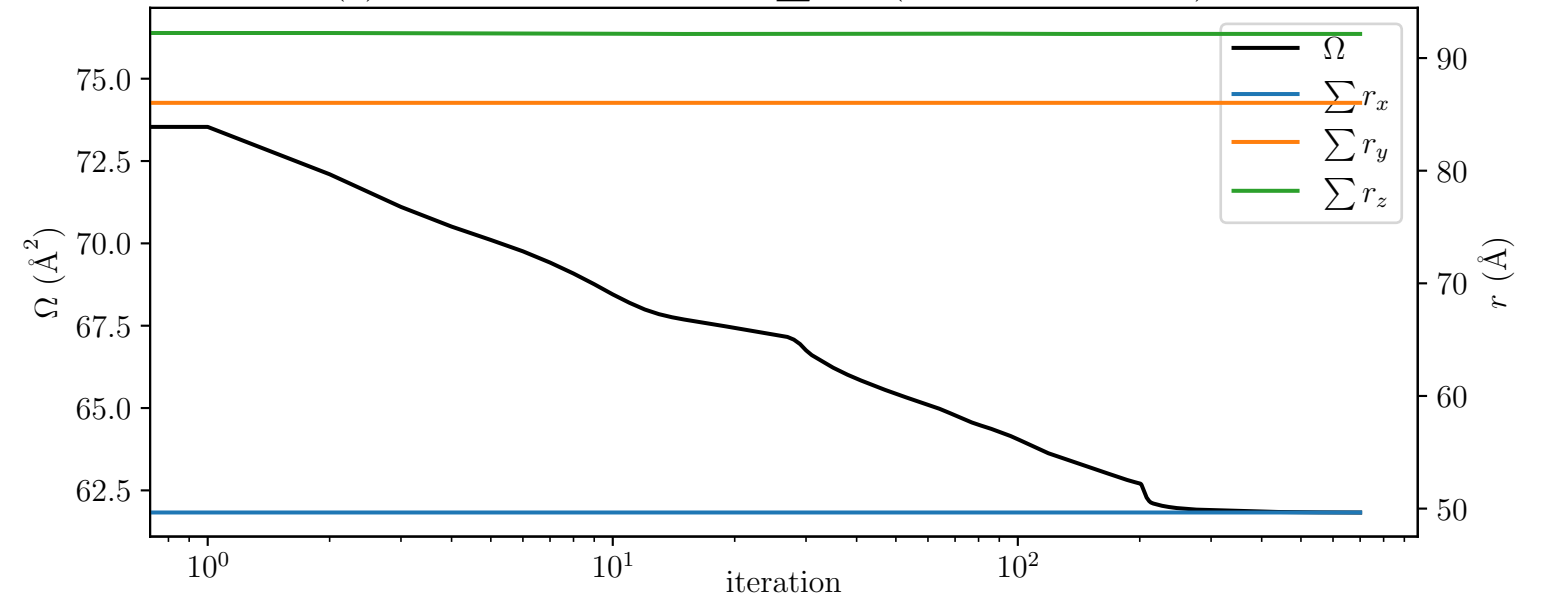
C₃Ag₃N₃ (exclude semicore)
PW AiiDA UUID: 08720073-7c39-44c3-8cf9-e8a7ee72d626
W90 AiiDA UUID: 8ff527b4-082c-4dab-93b6-fb5f00a877e1



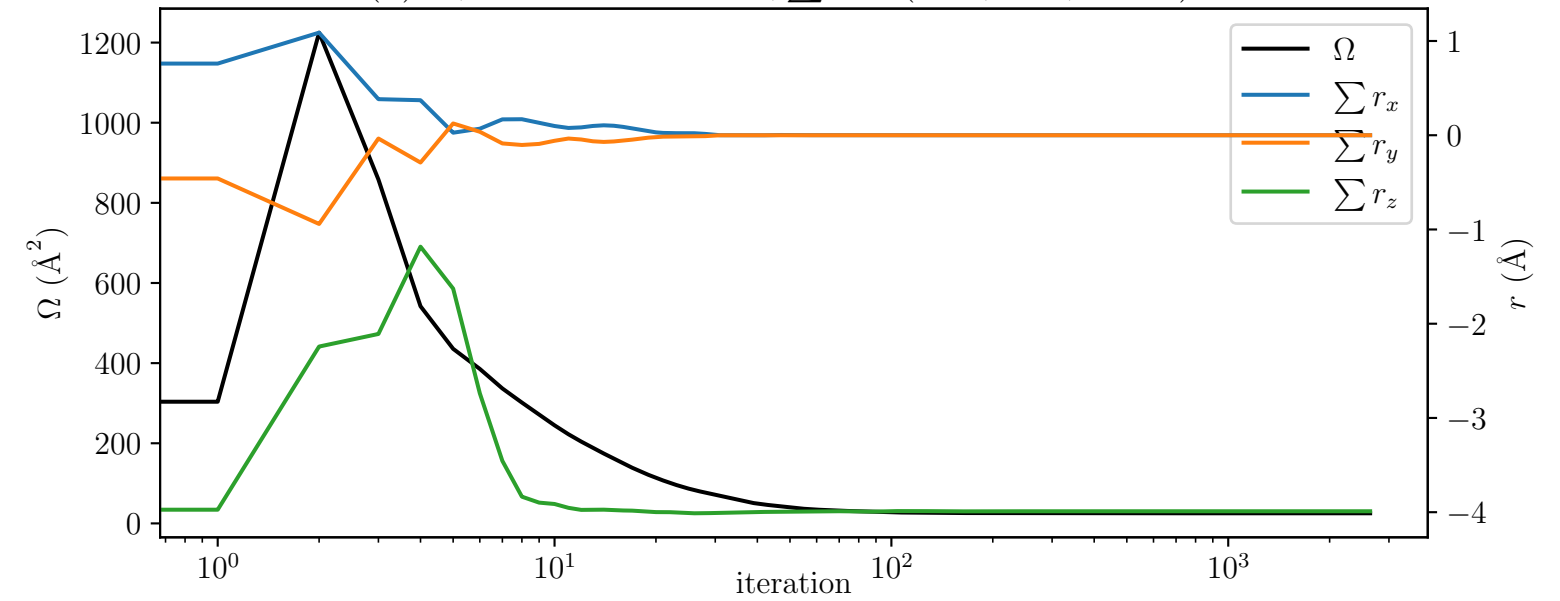
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.7	0.9	0.0	0.9	7.8	8.7	2.1
η_{max}	12.3	5.2	0.2	5.0	12.3	14.1	12.3

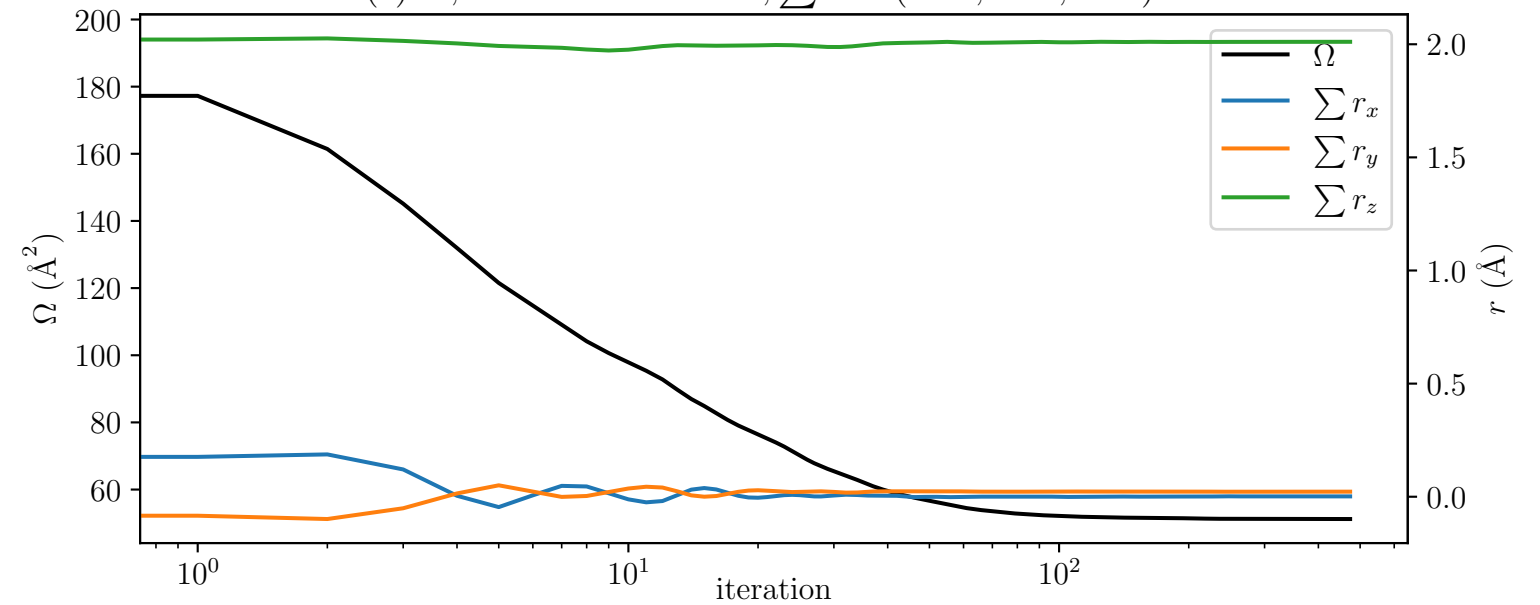
(a) VC; final $\Omega = 61.83 \text{ \AA}^2$, $\sum r = (49.66, 86.02, 92.14) \text{ \AA}$



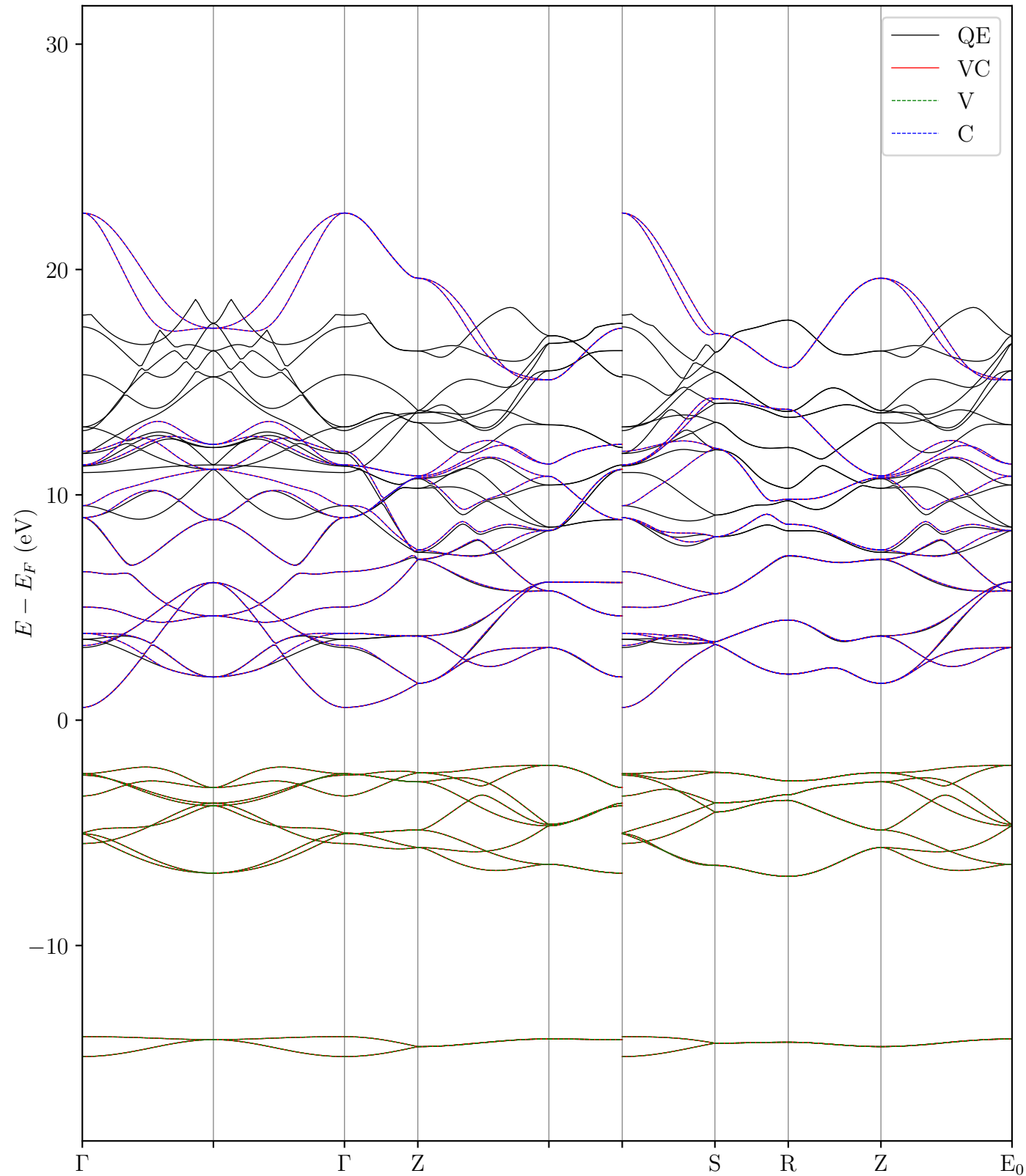
(b) V; final $\Omega = 25.27 \text{ \AA}^2$, $\sum r = (0.00, 0.00, -3.99) \text{ \AA}$



(c) C; final $\Omega = 51.22 \text{ \AA}^2$, $\sum r = (0.00, 0.02, 2.01) \text{ \AA}$

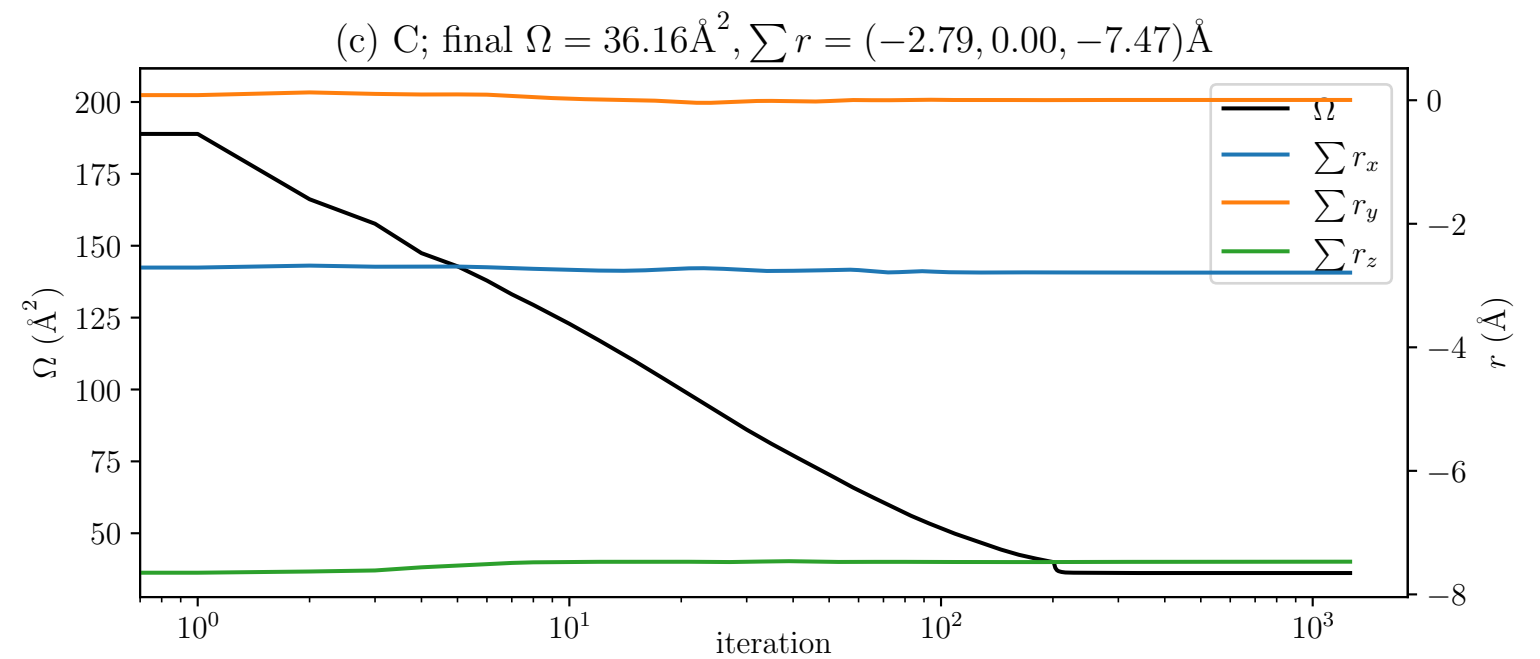
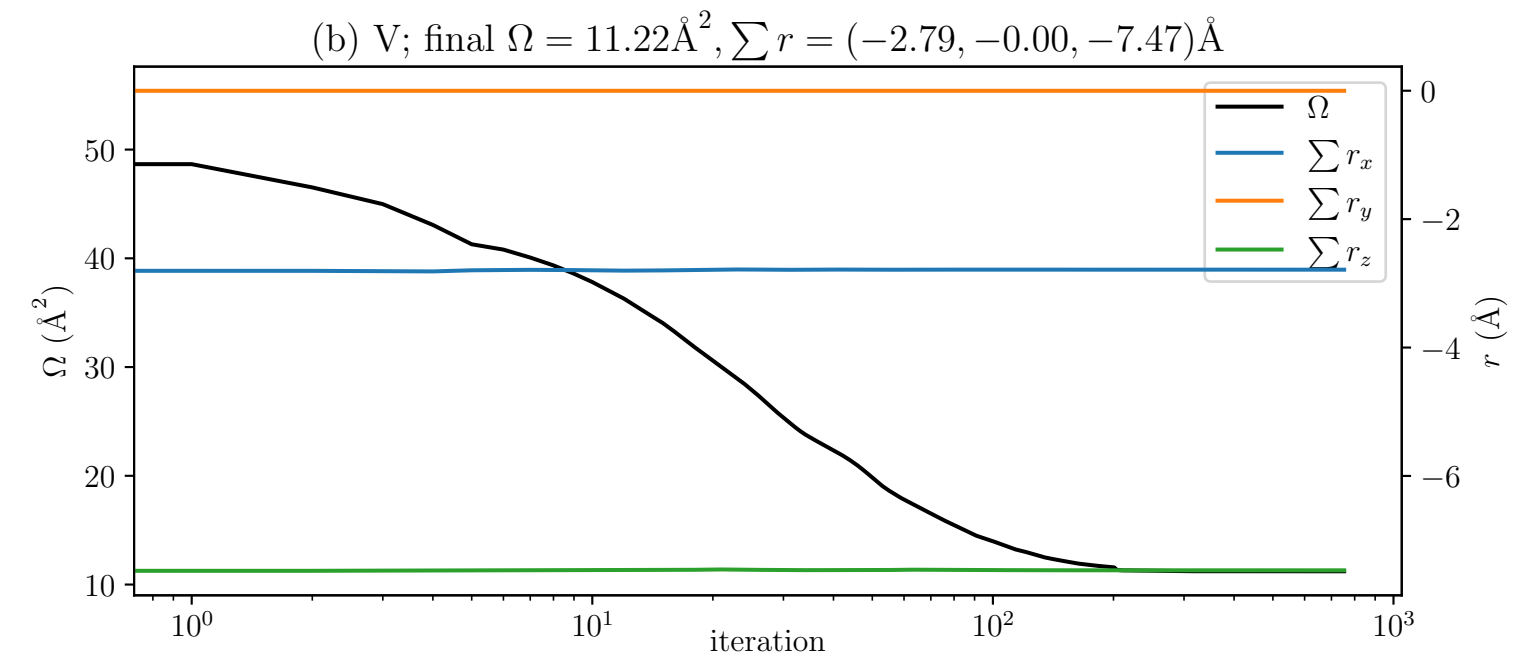
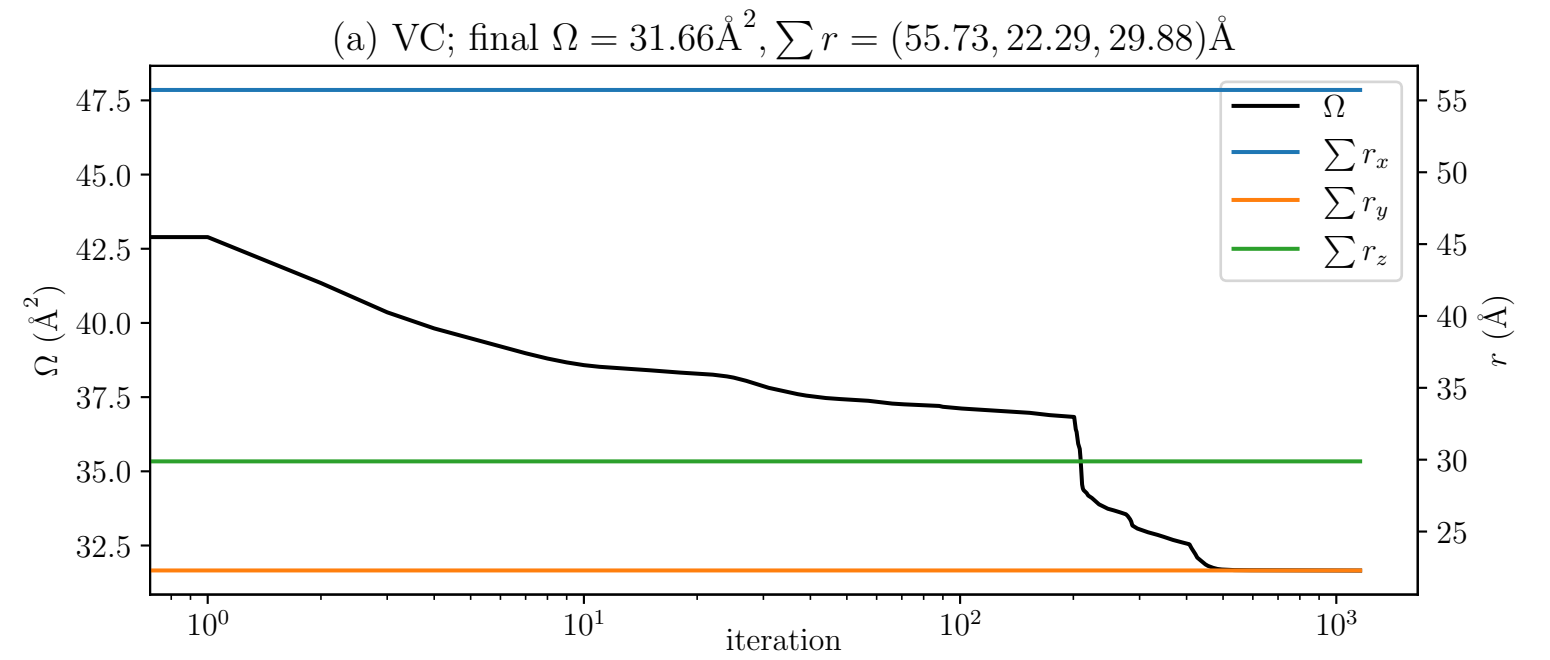


C₄Mg₂ (exclude semicore)
PW AiiDA UUID: 14adf787-7ba3-49fb-8ee1-4eb4fd6076c9
W90 AiiDA UUID: ad2e488b-5590-4080-a0e0-c54cc0cf026a

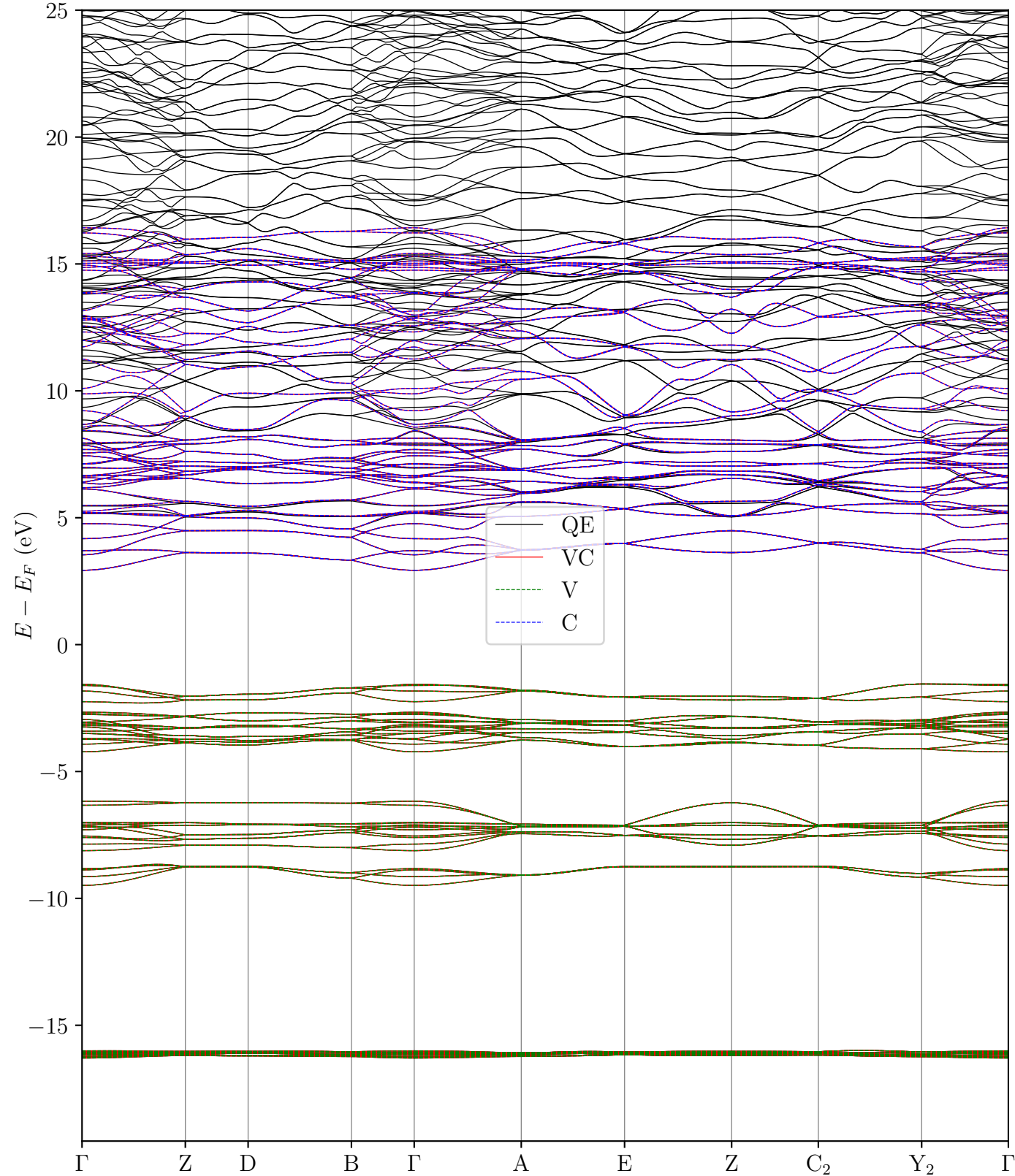


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	2.0	1.7	0.1	1.7	5.0	5.6	3.0
η_{max}	10.7	10.0	0.9	9.8	10.7	9.9	20.2



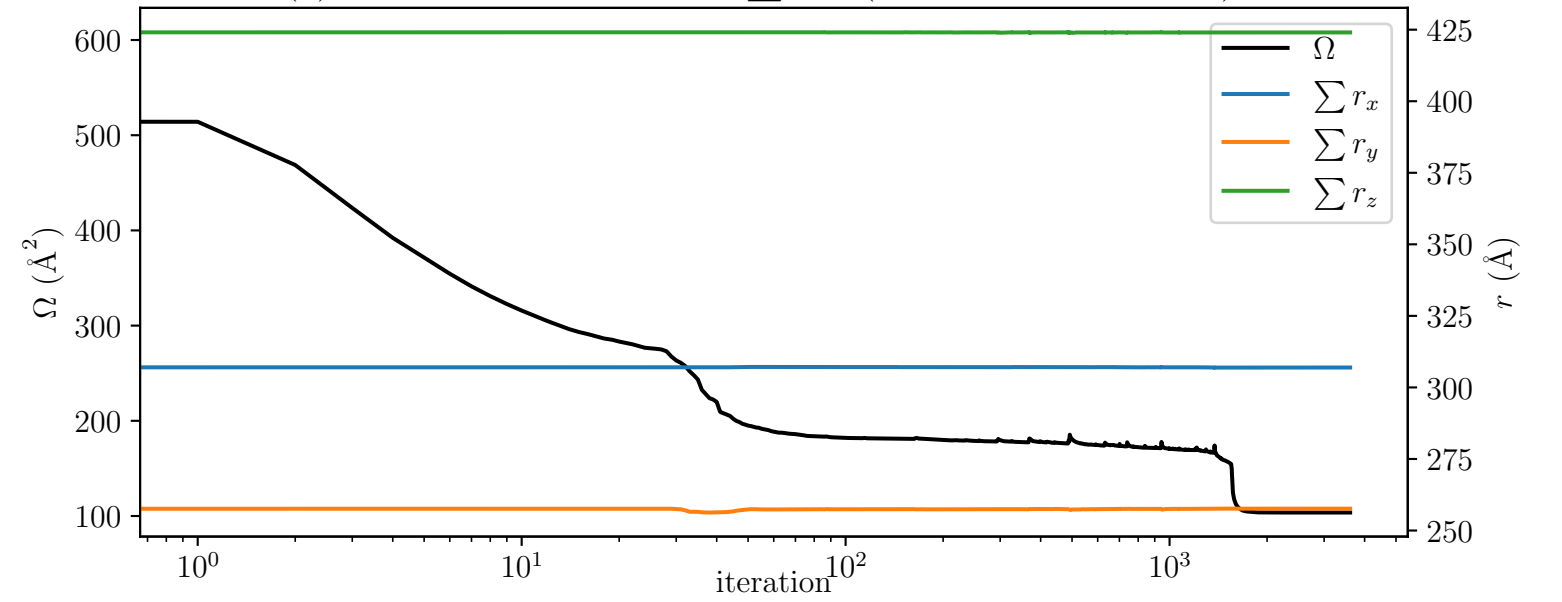
C₄O₁₂Sr₄ (exclude semicore)
PW AiiDA UUID: e51e060a-b39e-471f-9299-6488b4d58ab7
W90 AiiDA UUID: 1bc3dfa9-eab9-49de-869e-f0df5c8d5b54



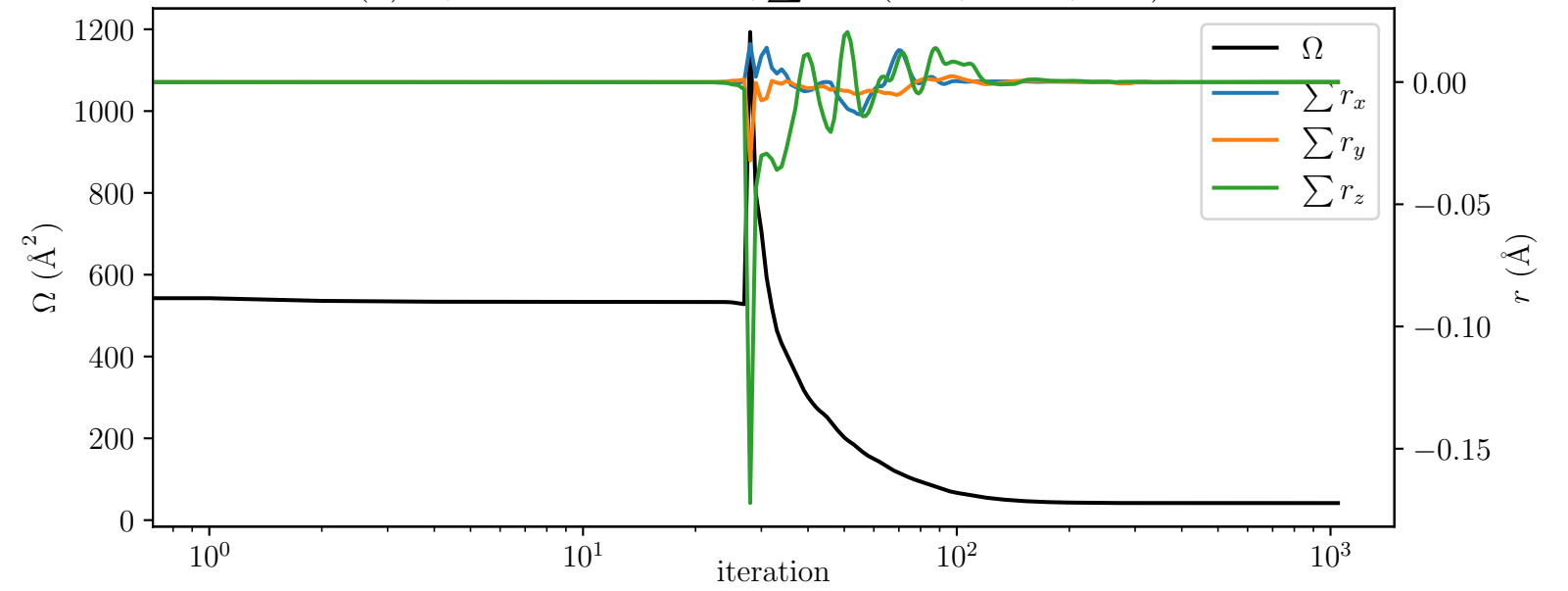
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.3	0.3	0.0	0.3	0.1	0.1	0.5
η_{max}	2.0	2.0	0.0	2.0	0.0	0.0	3.6

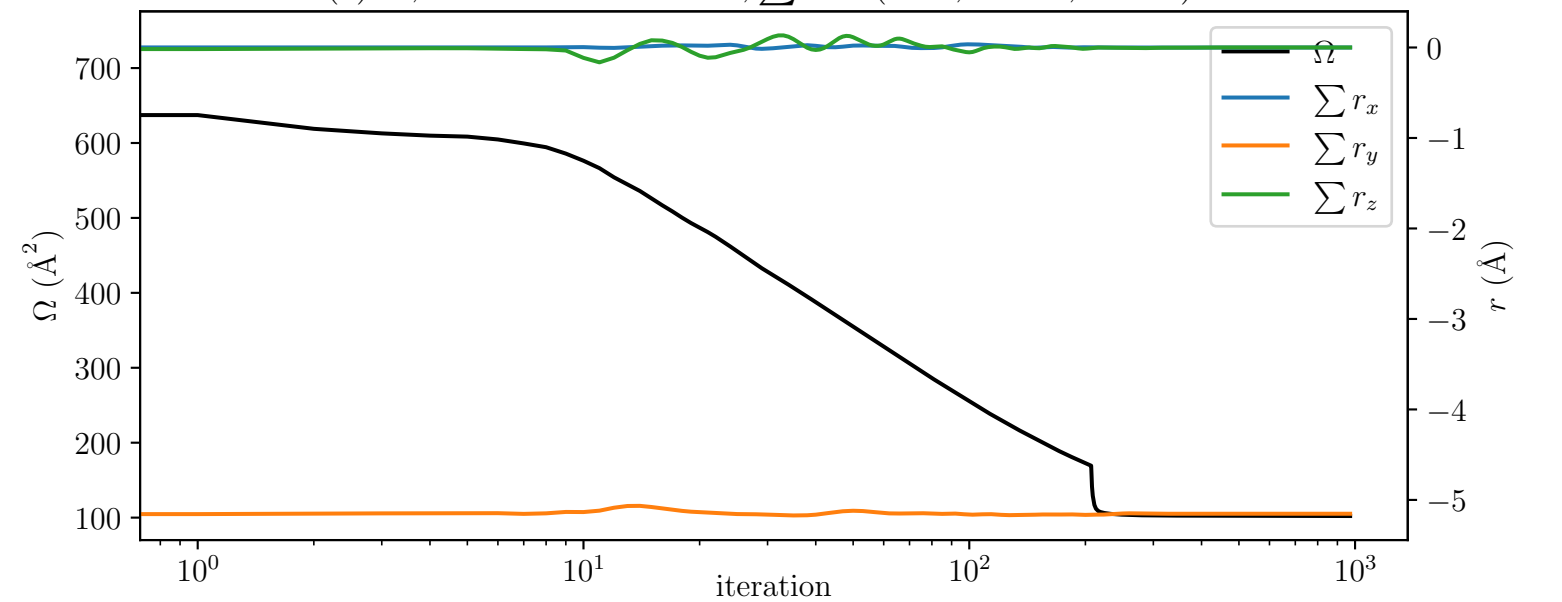
(a) VC; final $\Omega = 103.65 \text{ \AA}^2$, $\sum r = (306.96, 257.64, 424.04) \text{ \AA}$



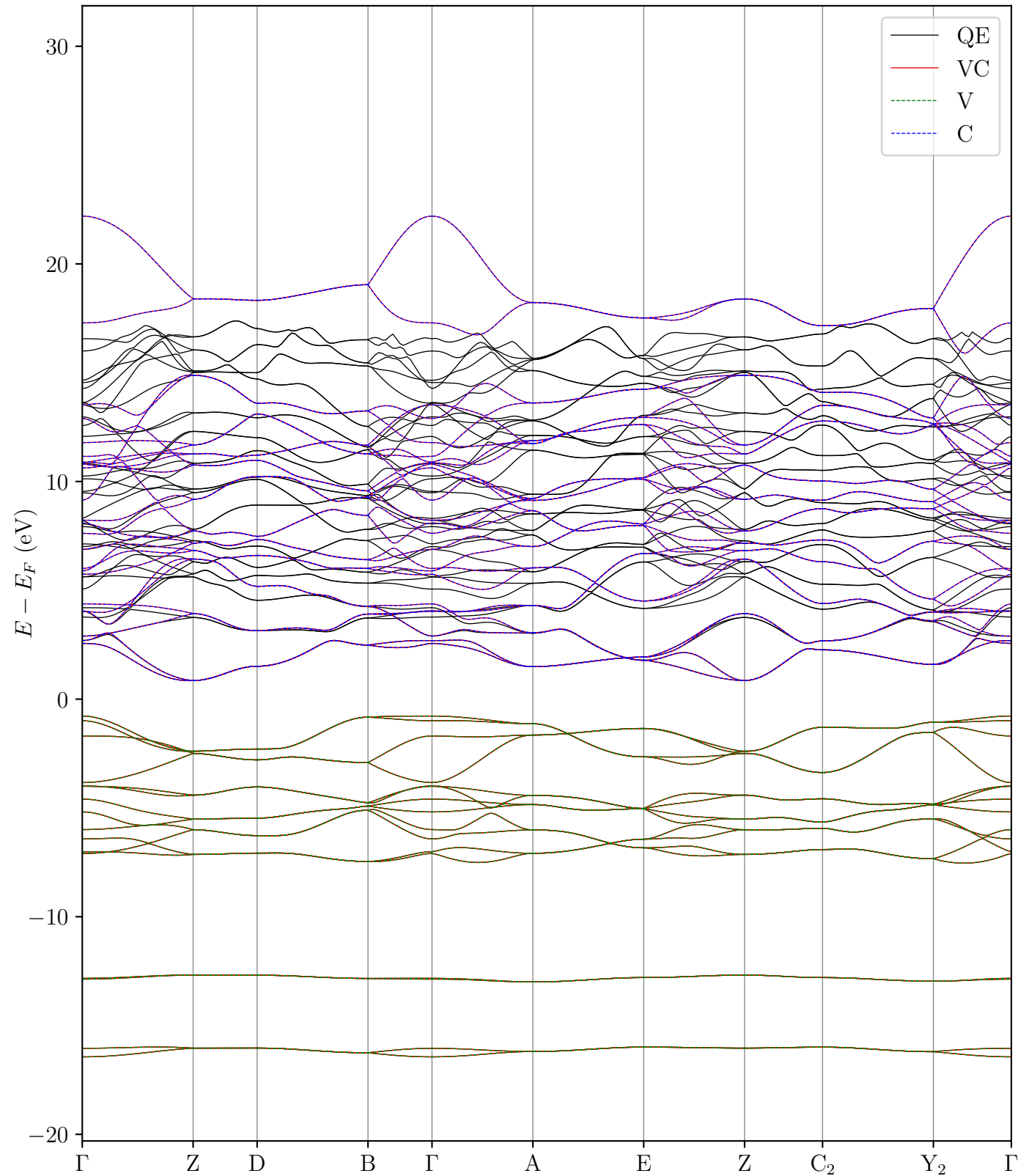
(b) V; final $\Omega = 41.72 \text{ \AA}^2$, $\sum r = (0.00, -0.00, 0.00) \text{ \AA}$



(c) C; final $\Omega = 102.13 \text{ \AA}^2$, $\sum r = (0.00, -5.15, -0.00) \text{ \AA}$

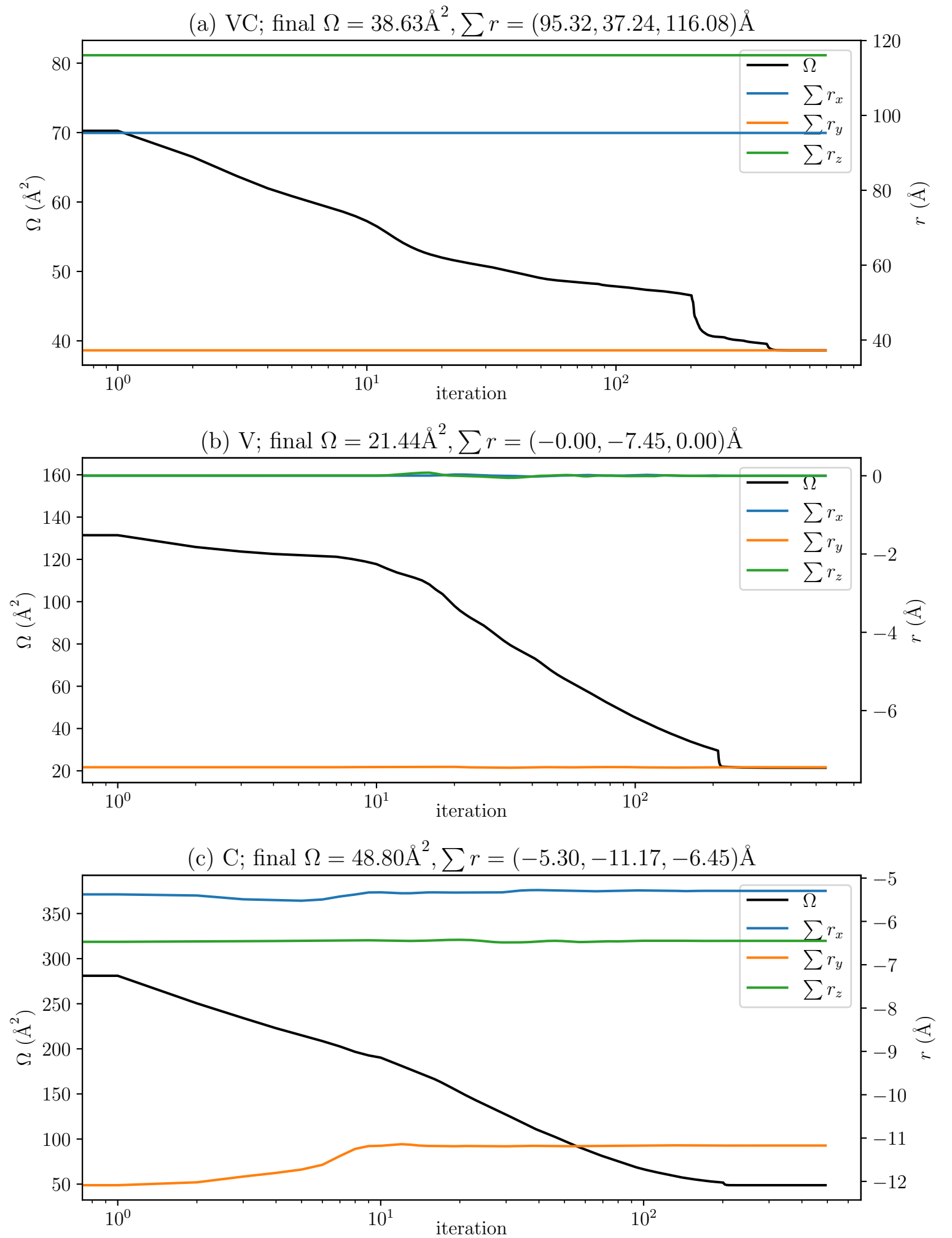


C₆Mg₄ (exclude semicore)
PW AiiDA UUID: 37c6e6e6-82b8-4991-aedf-32536d915935
W90 AiiDA UUID: 9b8dee94-6aa6-406a-96a1-af8f68ab2261

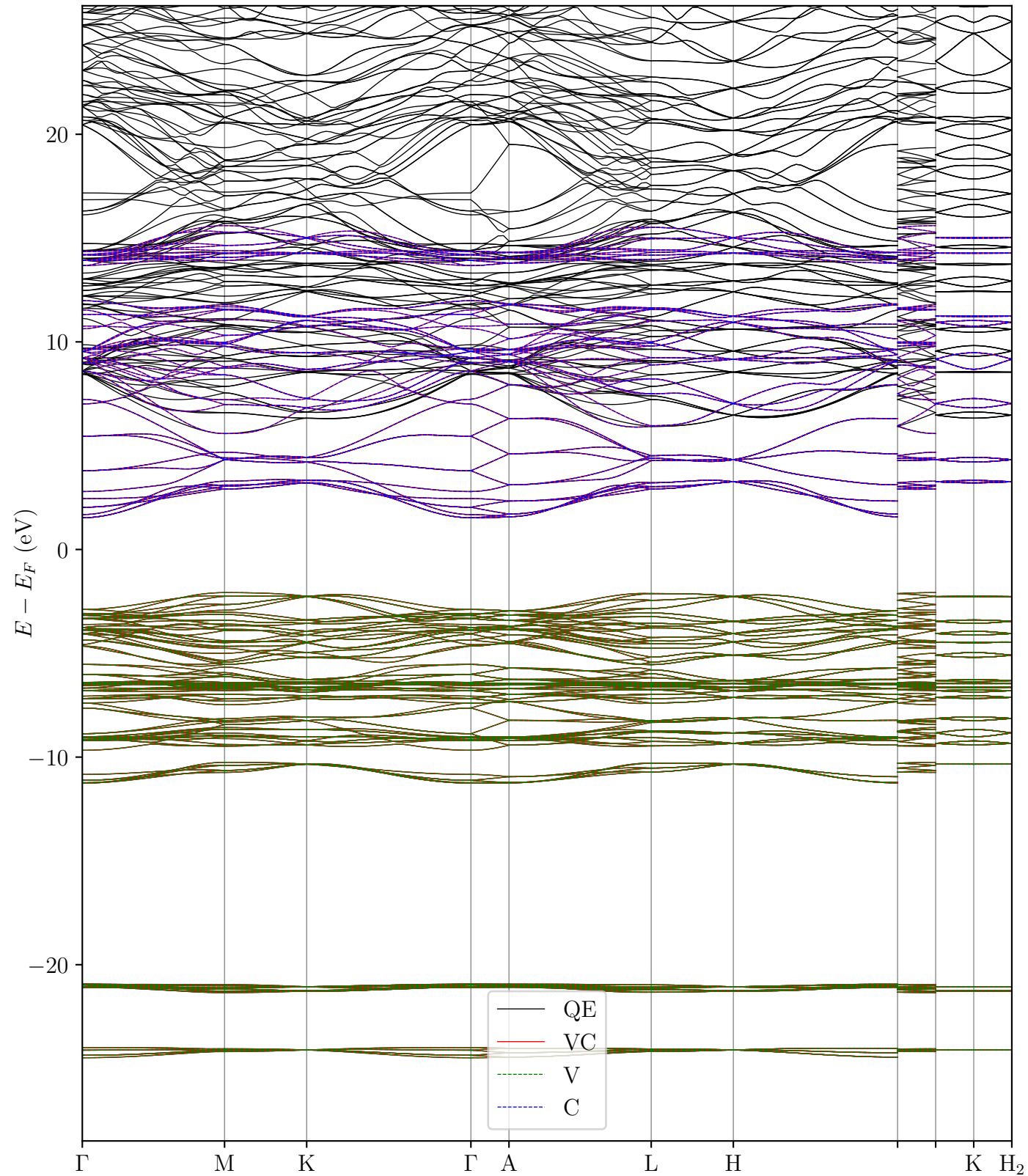


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	2.0	1.8	0.4	1.8	4.0	4.5	2.8
η_{max}	13.2	13.2	6.3	13.4	10.6	13.6	17.3



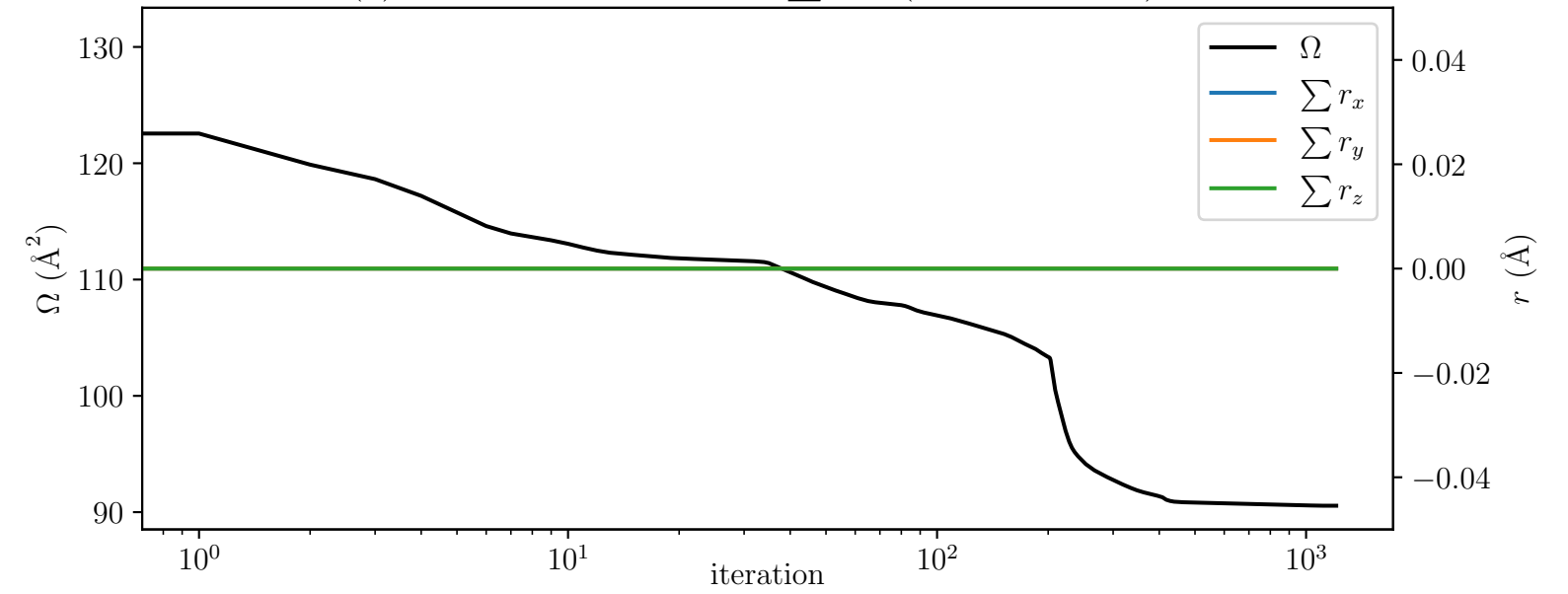
$\text{C}_6\text{O}_{18}\text{Zn}_6$ (exclude semicore)
PW AiiDA UUID: dc84cc0a-8980-482f-98eb-4bd0b696d0a4
W90 AiiDA UUID: 5cef75f2-ed69-45fe-adcf-593f102c935a



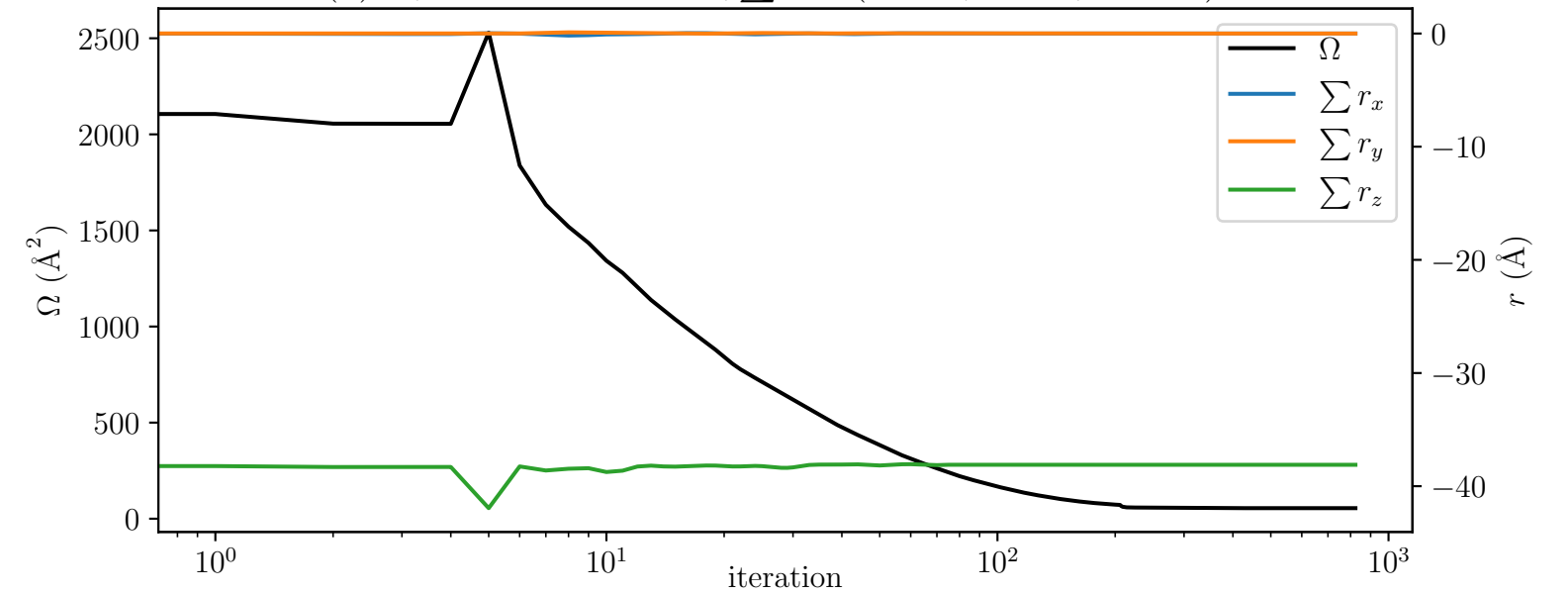
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.3	0.3	0.0	0.3	0.5	0.4	1.2
η_{max}	2.6	2.6	0.0	2.6	0.9	1.4	15.3

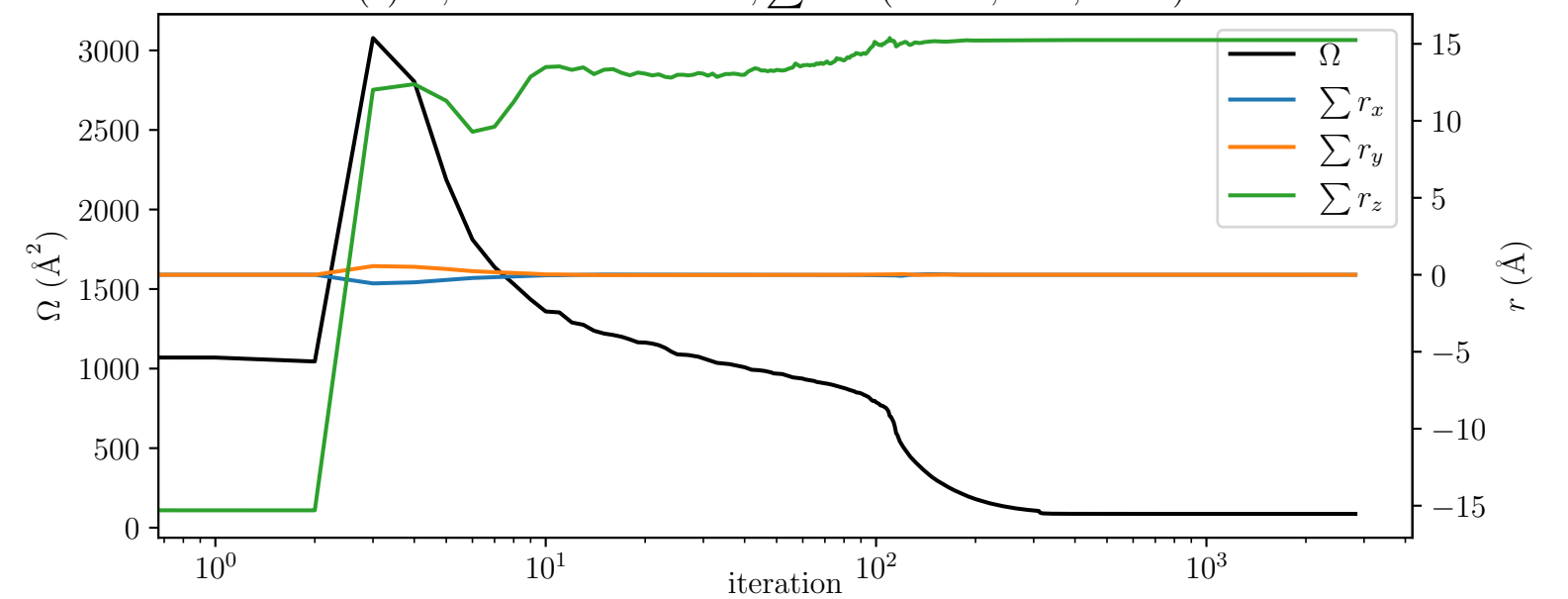
(a) VC; final $\Omega = 90.55 \text{\AA}^2$, $\sum r = (0.00, 0.00, 0.00) \text{\AA}$



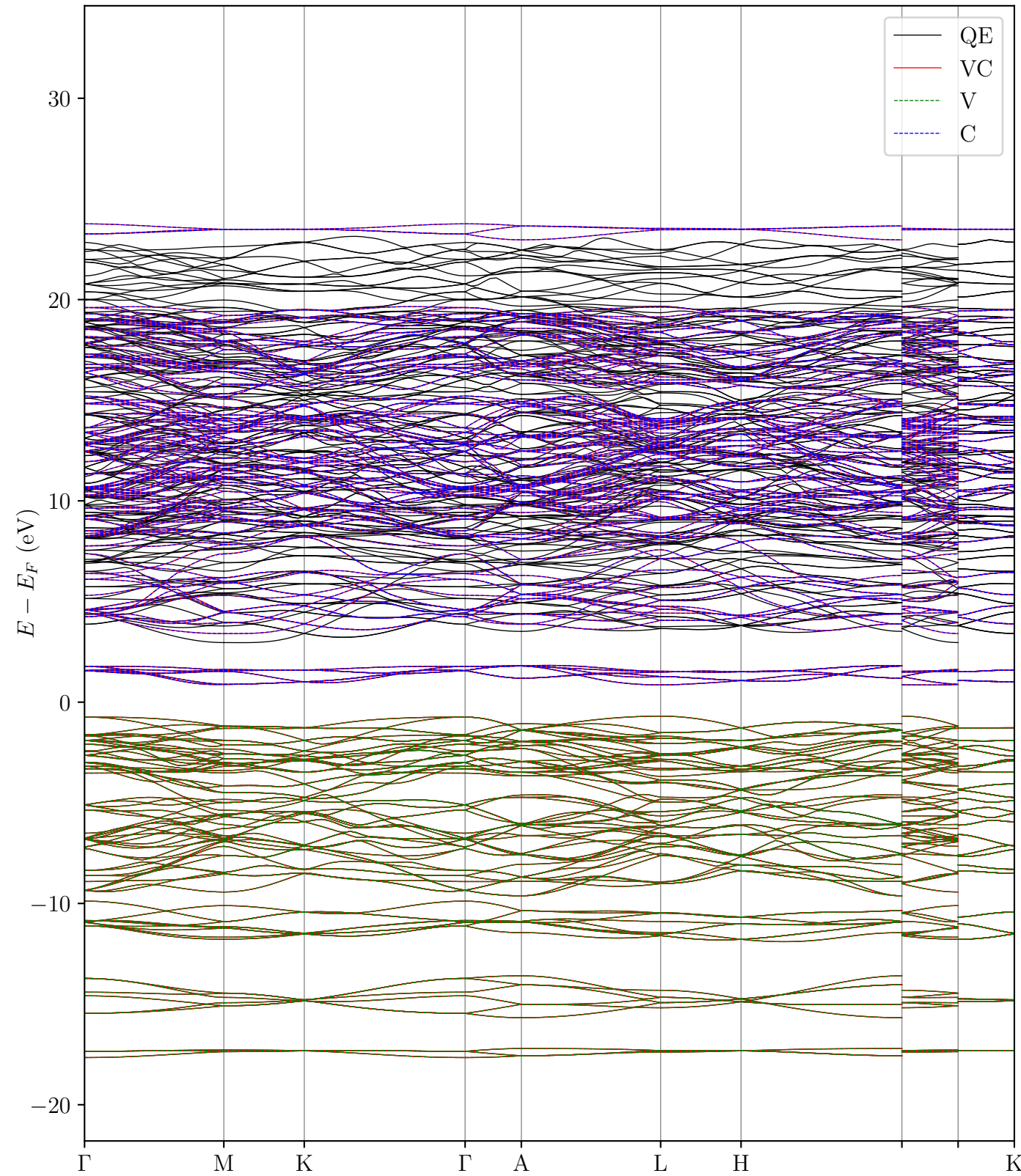
(b) V; final $\Omega = 54.88 \text{\AA}^2$, $\sum r = (-0.00, -0.00, -38.11) \text{\AA}$



(c) C; final $\Omega = 86.87 \text{\AA}^2$, $\sum r = (-0.00, 0.00, 15.25) \text{\AA}$

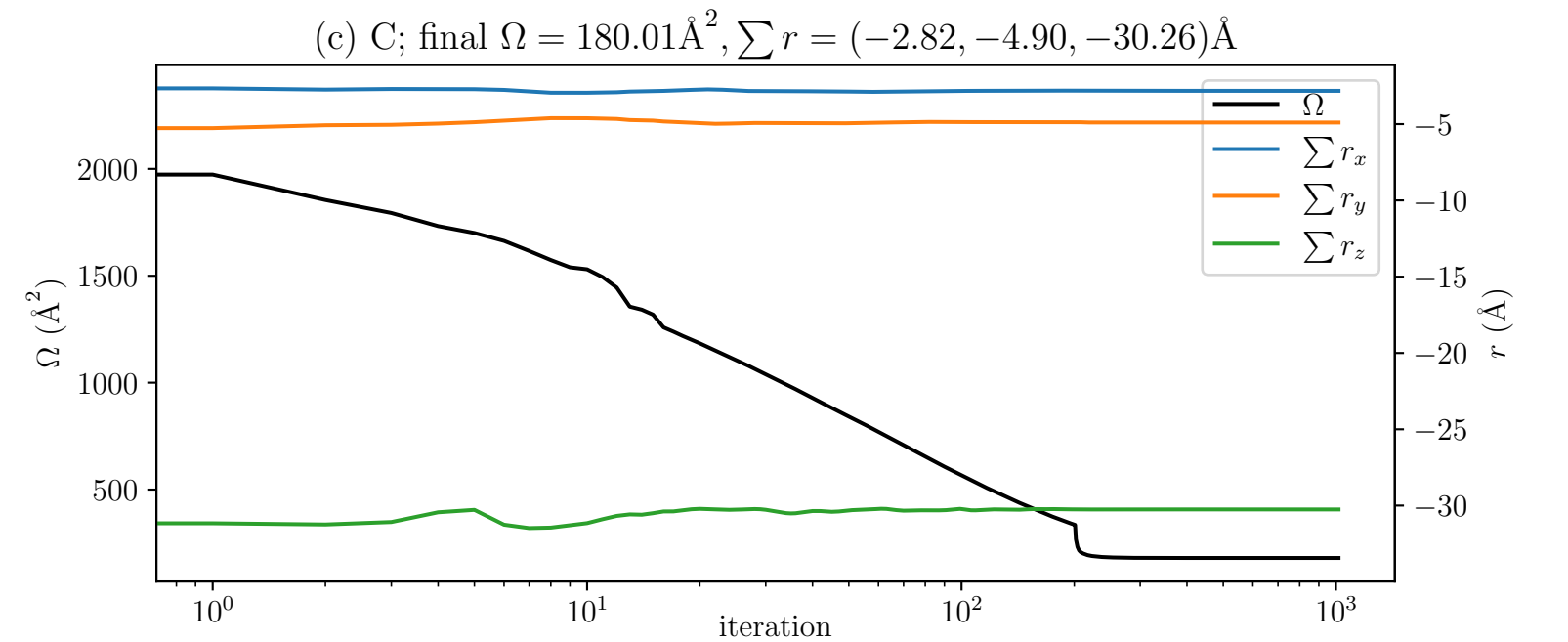
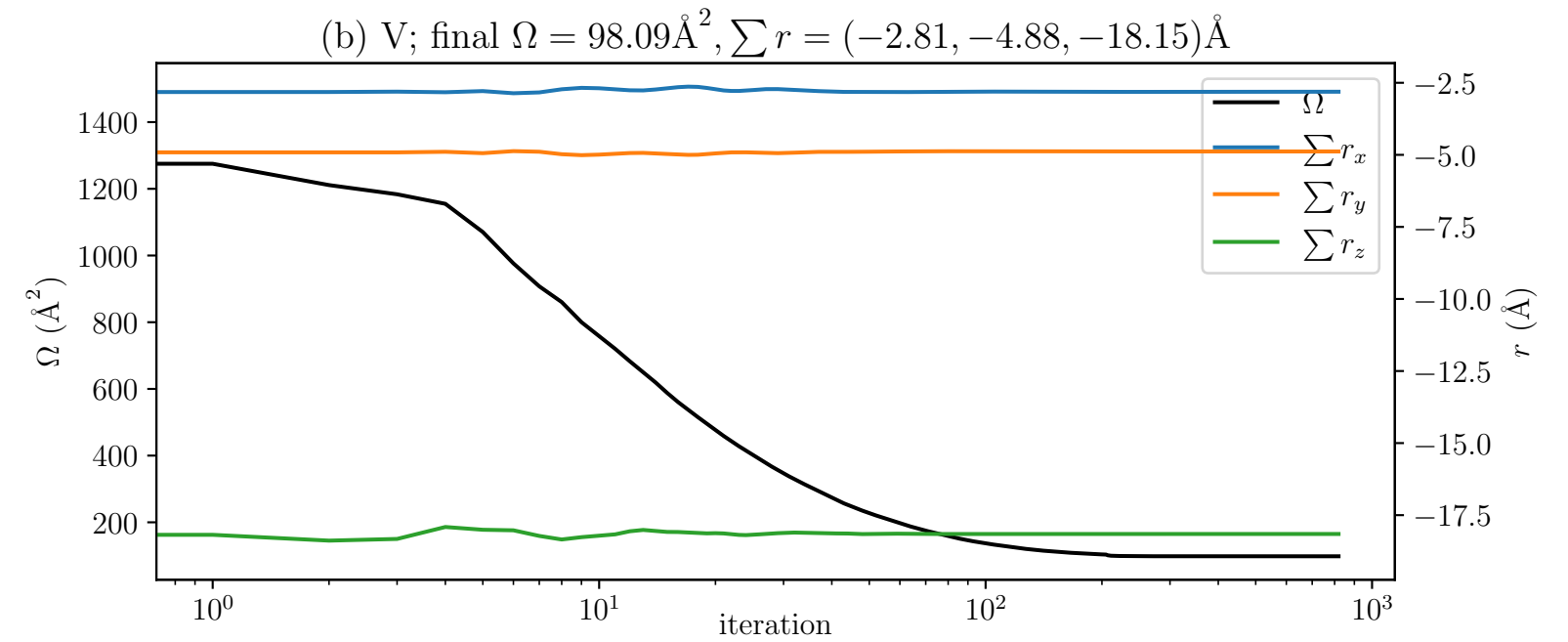
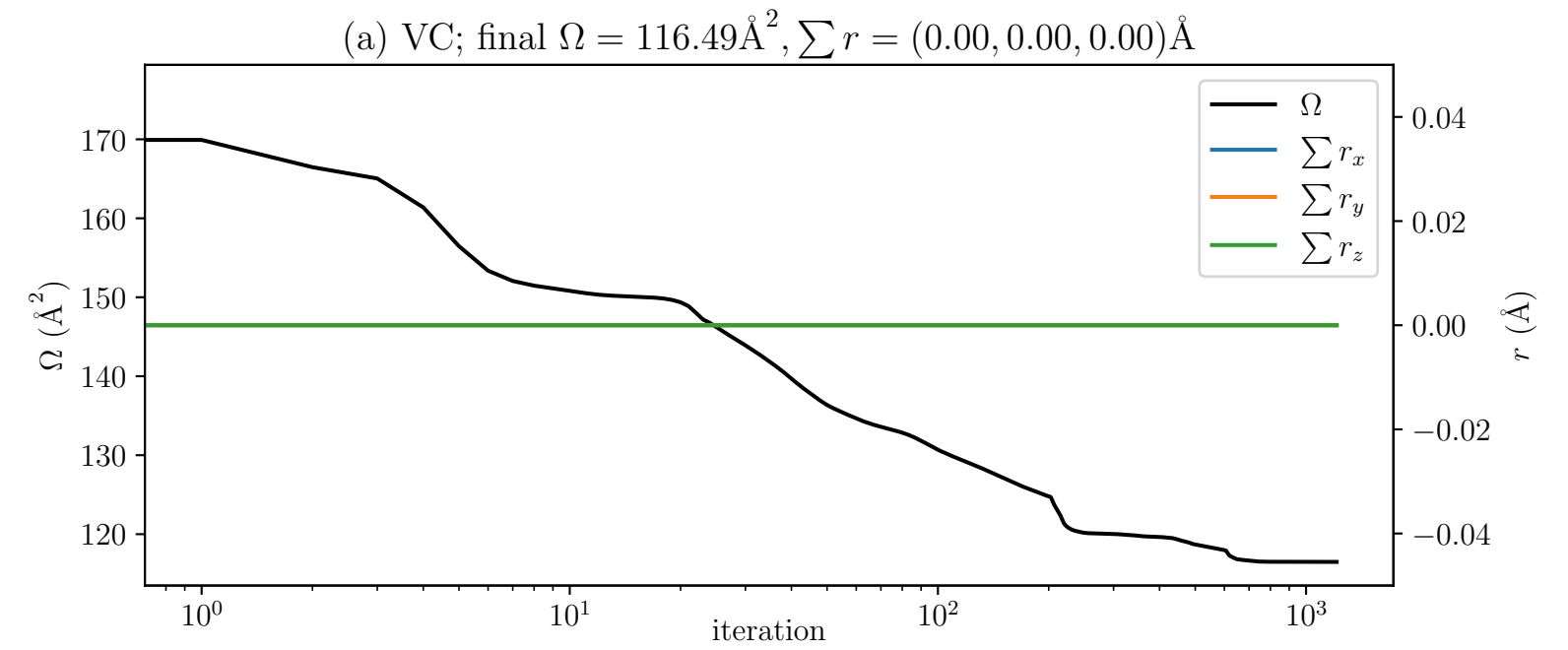


C₉B₃₆ (exclude semicore)
PW AiiDA UUID: ffe6d1d7-a646-4500-be2d-c70997e79c73
W90 AiiDA UUID: fefff387-f676-4591-94db-f9df151a65eb

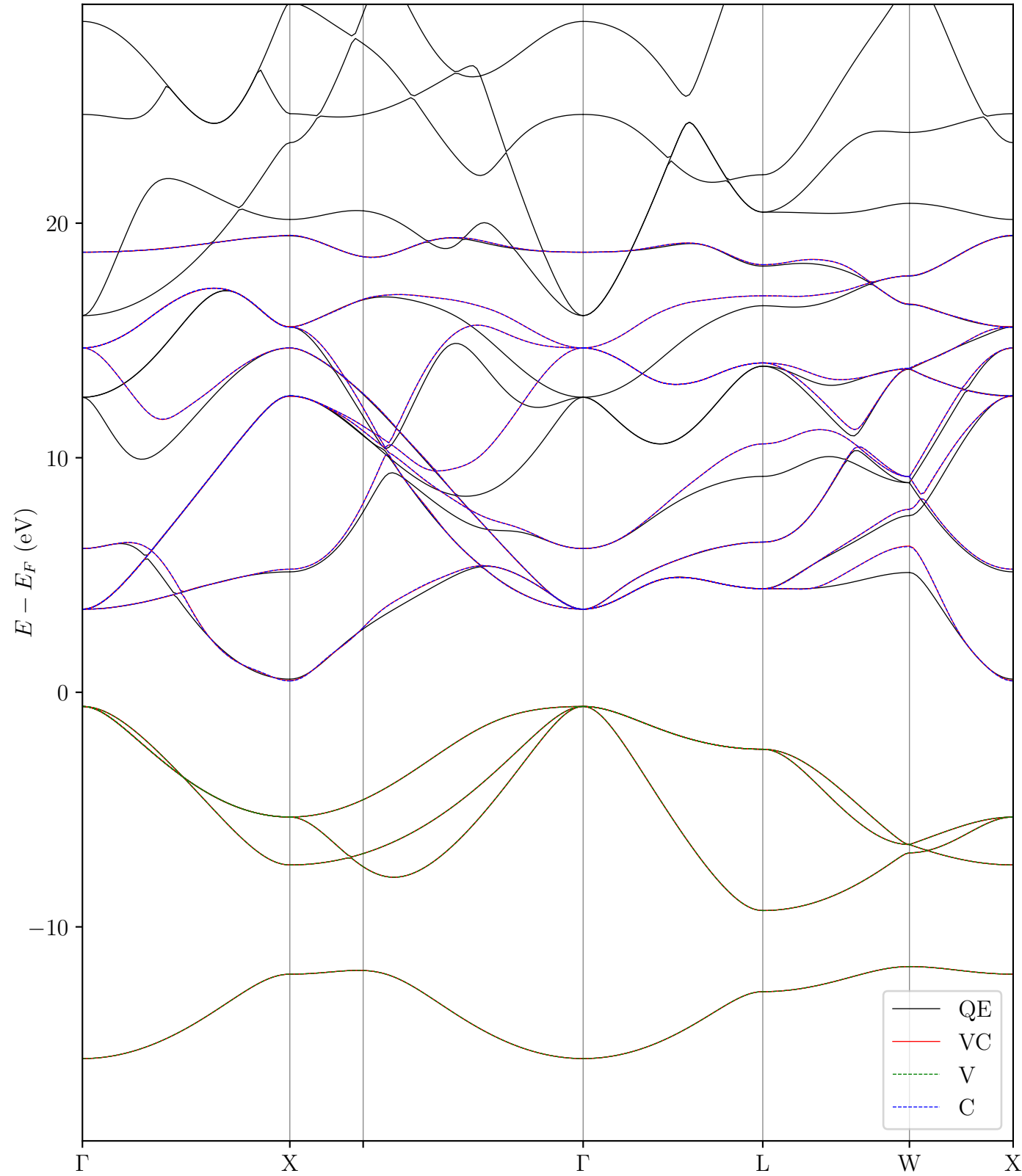


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.6	1.6	0.2	1.6	1.6	1.5	2.3
η_{max}	12.9	12.9	3.1	13.0	6.8	7.5	20.0



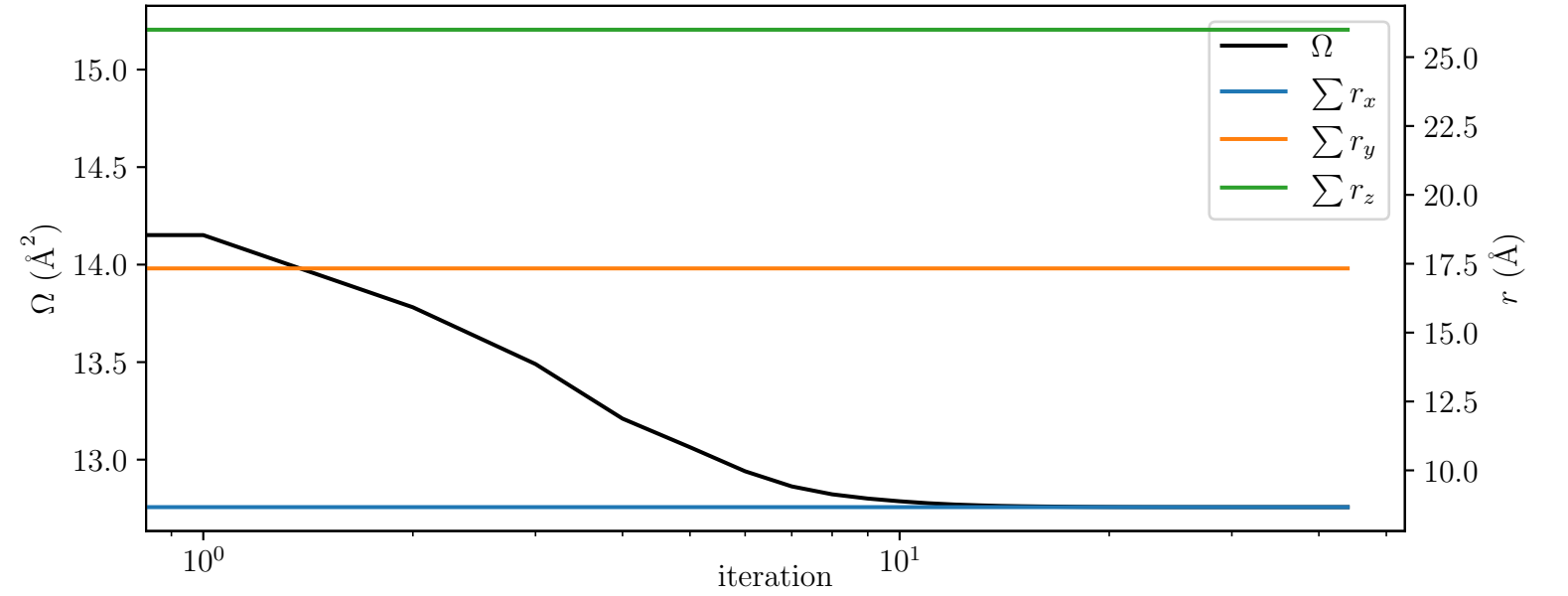
CBe₂ (exclude semicore)
PW AiiDA UUID: 8435169a-11e0-4a7f-8e19-e9075d8e7311
W90 AiiDA UUID: e26bee78-0a81-4949-be70-bd6c1c54294f



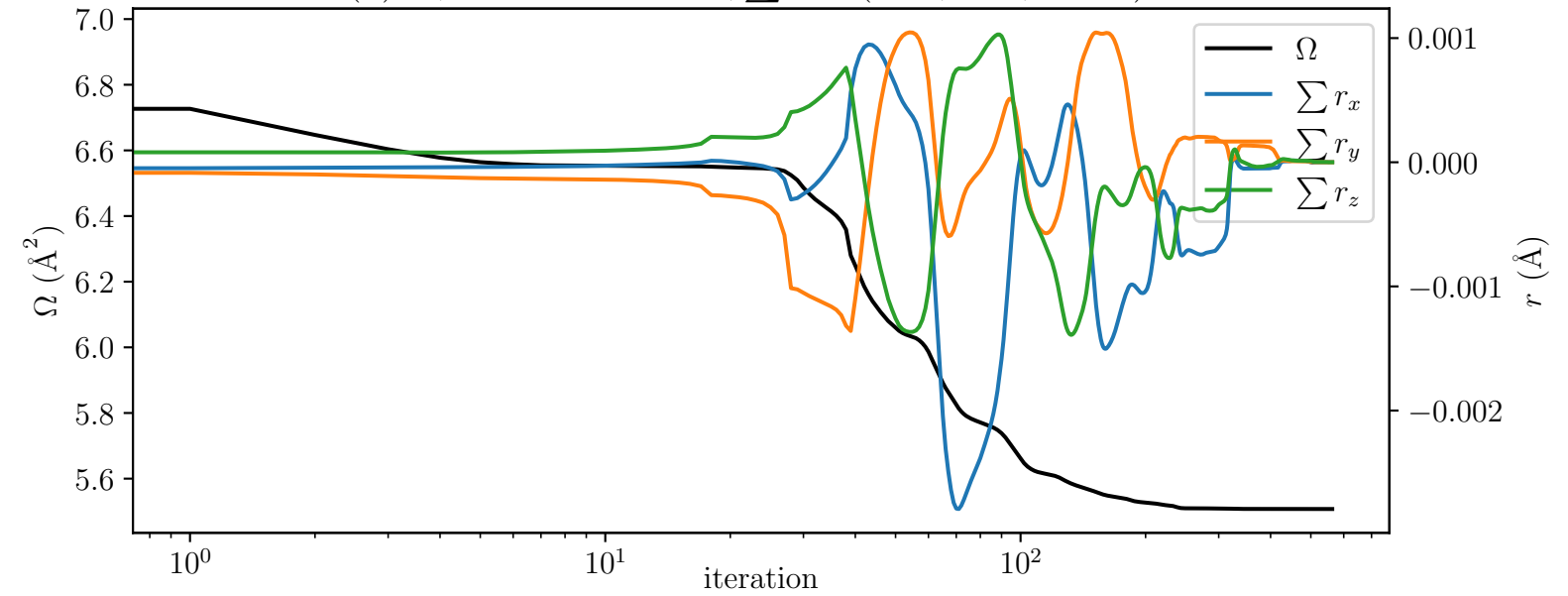
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	7.8	1.6	0.6	1.9	36.6	46.5	5.9
η_{max}	60.1	6.3	3.3	7.4	60.1	80.8	28.4

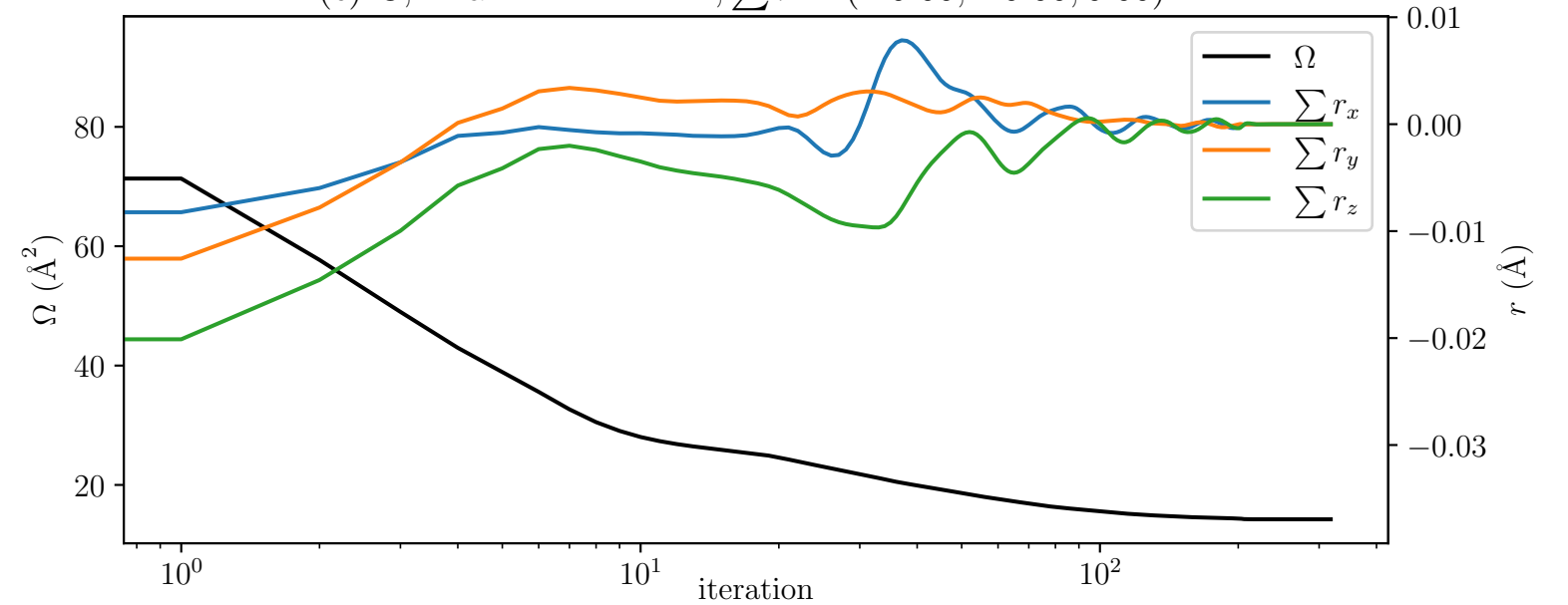
(a) VC; final $\Omega = 12.76 \text{ \AA}^2$, $\sum r = (8.67, 17.33, 26.00) \text{ \AA}$



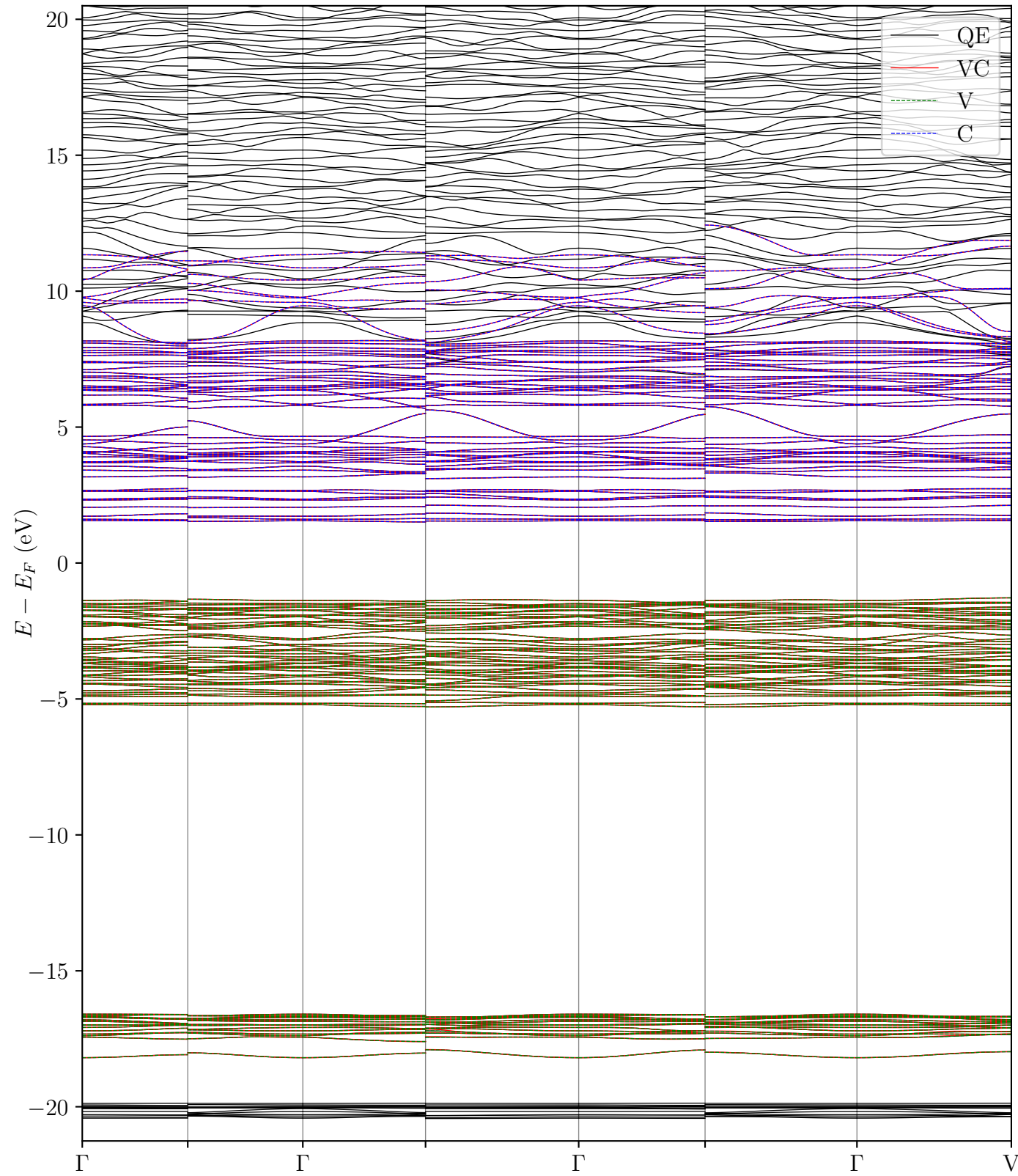
(b) V; final $\Omega = 5.51 \text{ \AA}^2$, $\sum r = (0.00, 0.00, -0.00) \text{ \AA}$



(c) C; final $\Omega = 14.24 \text{ \AA}^2$, $\sum r = (-0.00, -0.00, 0.00) \text{ \AA}$

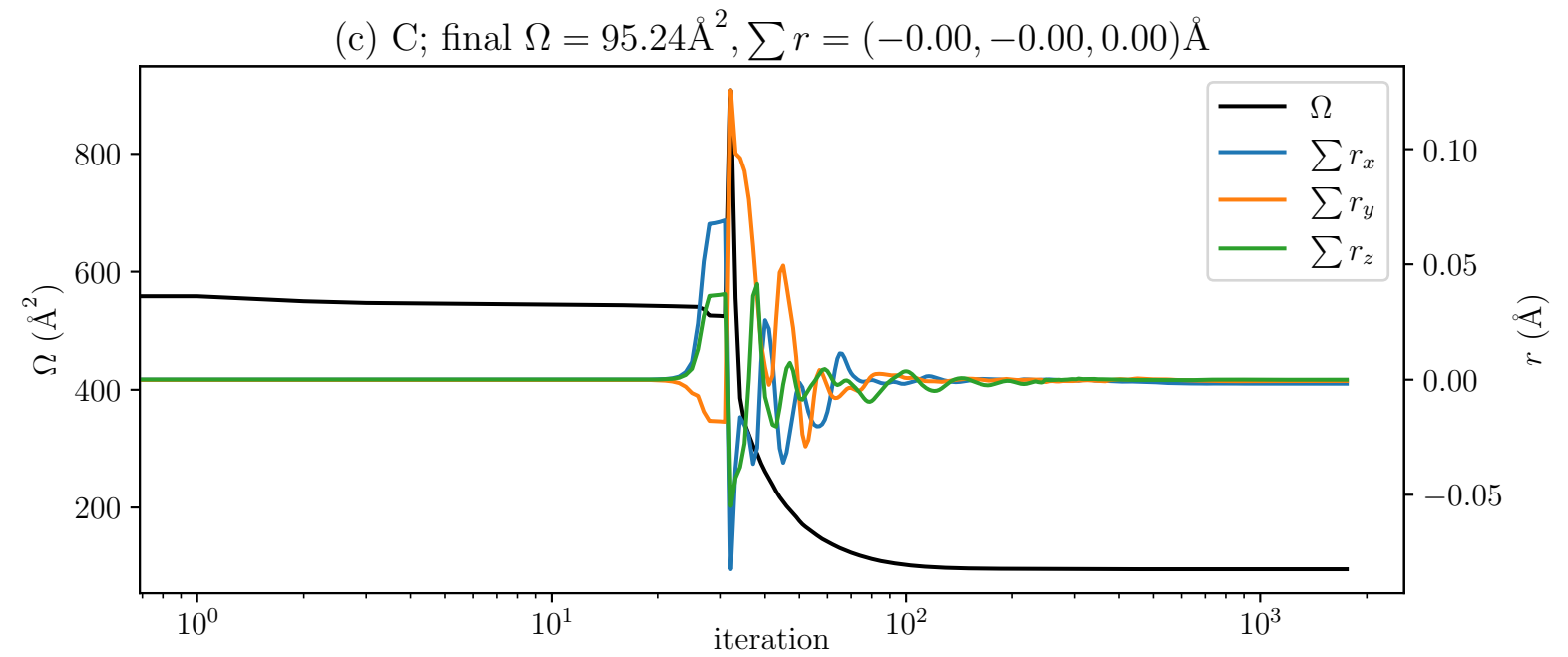
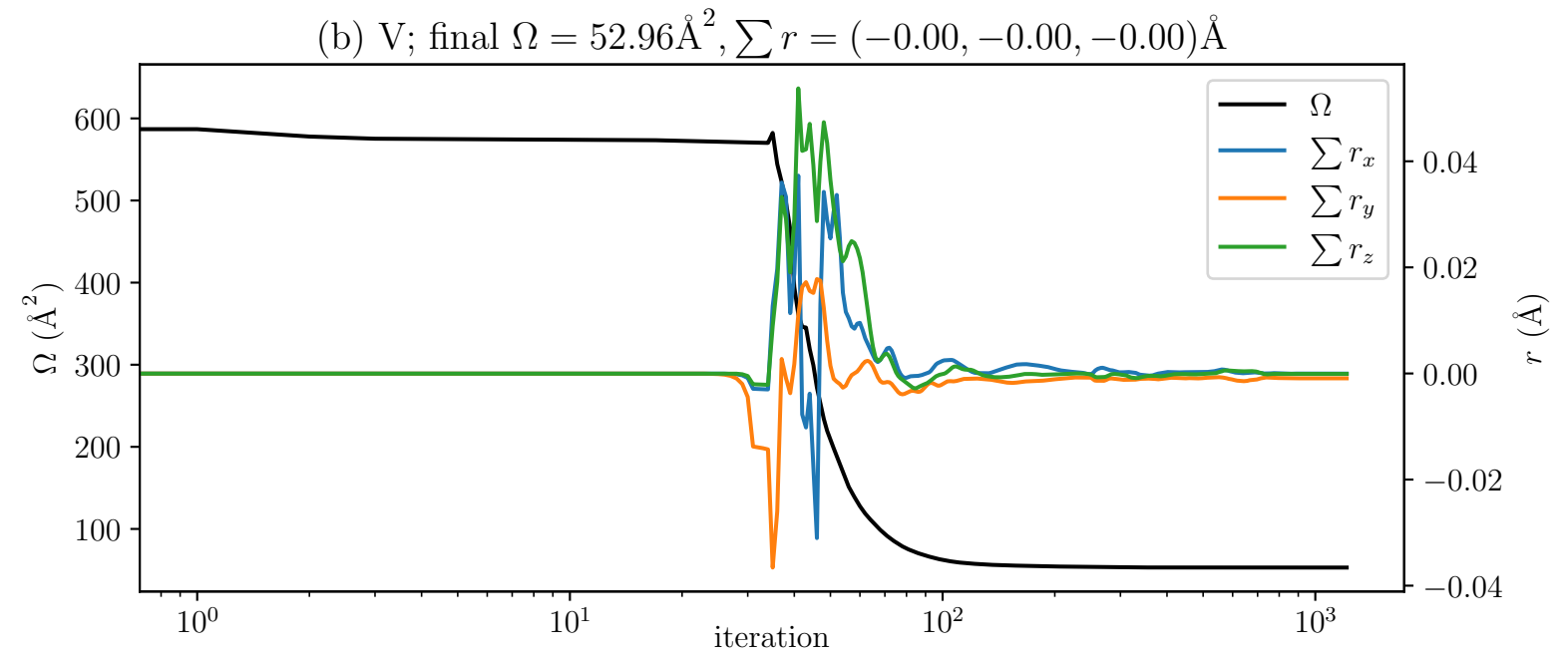
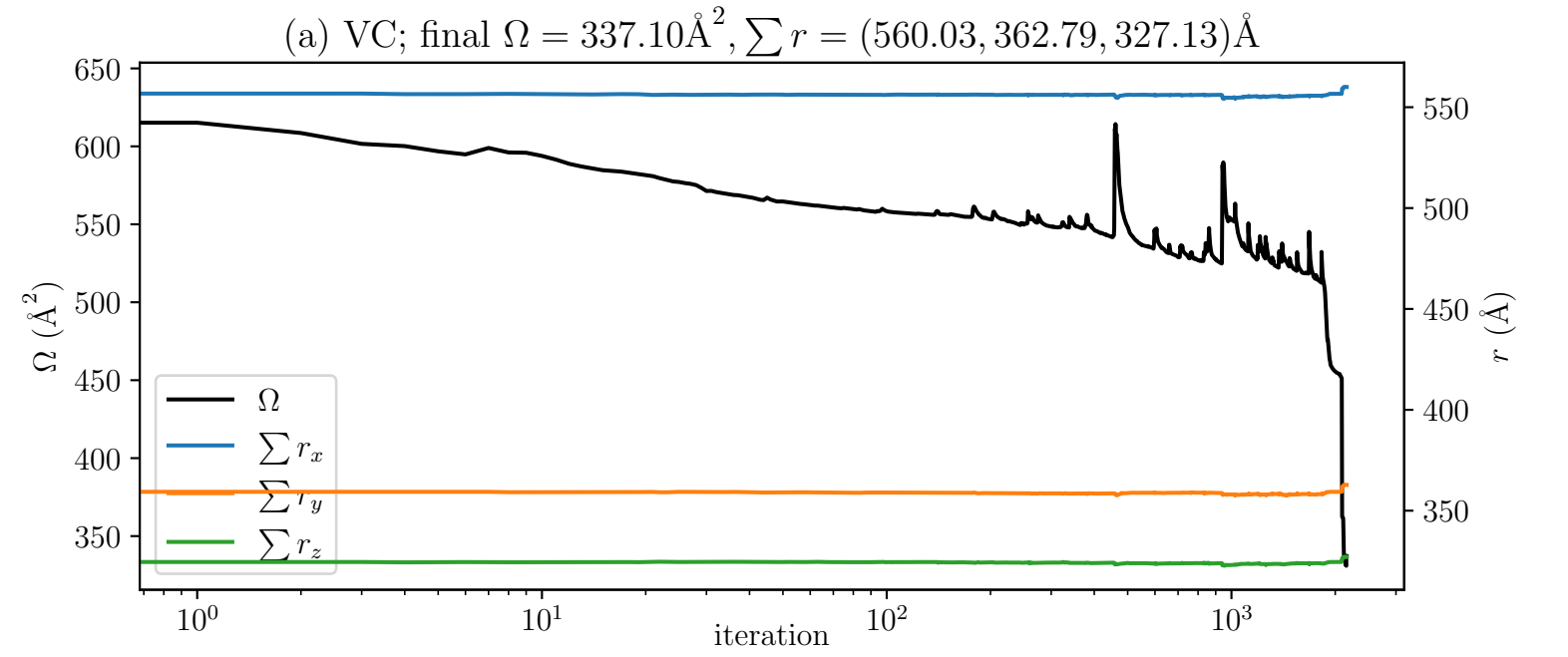


Ca₄O₁₄V₄ (exclude semicore)
PW AiiDA UUID: 60de1e59-73f1-4d8b-a8b2-def5ac34347c
W90 AiiDA UUID: b66f0e9d-7e17-40c4-9596-e41f0b11adbf

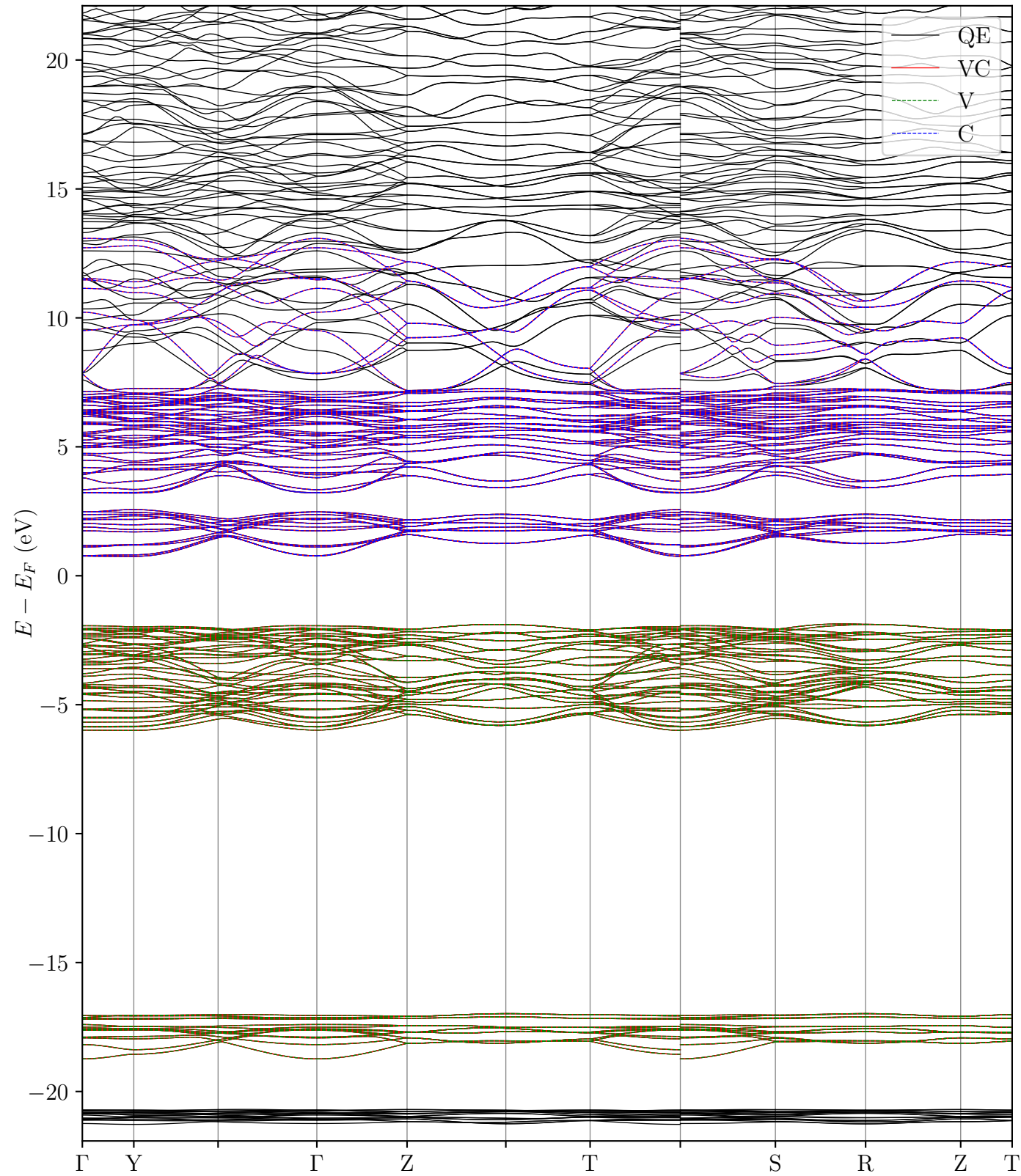


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	2.7	2.8	0.0	2.8	0.5	0.0	0.8
η_{max}	63.1	63.1	0.0	63.1	2.0	0.1	9.8



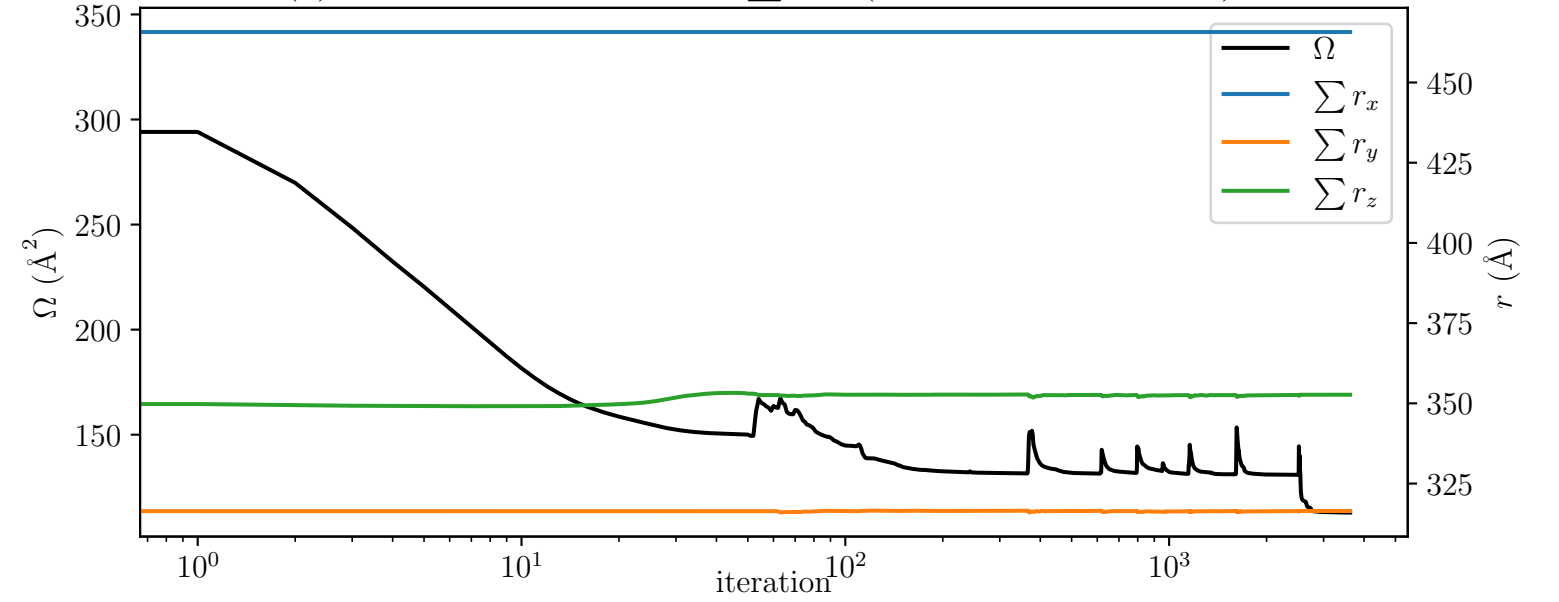
Ca₆O₁₄Ti₄ (exclude semicore)
PW AiiDA UUID: 1eba4941-5893-4214-9acd-1823802f2e14
W90 AiiDA UUID: 314bb490-1f42-4728-b676-6fb6afebeb03



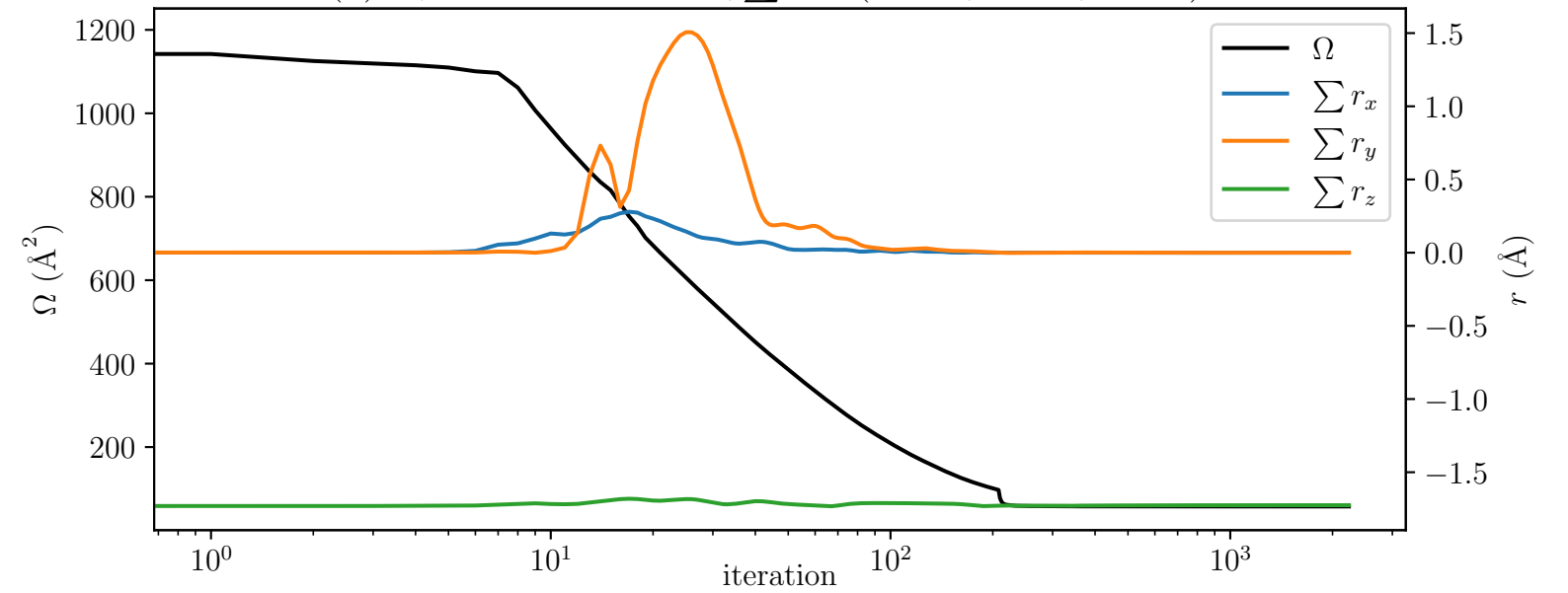
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.0	0.0	0.0	0.1	0.0	0.0	0.1
η_{max}	0.3	0.3	0.5	0.6	0.1	0.3	1.7

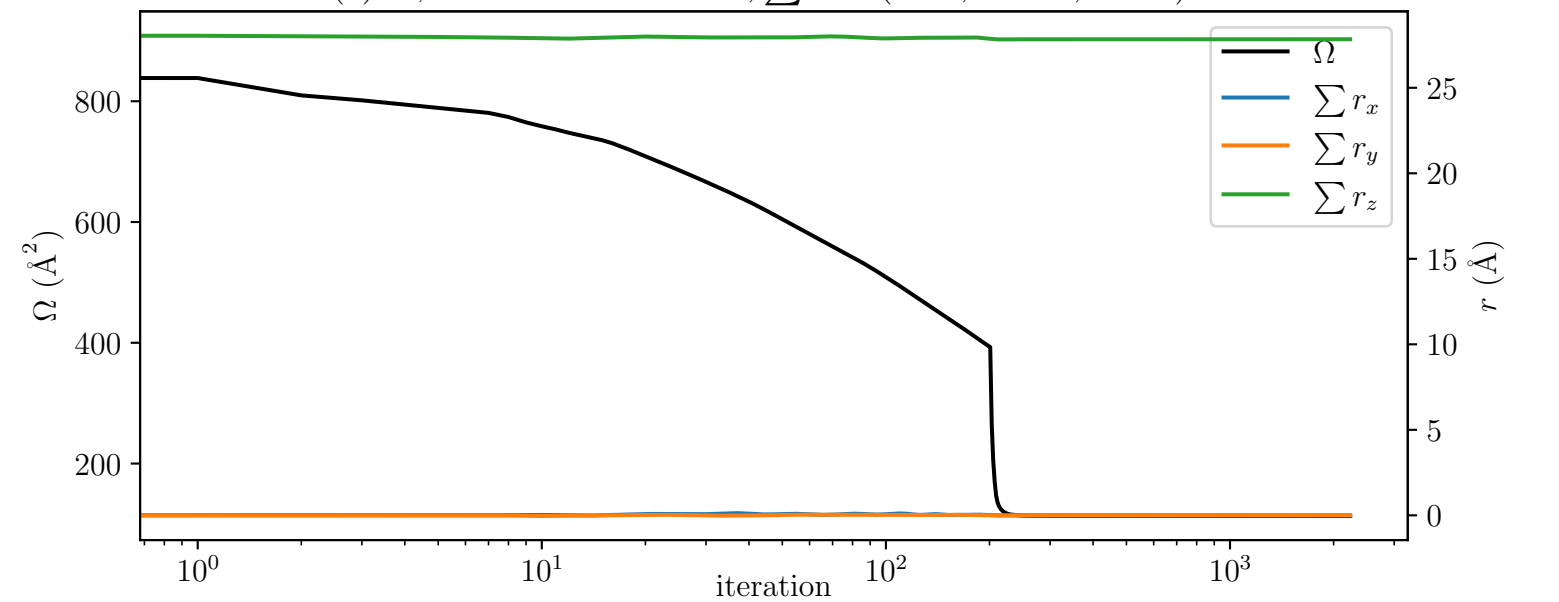
(a) VC; final $\Omega = 112.95 \text{ \AA}^2$, $\sum r = (465.73, 316.45, 352.68) \text{ \AA}$



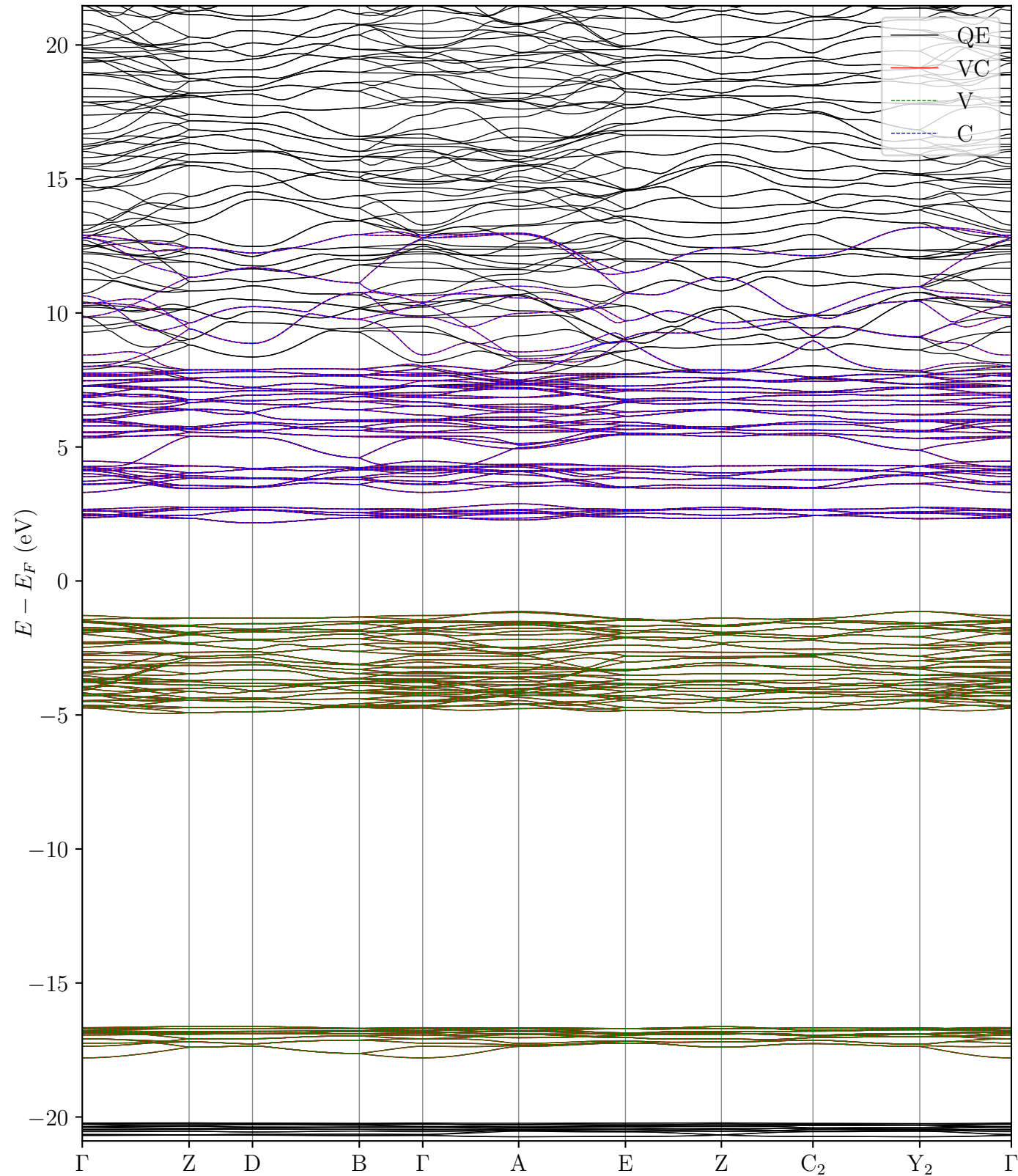
(b) V; final $\Omega = 57.68 \text{ \AA}^2$, $\sum r = (-0.00, -0.00, -1.73) \text{ \AA}$



(c) C; final $\Omega = 113.10 \text{ \AA}^2$, $\sum r = (0.00, -0.00, 27.84) \text{ \AA}$

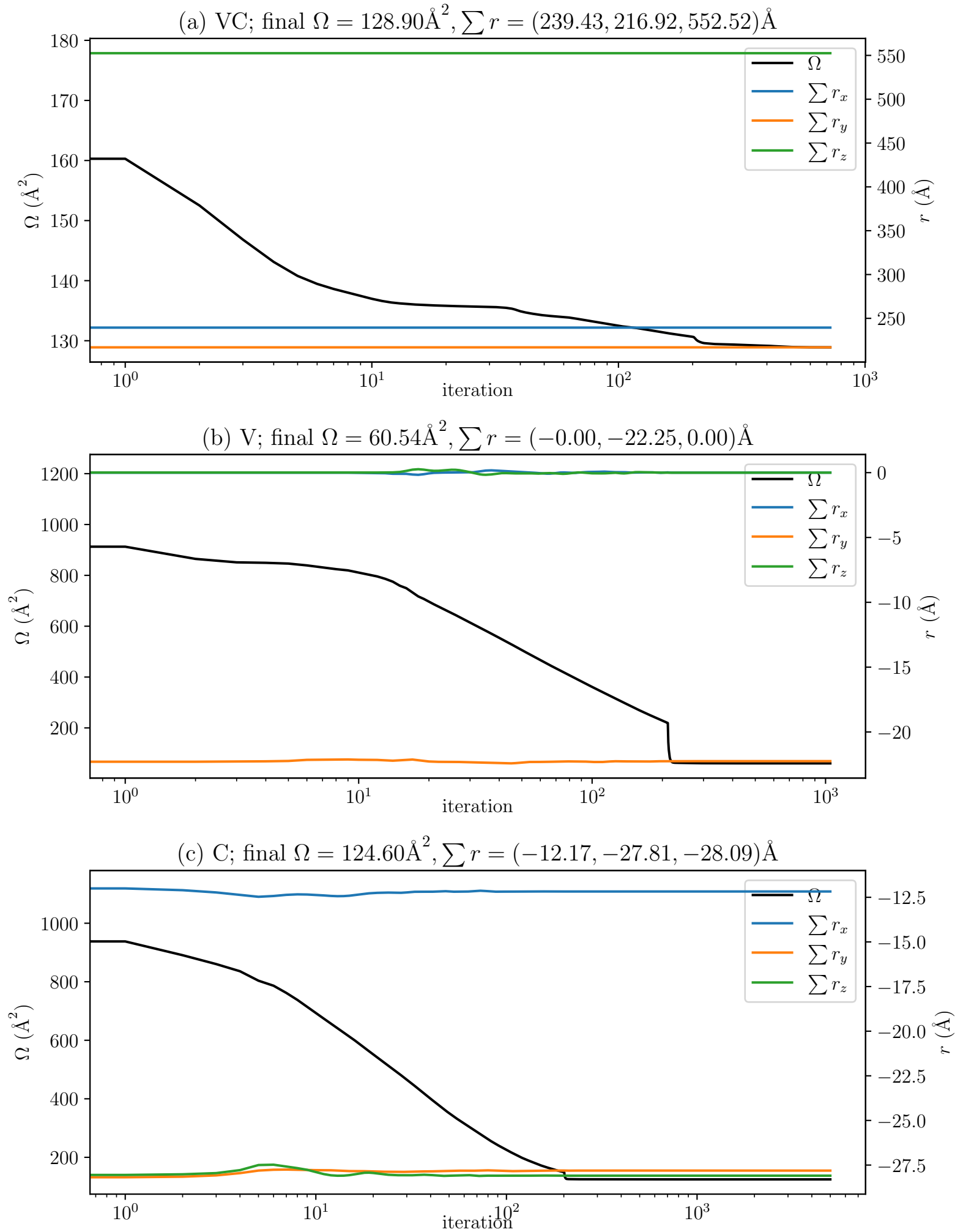


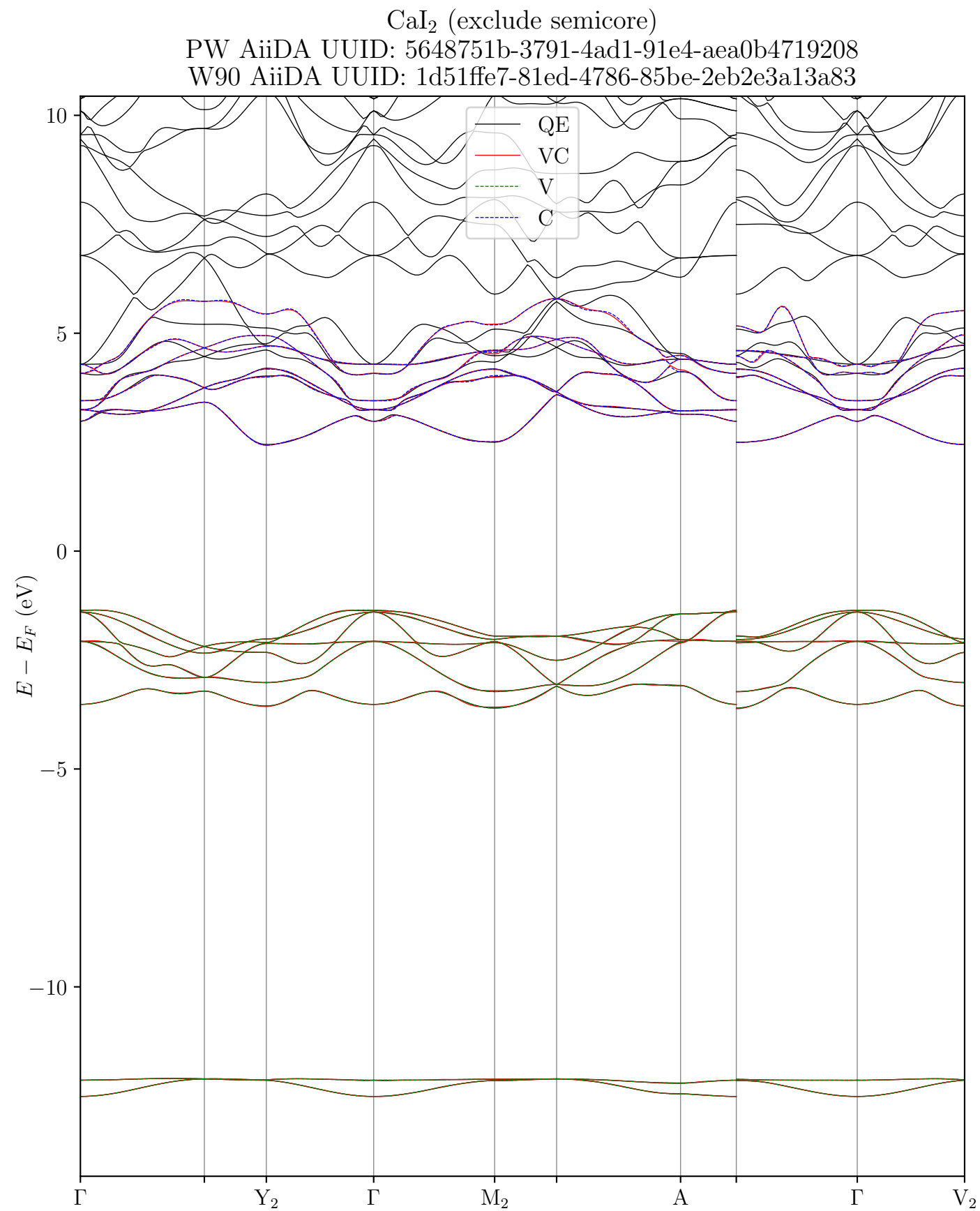
Ca₆O₁₆V₄ (exclude semicore)
PW AiiDA UUID: 6a8c65f8-a707-4dc6-865b-7fe7a818b059
W90 AiiDA UUID: fe56fe5e-c54c-40a0-abf8-af37a8028016



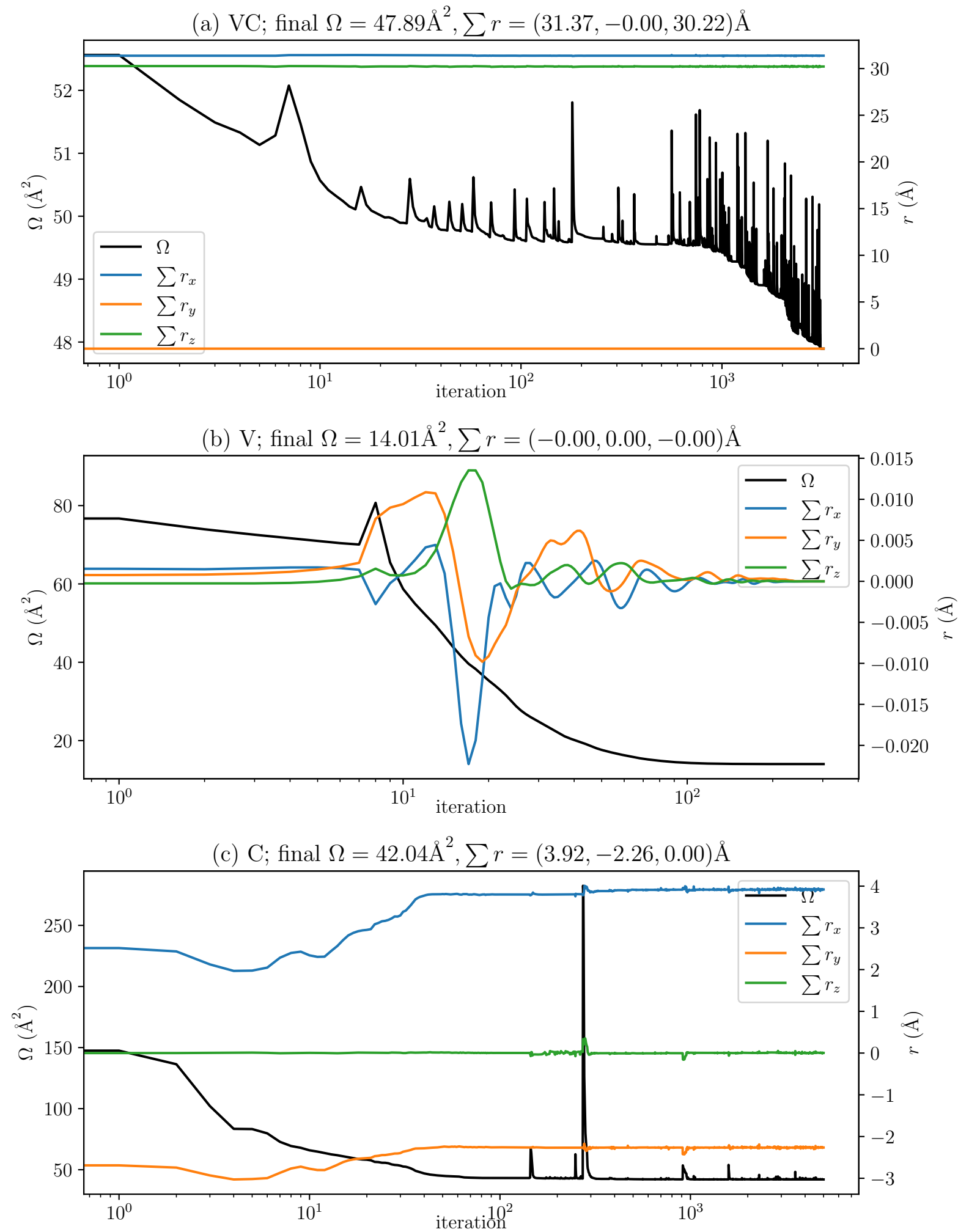
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.1	0.1	0.0	0.1	0.1	0.1	0.4
η_{max}	2.0	2.0	0.0	2.0	0.0	0.0	3.1

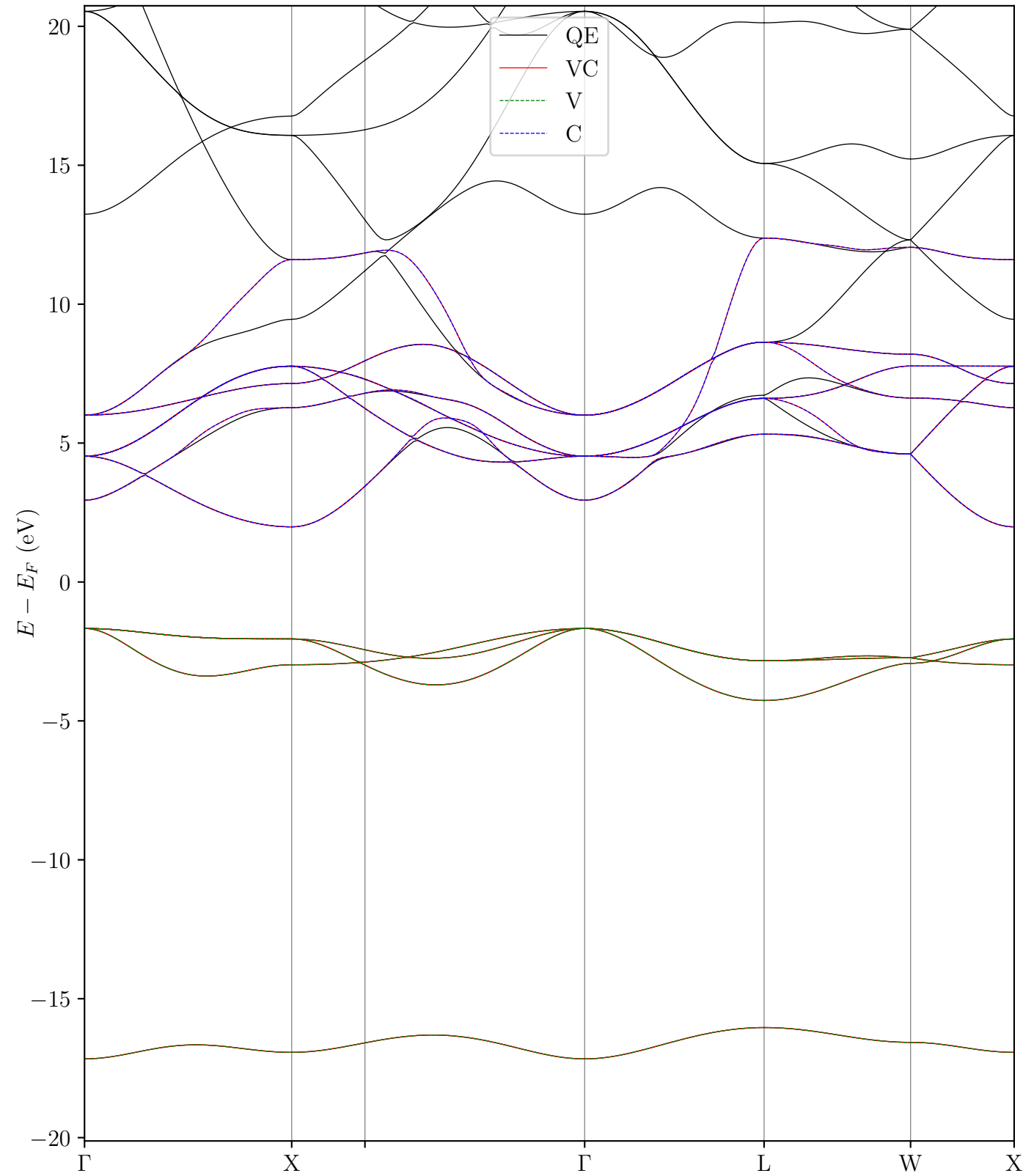




	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	5.7	5.7	0.1	5.7	7.6	7.5	8.1
η_{max}	34.0	34.0	0.6	34.0	0.2	0.2	50.3

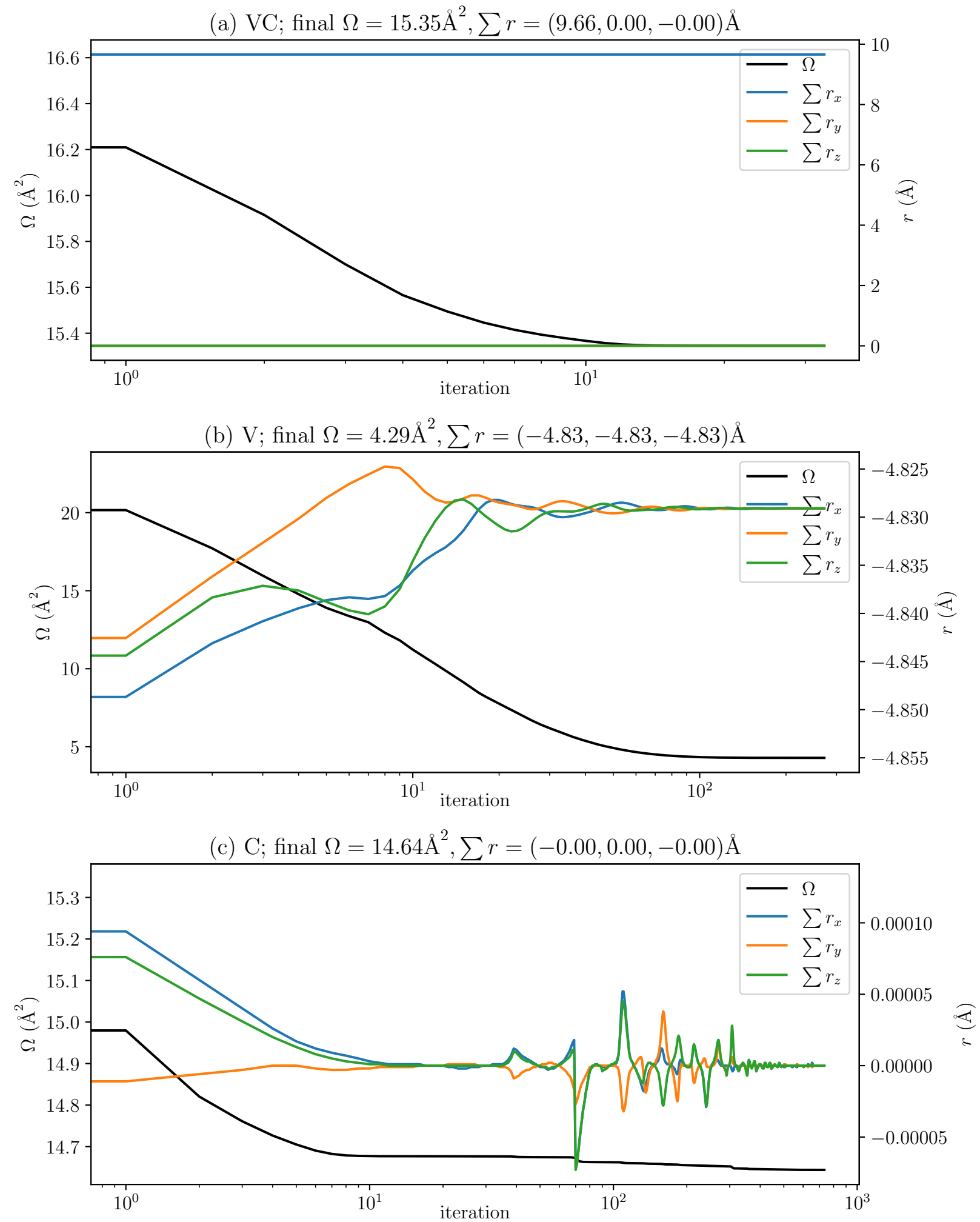


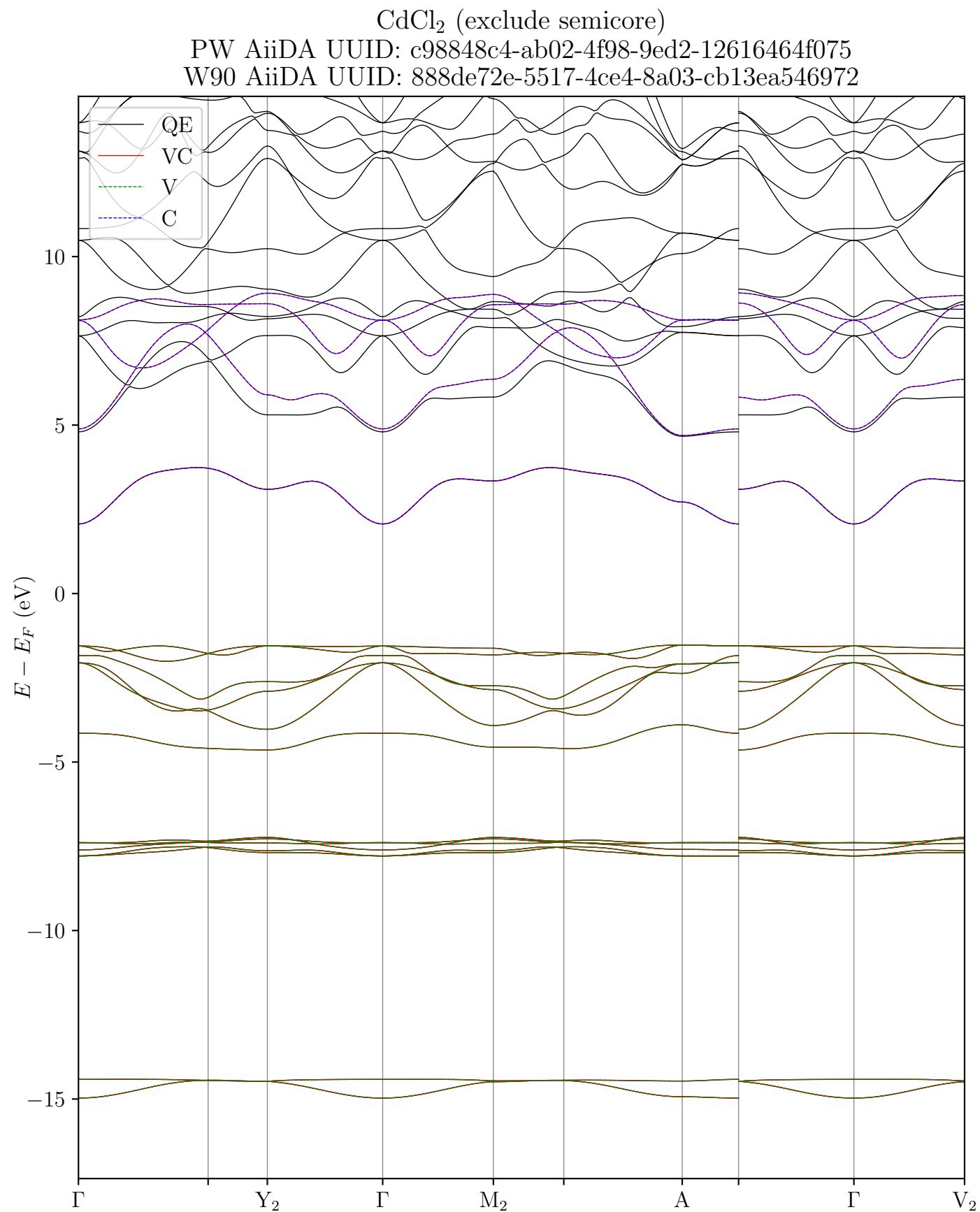
CaO (exclude semicore)
PW AiiDA UUID: 57f75c4f-a2d1-492d-96b9-153802fbf028
W90 AiiDA UUID: 596dc626-b793-4eae-a7cc-51ab9bc9a423



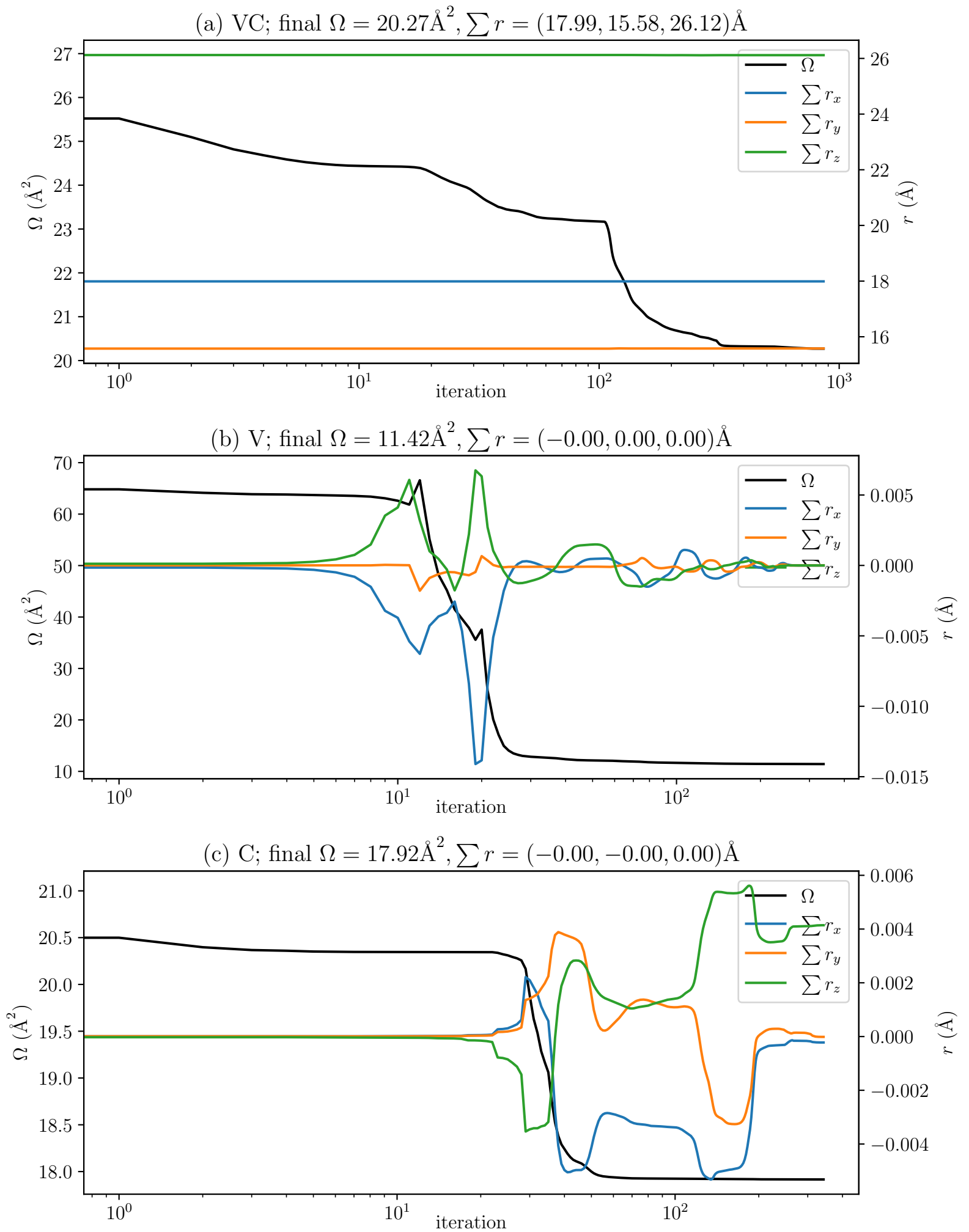
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.4	1.4	0.0	1.4	0.2	0.3	0.9
η_{max}	8.5	8.5	0.2	8.6	0.2	0.3	4.6

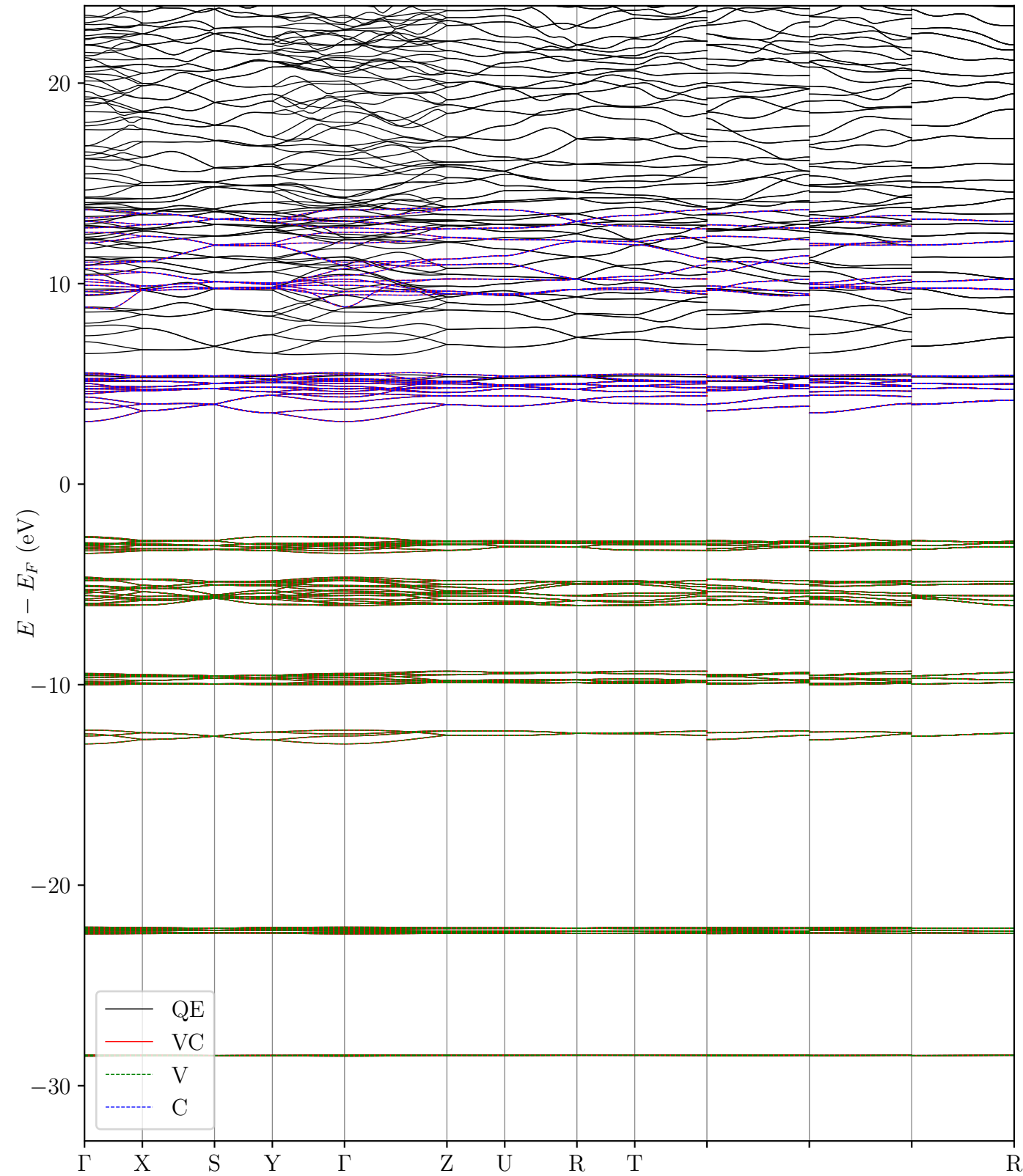




	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.4	0.4	0.0	0.4	0.3	0.4	1.1
η_{max}	3.1	3.1	0.3	3.1	0.1	0.2	6.1



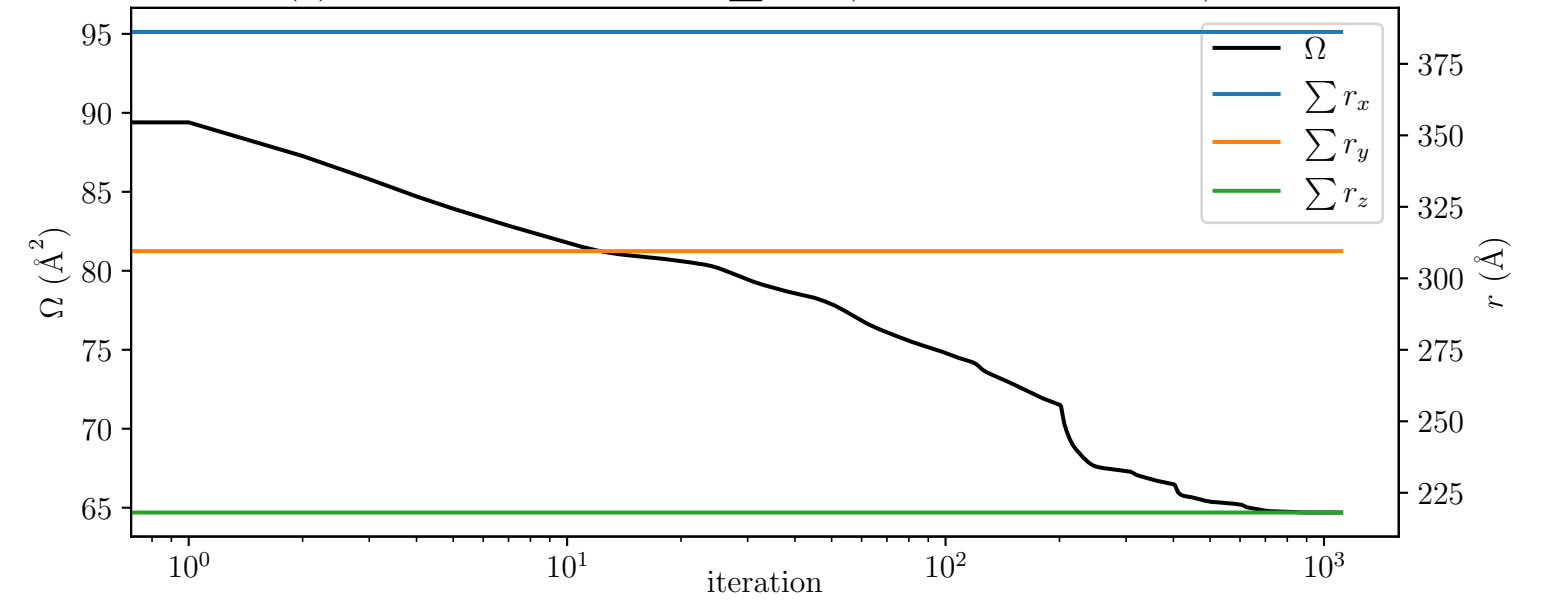
Cl₄Li₄O₁₆ (exclude semicore)
PW AiiDA UUID: 5f8bd061-a5a6-47a1-907a-4485b9b859c4
W90 AiiDA UUID: 84f9d7d2-a1e9-4216-847d-80cfedf5d0f9



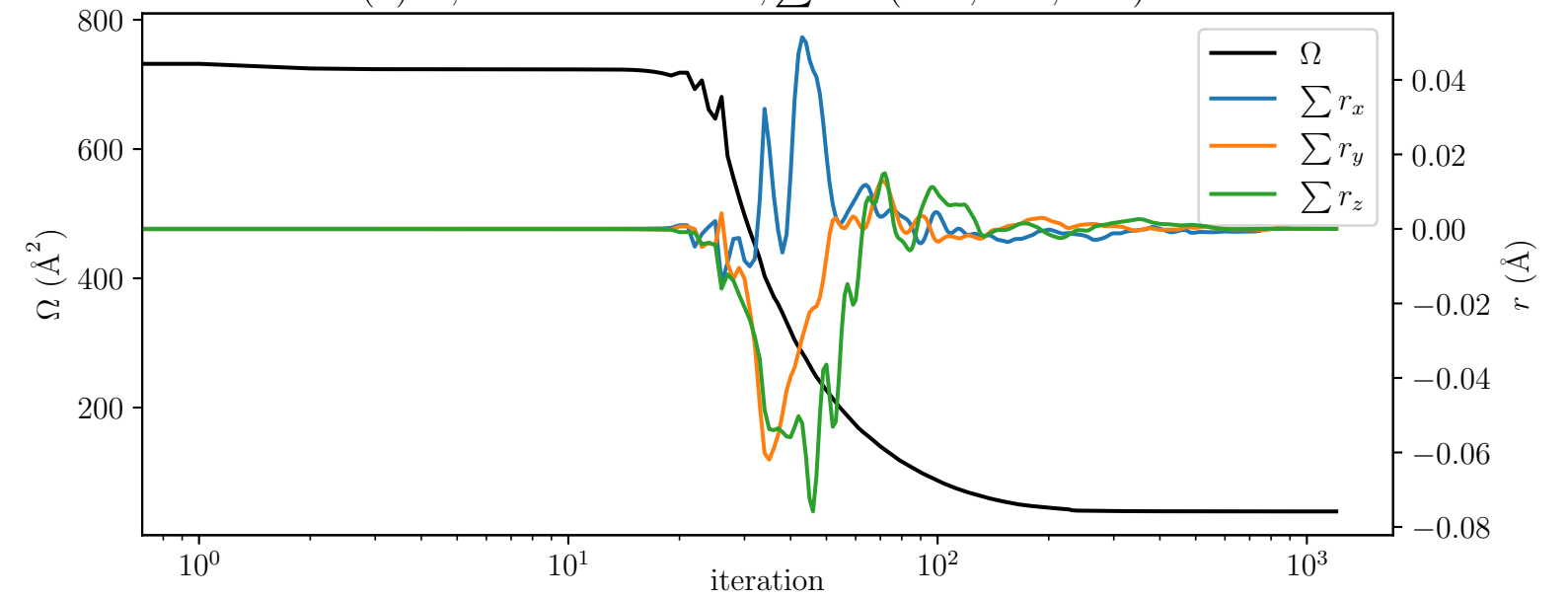
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.1	0.1	0.0	0.1	0.1	0.1	1.6
η_{max}	1.5	1.5	0.0	1.5	0.0	0.0	18.0

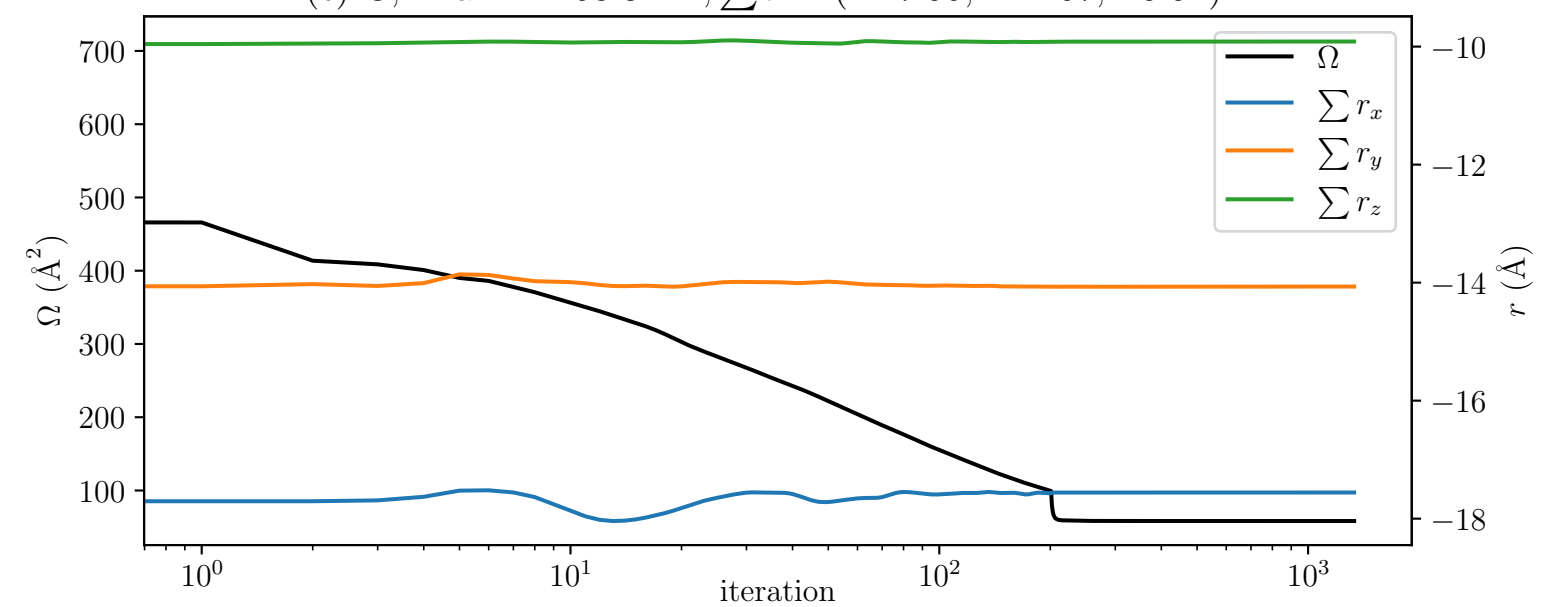
(a) VC; final $\Omega = 64.69 \text{ \AA}^2$, $\sum r = (386.17, 309.51, 218.09) \text{ \AA}$



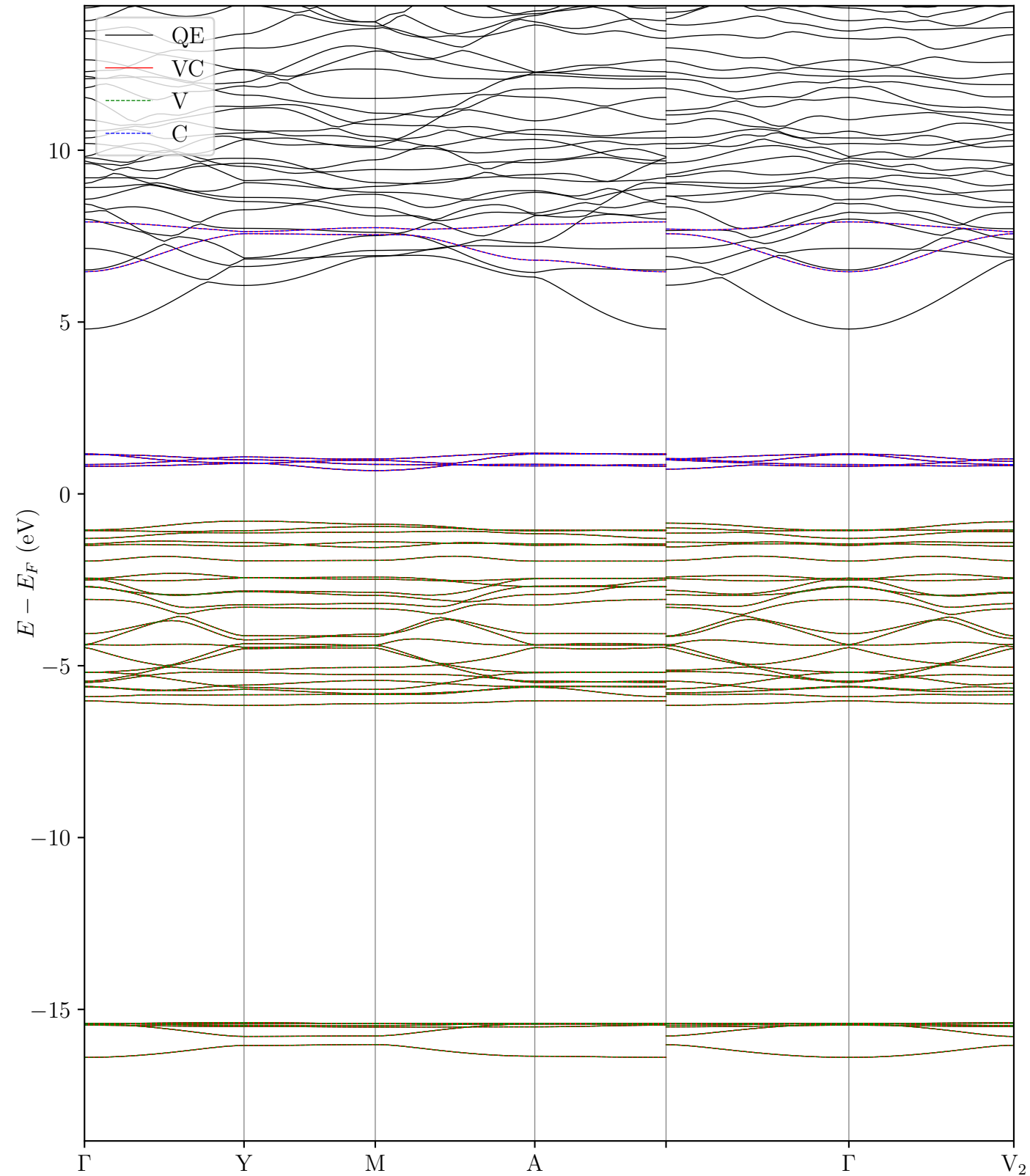
(b) V; final $\Omega = 39.26 \text{ \AA}^2$, $\sum r = (0.00, 0.00, 0.00) \text{ \AA}$



(c) C; final $\Omega = 58.32 \text{ \AA}^2$, $\sum r = (-17.56, -14.07, -9.91) \text{ \AA}$



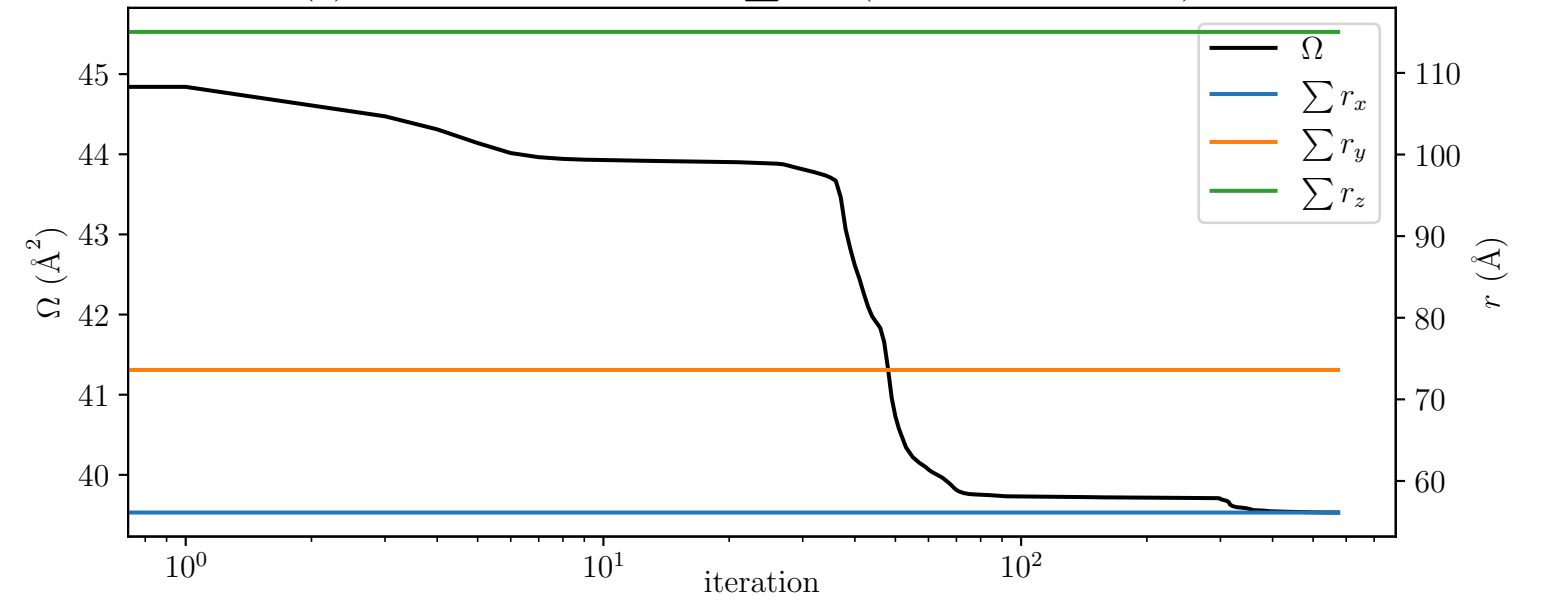
Cl₆Rh₂ (exclude semicore)
PW AiiDA UUID: 3146ce38-992a-497e-bcf5-493716ab5b03
W90 AiiDA UUID: 5681d817-851d-498e-b9a9-2d7e1ca633ed



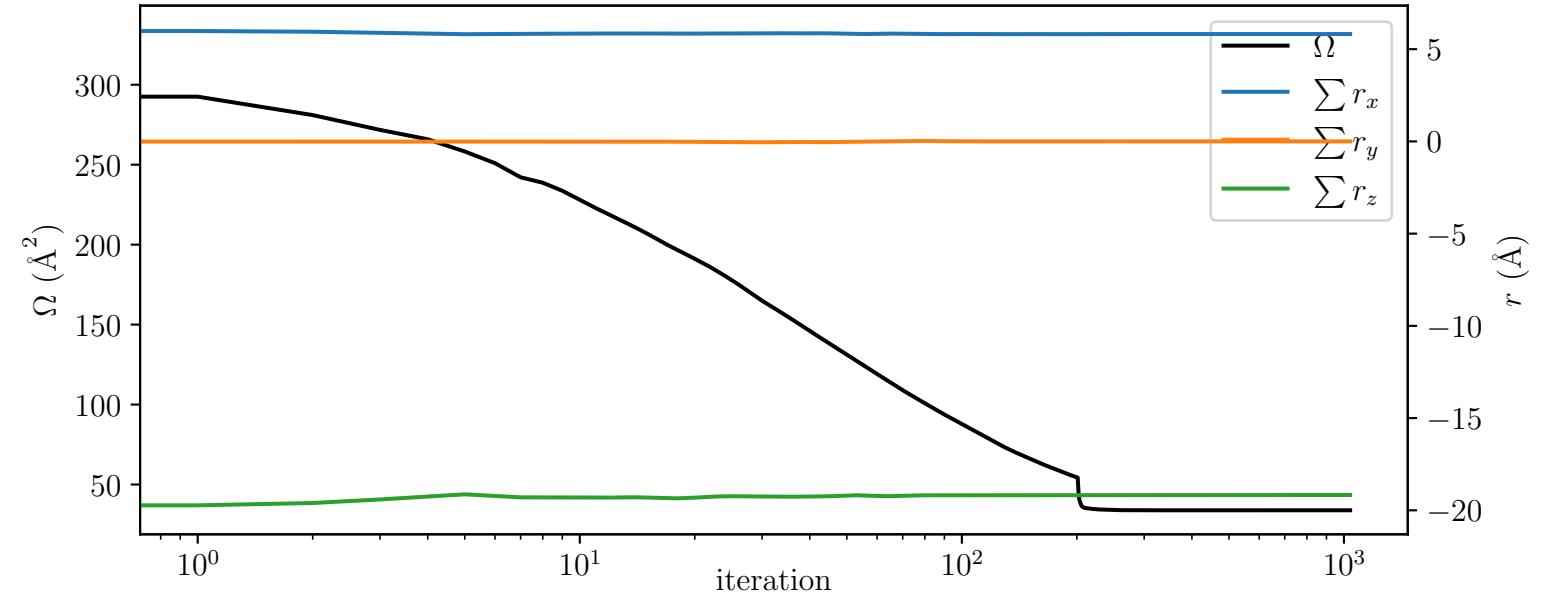
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.1	0.1	0.0	0.1	0.1	0.1	0.3
η_{max}	0.9	0.9	0.1	0.9	0.2	0.4	2.1

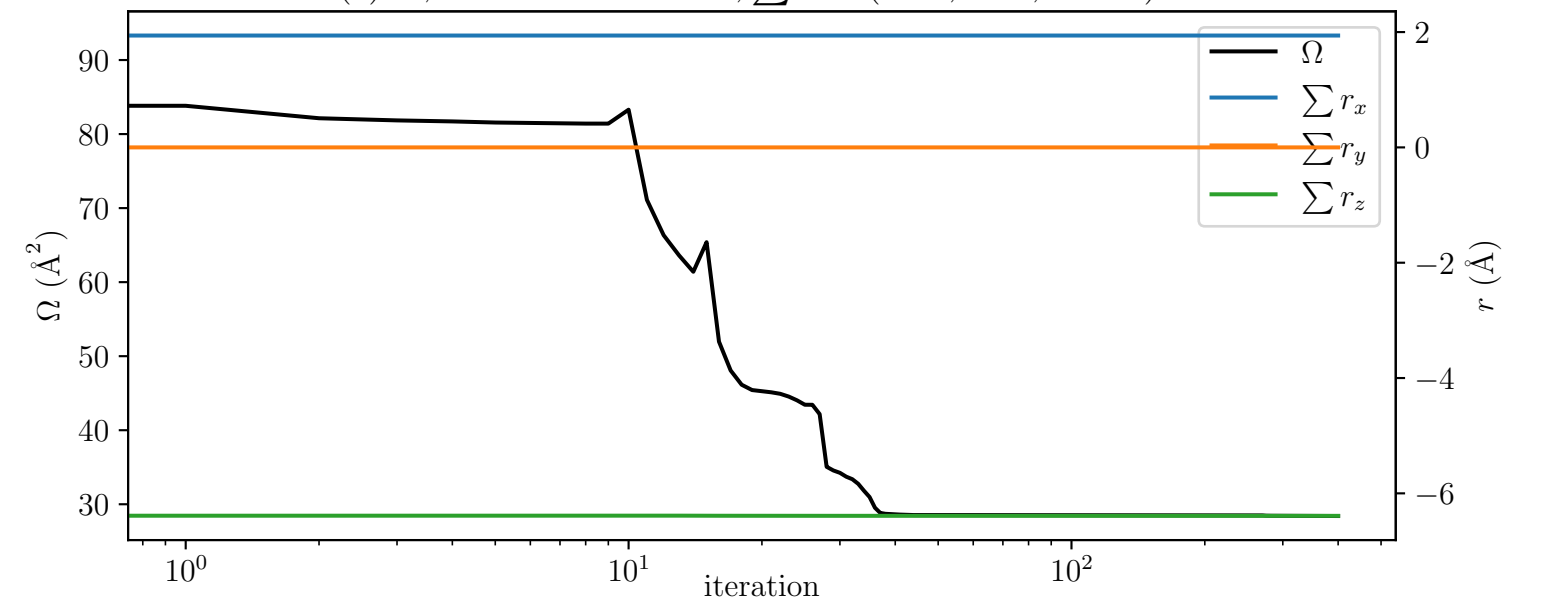
(a) VC; final $\Omega = 39.53 \text{ \AA}^2$, $\sum r = (56.13, 73.60, 115.02) \text{ \AA}$

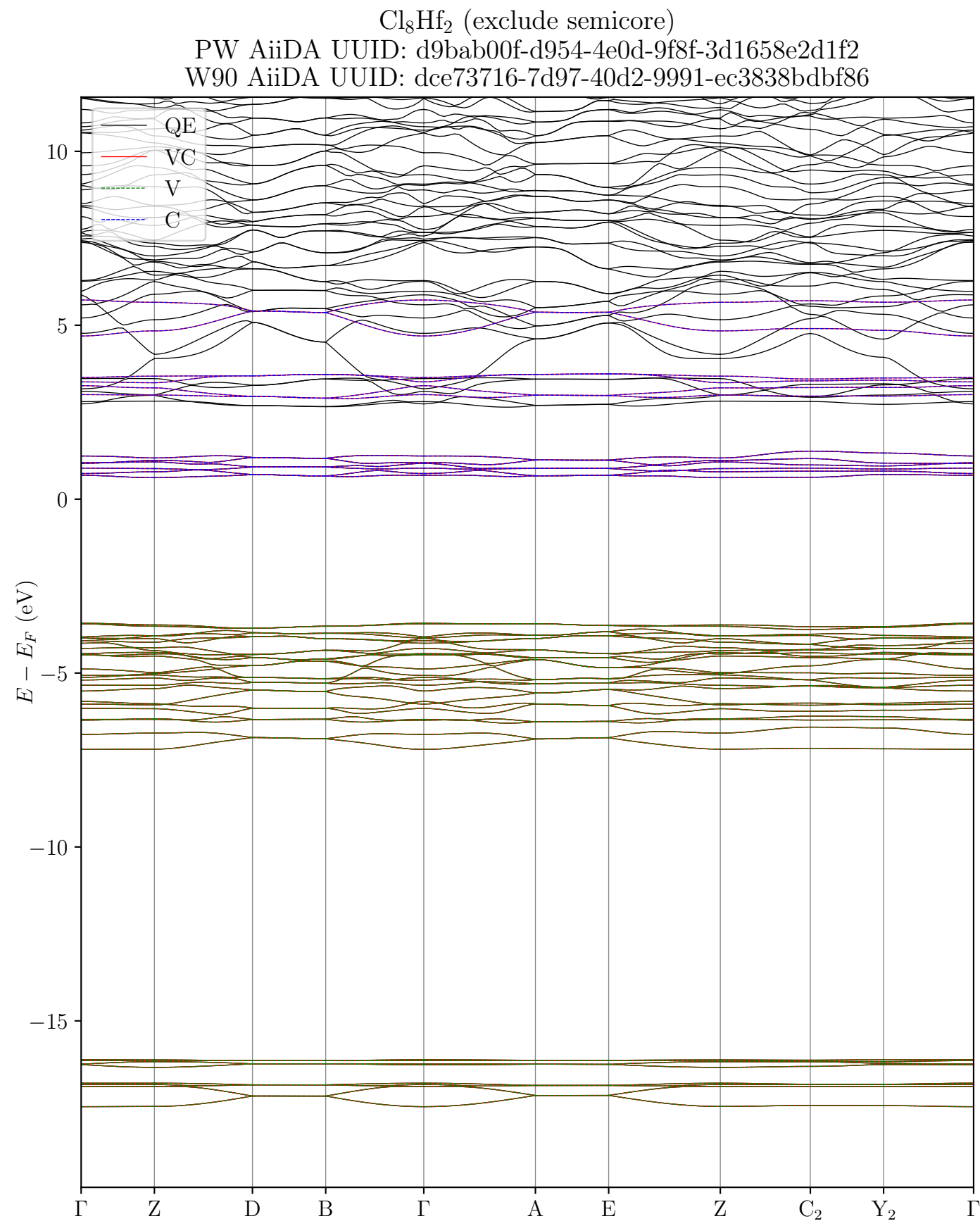


(b) V; final $\Omega = 33.89 \text{ \AA}^2$, $\sum r = (5.82, 0.00, -19.17) \text{ \AA}$



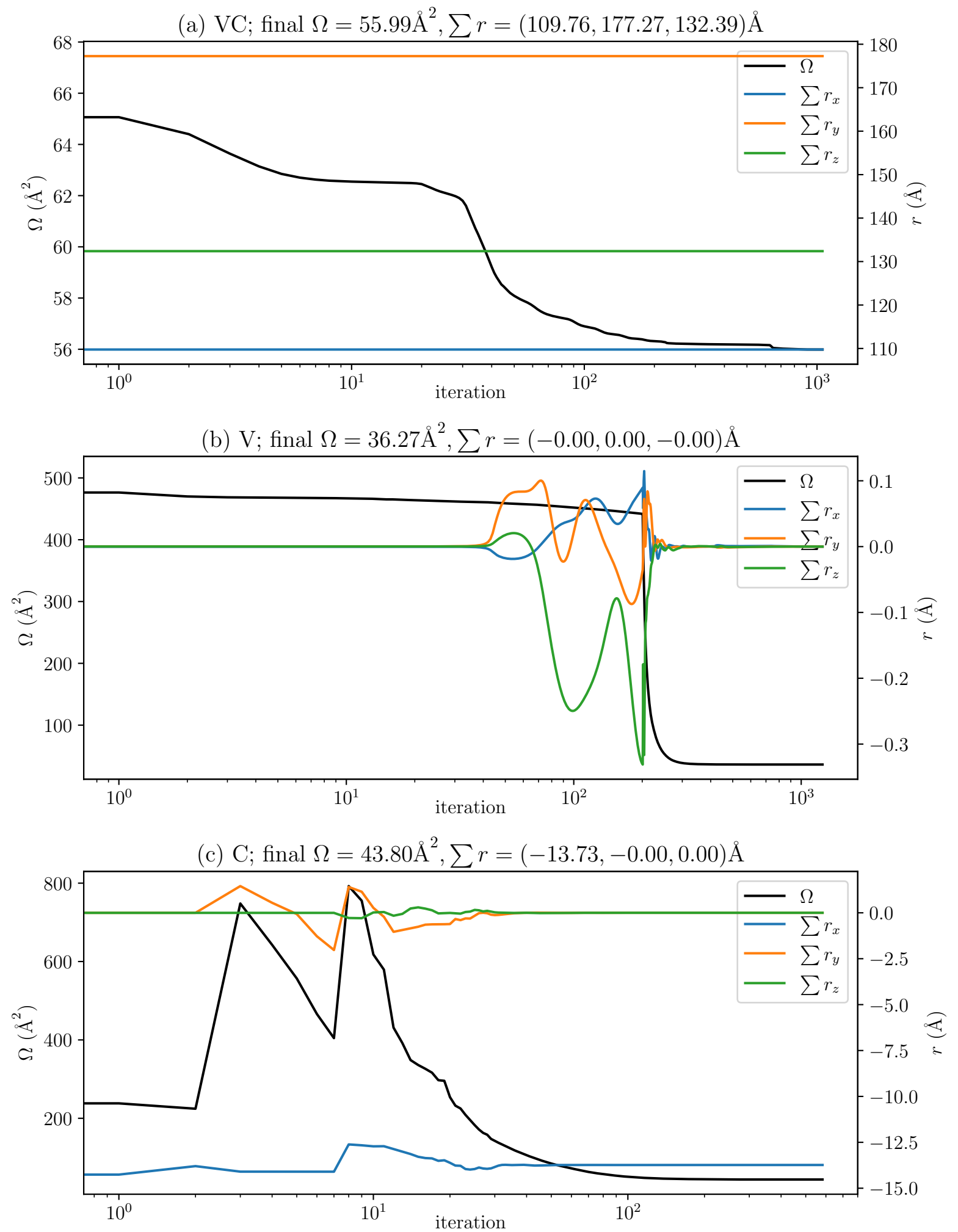
(c) C; final $\Omega = 28.41 \text{ \AA}^2$, $\sum r = (1.94, 0.00, -6.39) \text{ \AA}$

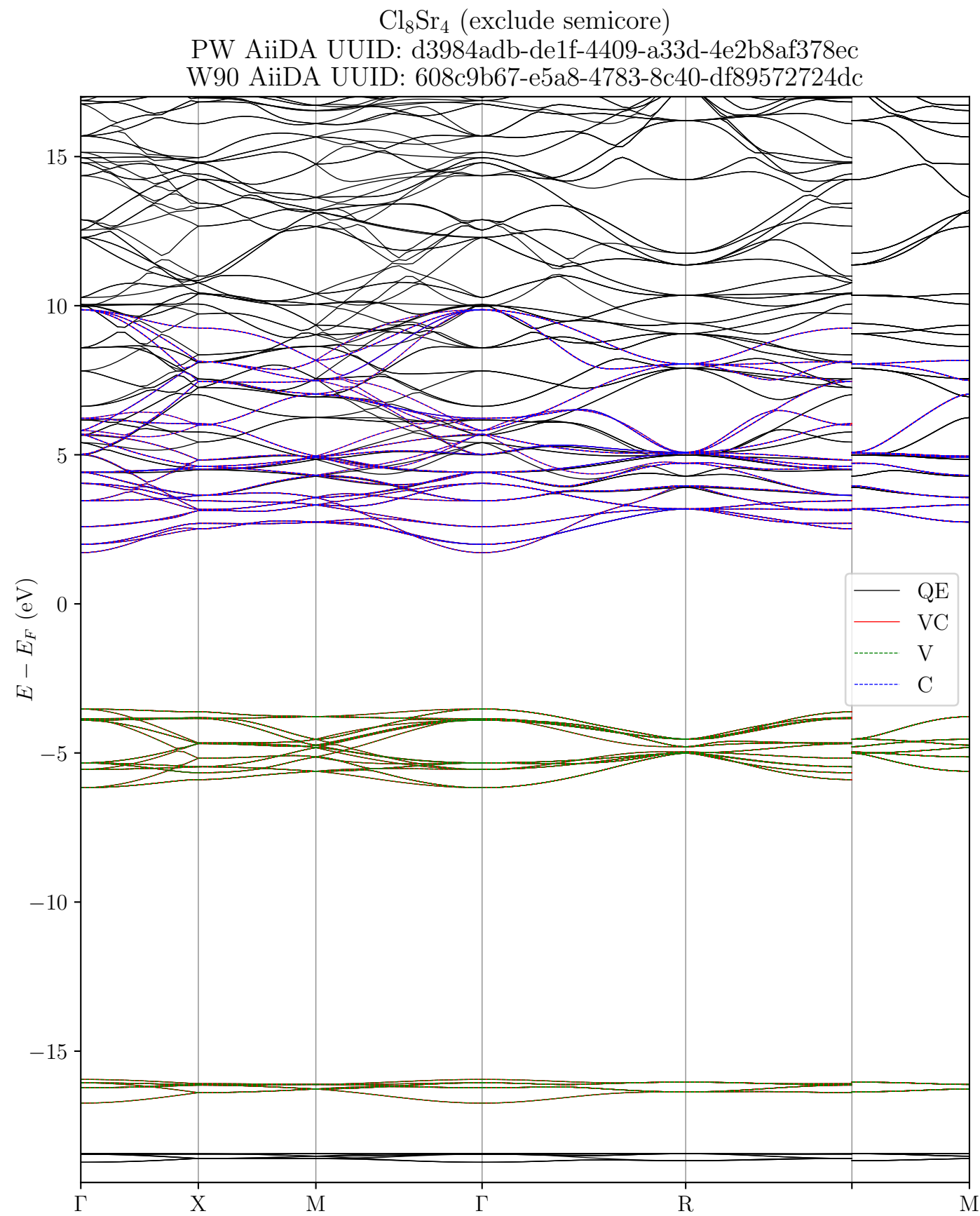




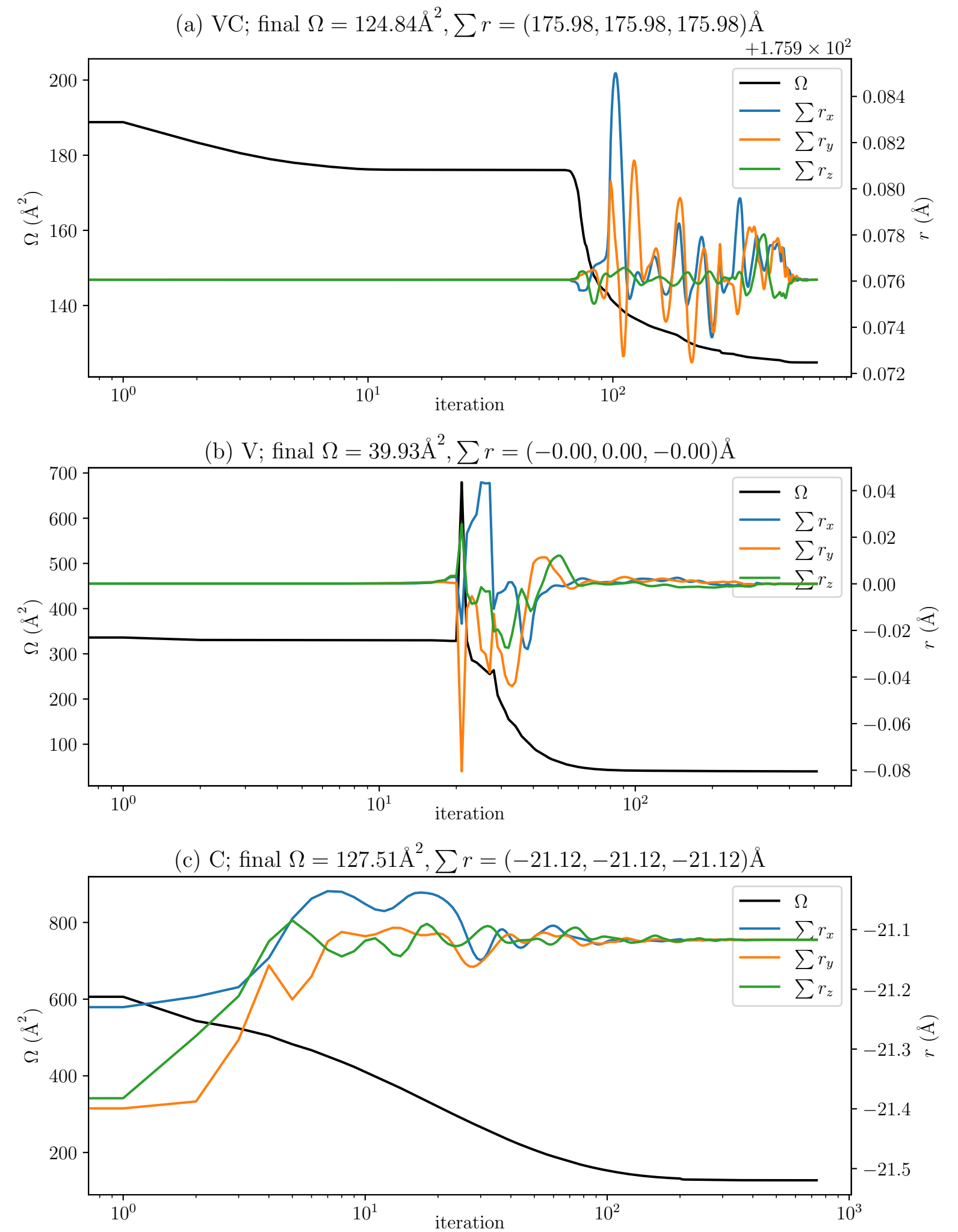
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.7	0.1	0.0	0.1	1.8	1.8	0.2
η_{max}	0.6	0.6	0.0	0.6	0.5	0.4	1.6

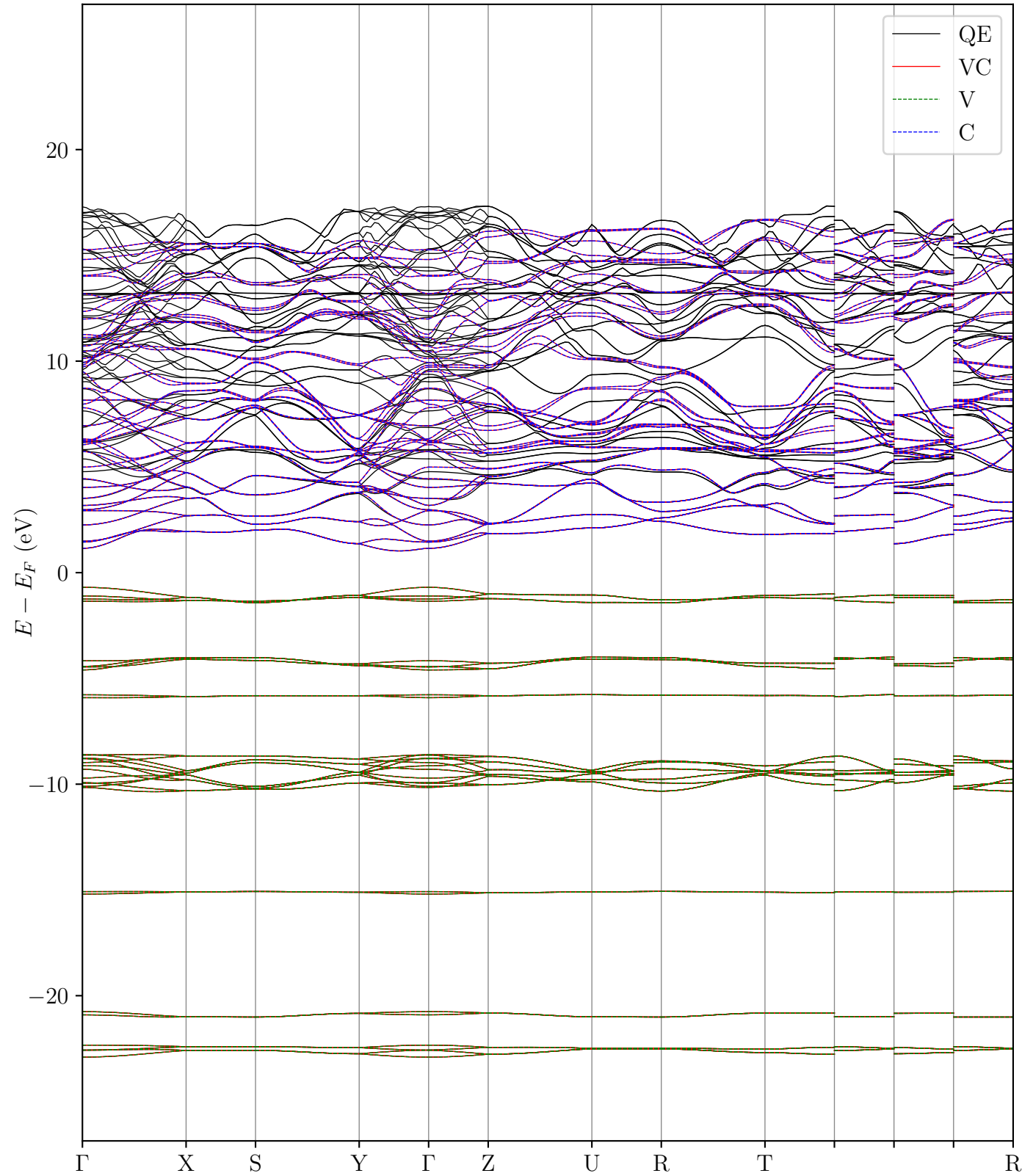




	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.6	0.6	0.1	0.6	0.9	0.6	0.8
η_{max}	3.8	3.8	0.5	3.6	1.7	1.2	4.8

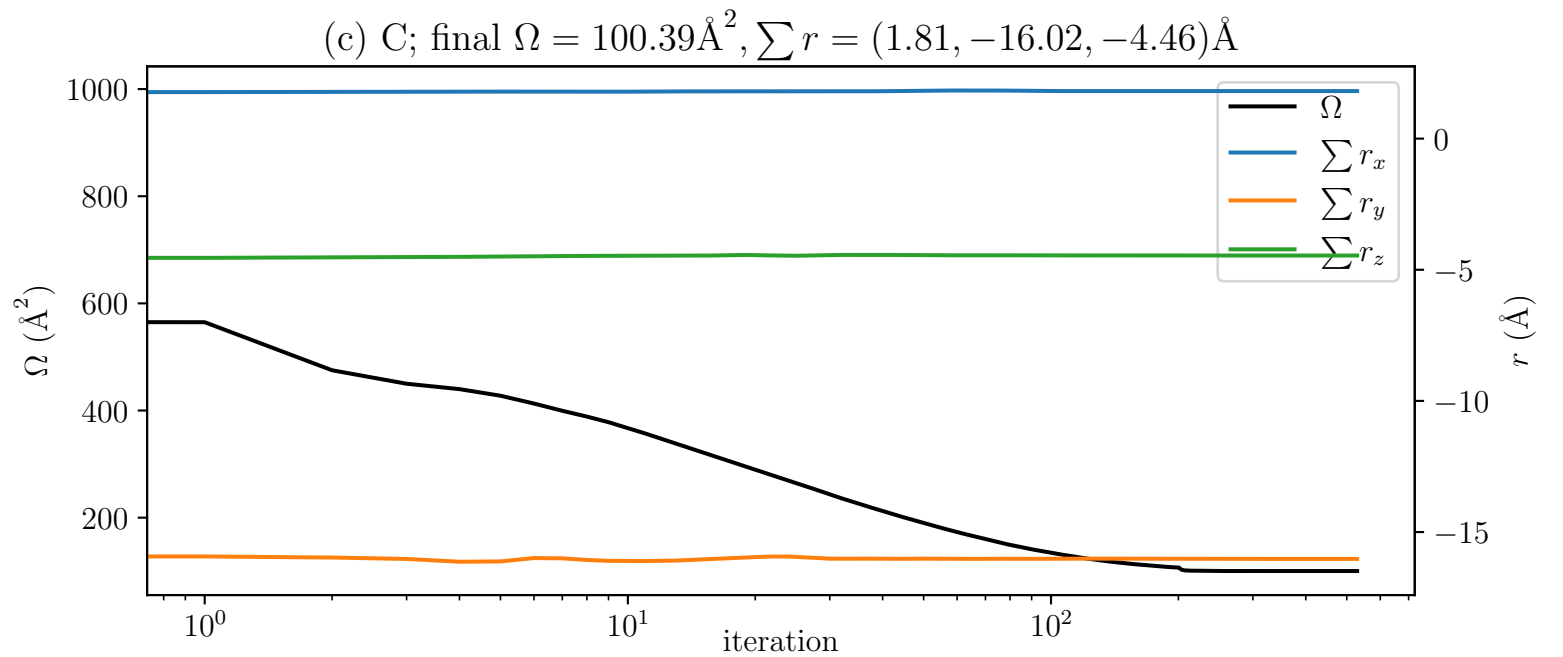
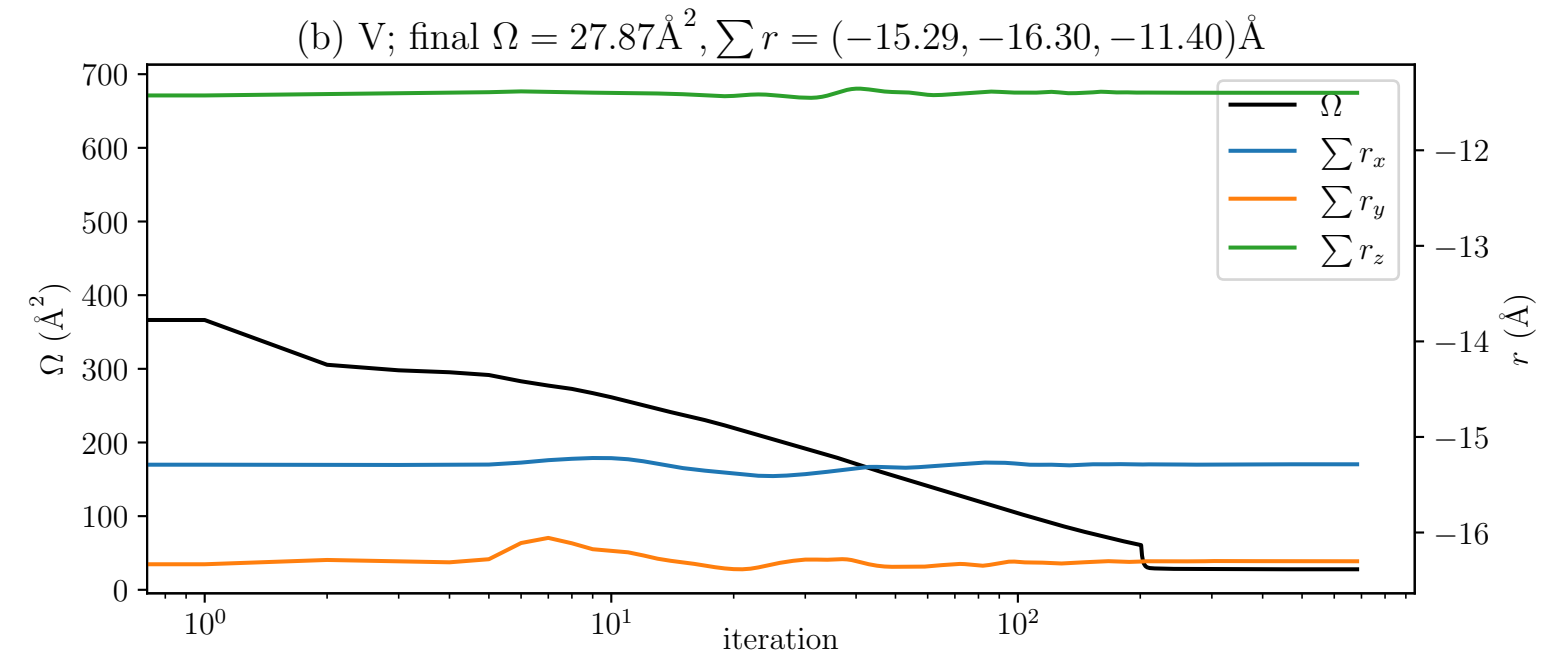
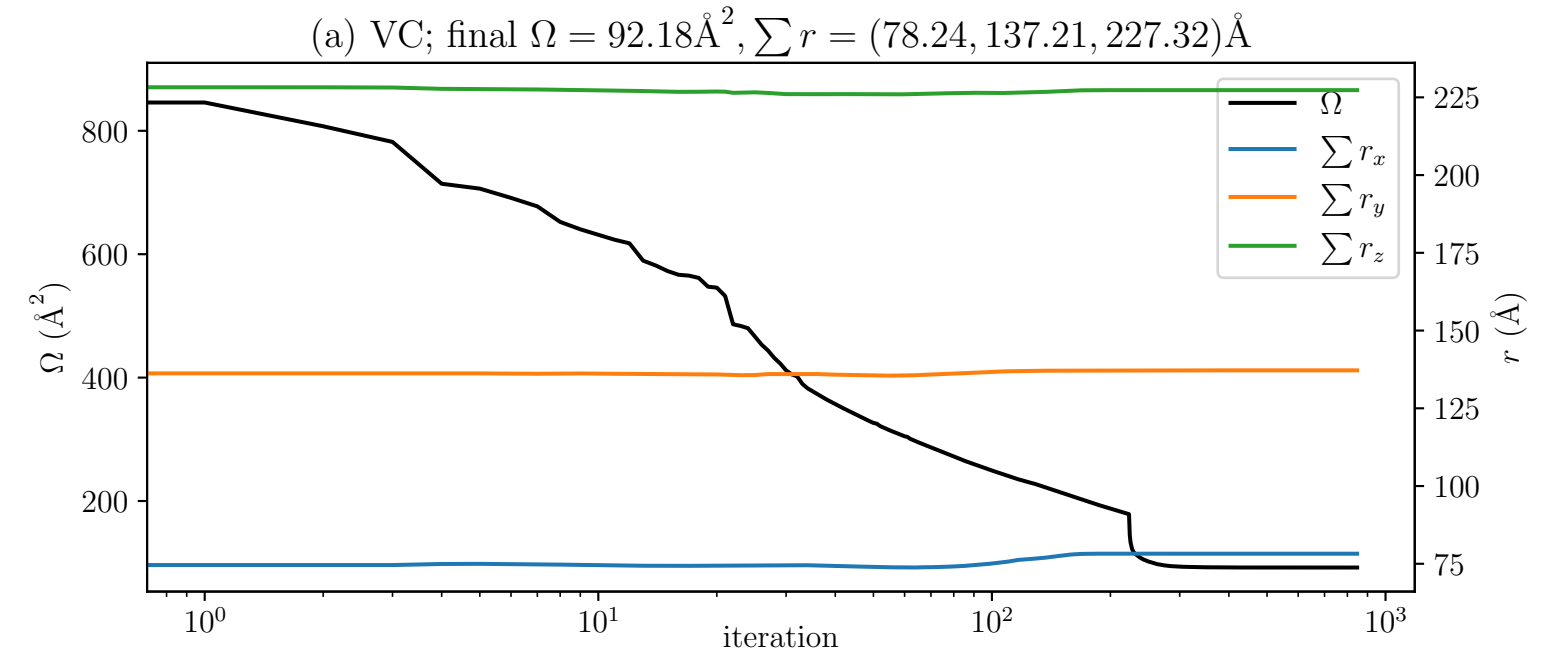


Cs₄O₄ (**include** semicore)
PW AiiDA UUID: 2a9e6492-dc17-4a33-a871-aaee78b5c8ce
W90 AiiDA UUID: af49ce79-7e78-45ea-ae0a-f490bffd5b0

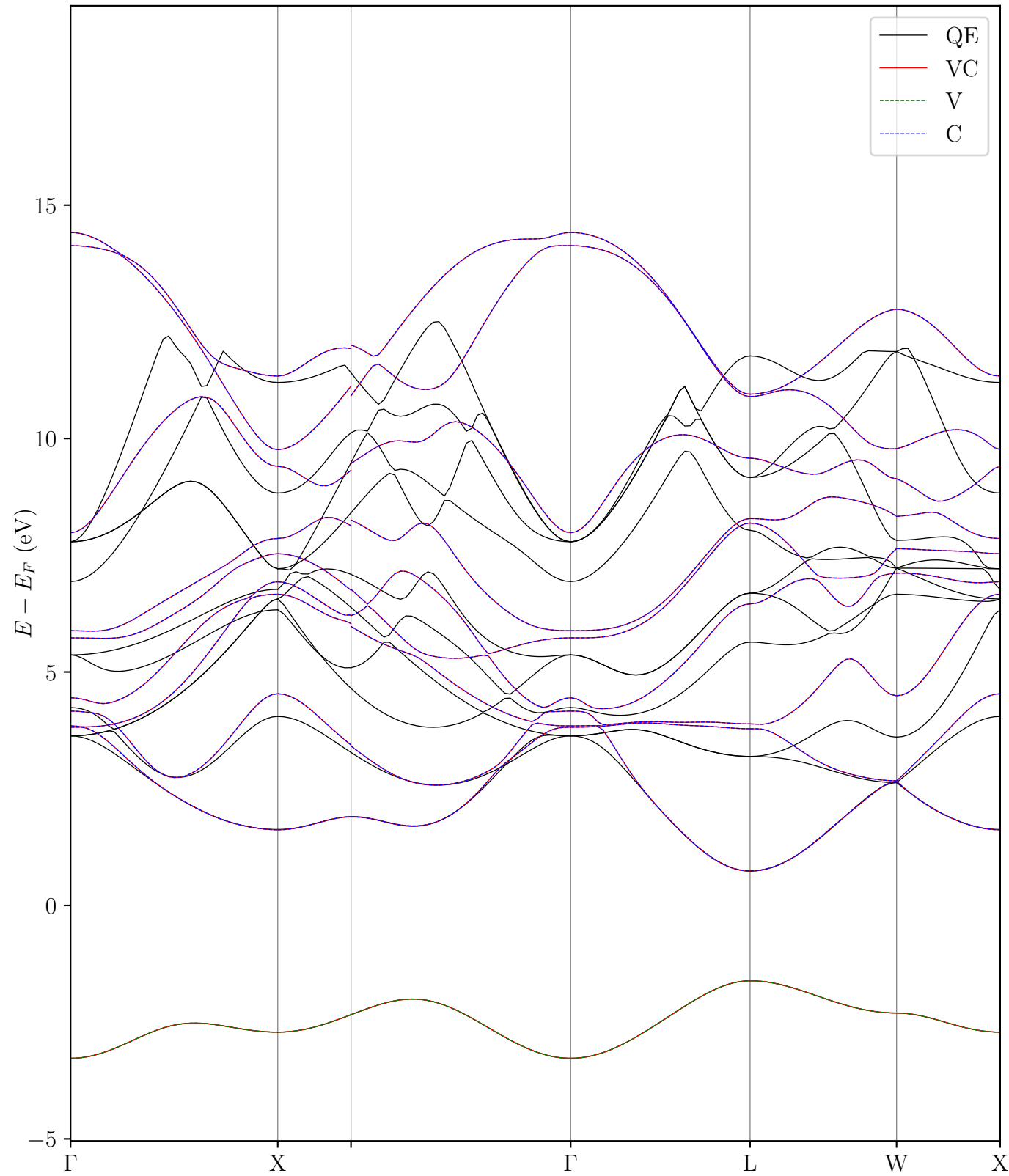


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.4	1.2	0.0	1.2	3.2	3.2	2.1
η_{max}	8.2	7.7	0.1	7.7	8.2	8.0	14.6

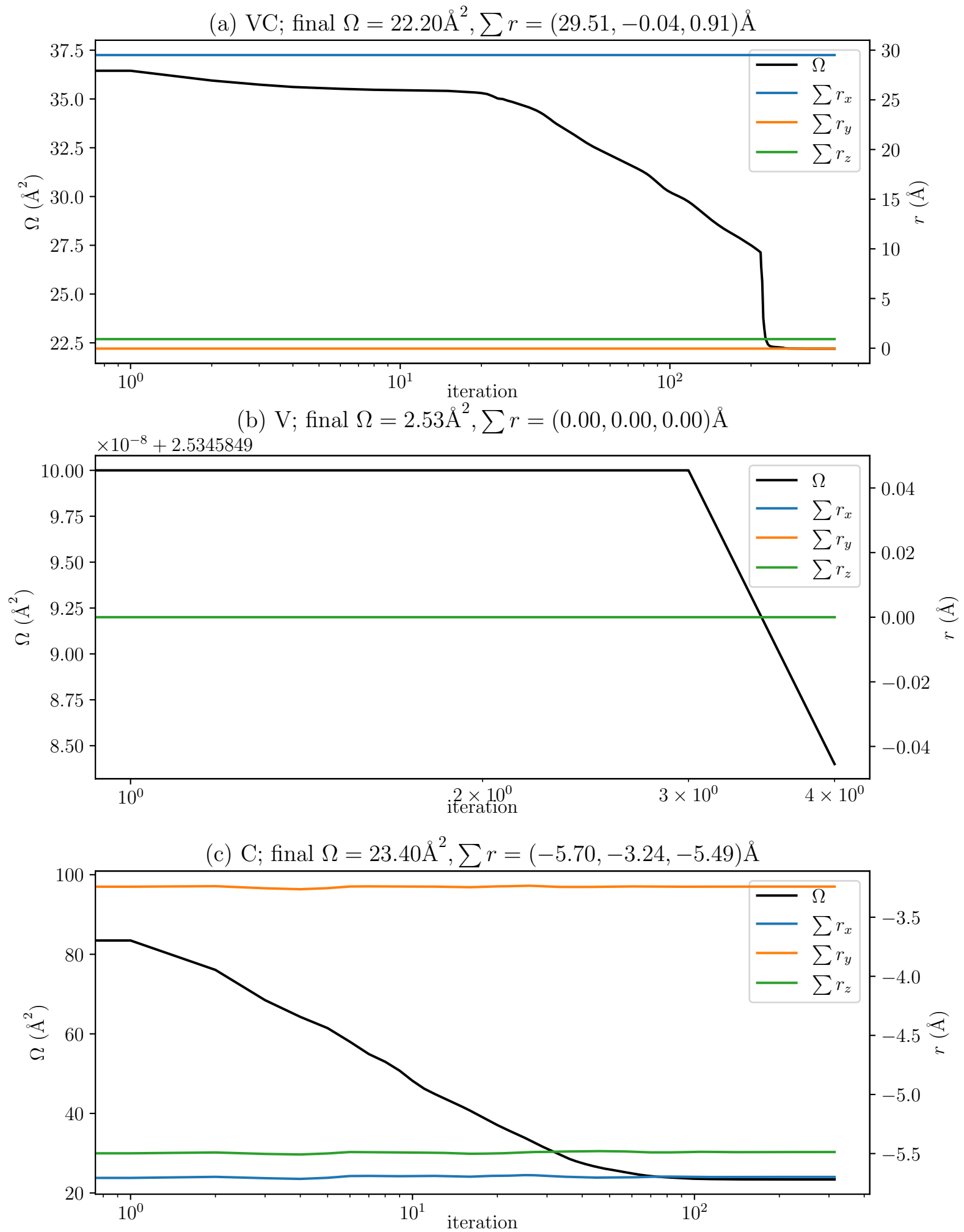


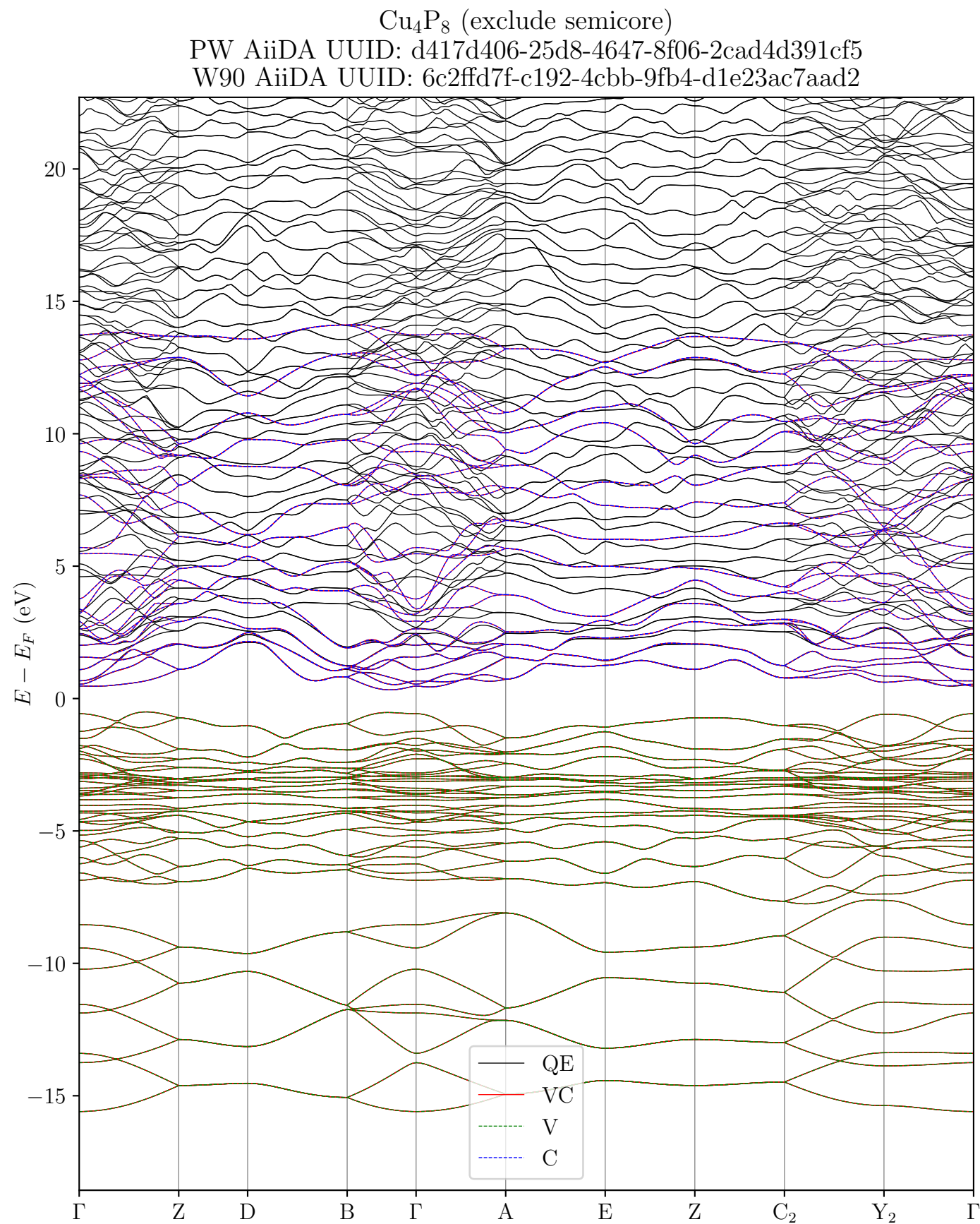
CsH (hydrogenic projection, energy disentanglement)
PW AiiDA UUID: 1717b625-2388-4909-8b7a-8003d9a35f4b
W90 AiiDA UUID: 3c2f8b61-2fc0-463a-82a6-6a030932b03a



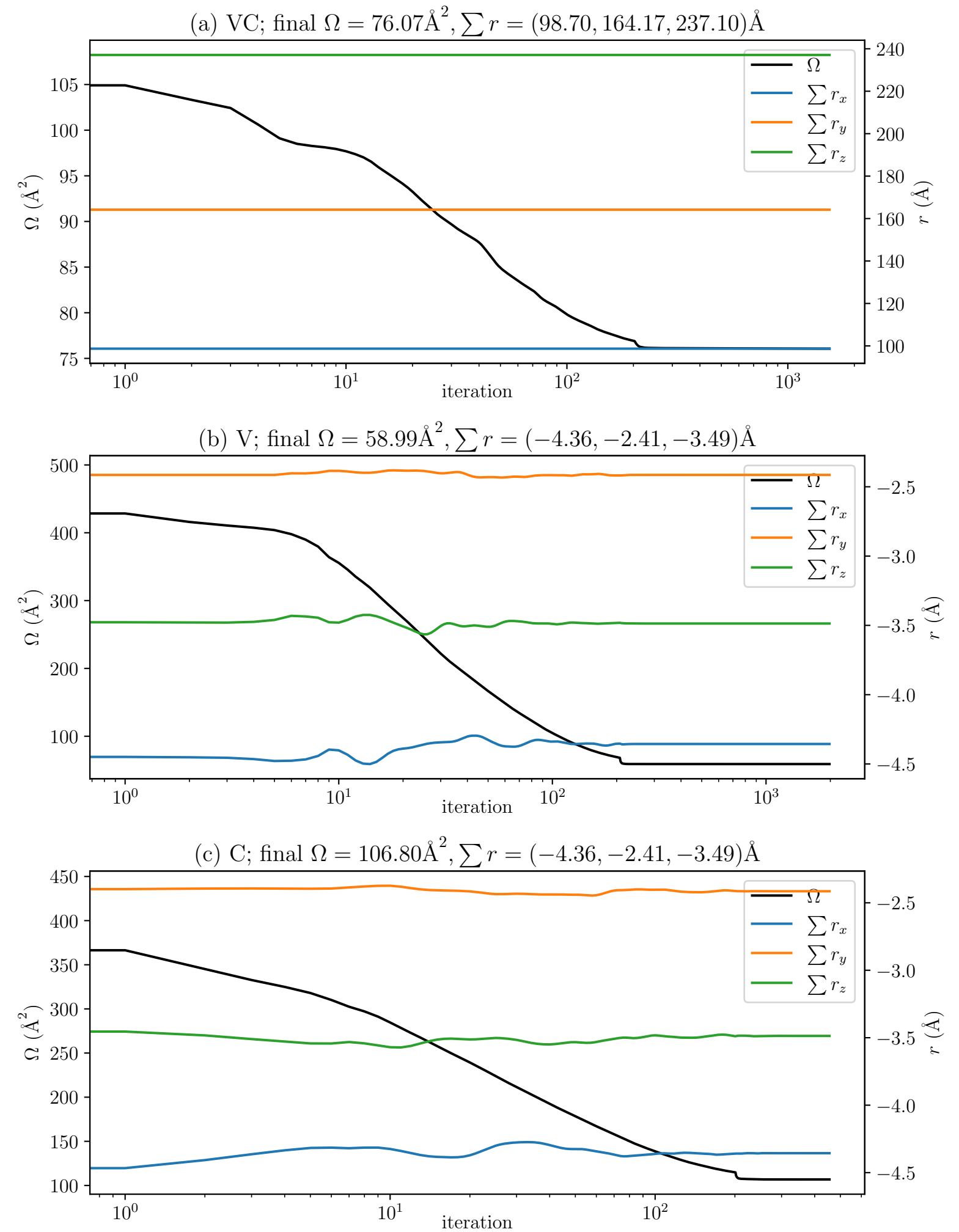
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	2.9	1.1	0.2	1.1	4.8	5.1	0.8
η_{max}	13.1	3.9	1.0	3.9	13.1	13.5	4.7

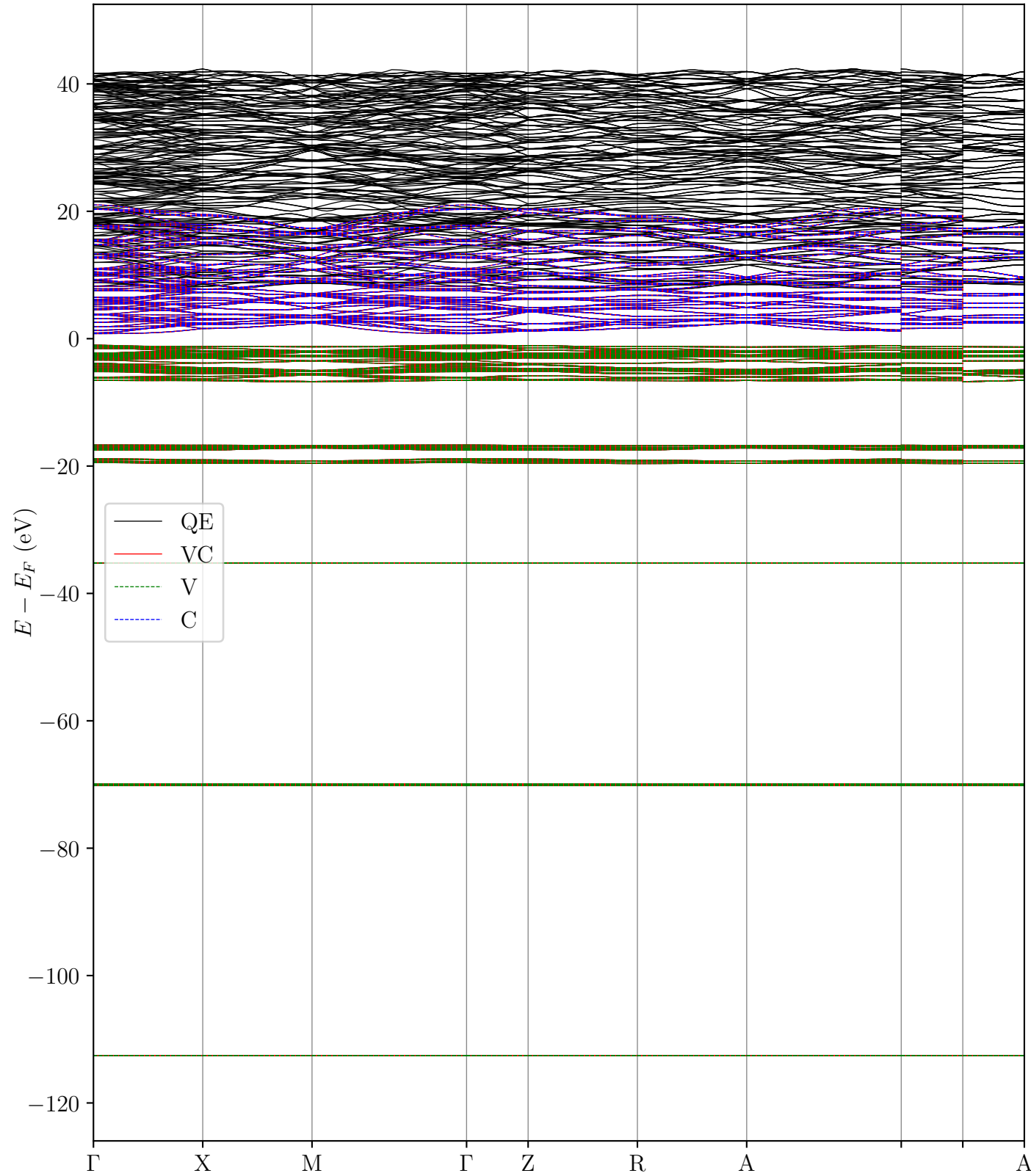




	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	4.0	1.4	0.8	1.6	12.3	13.4	4.1
η_{max}	47.3	8.9	7.3	10.6	47.3	46.9	18.7

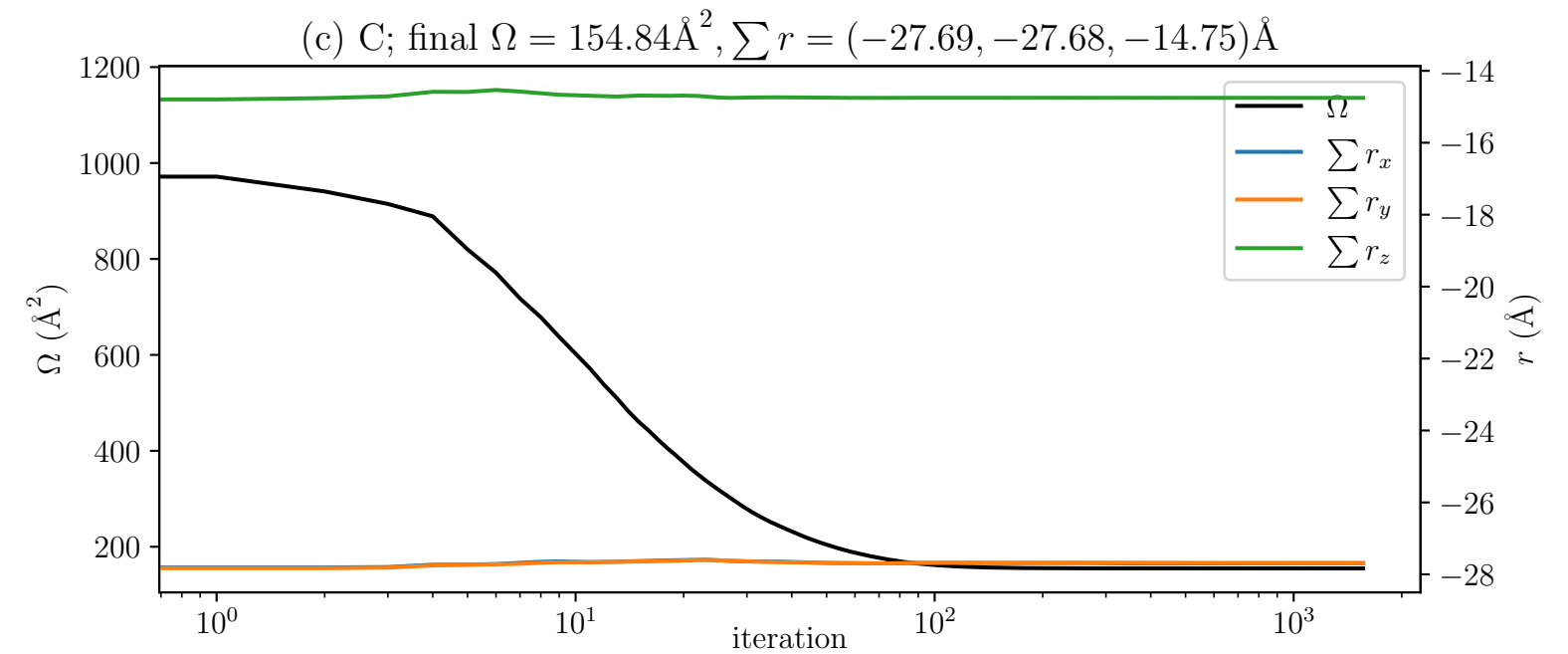
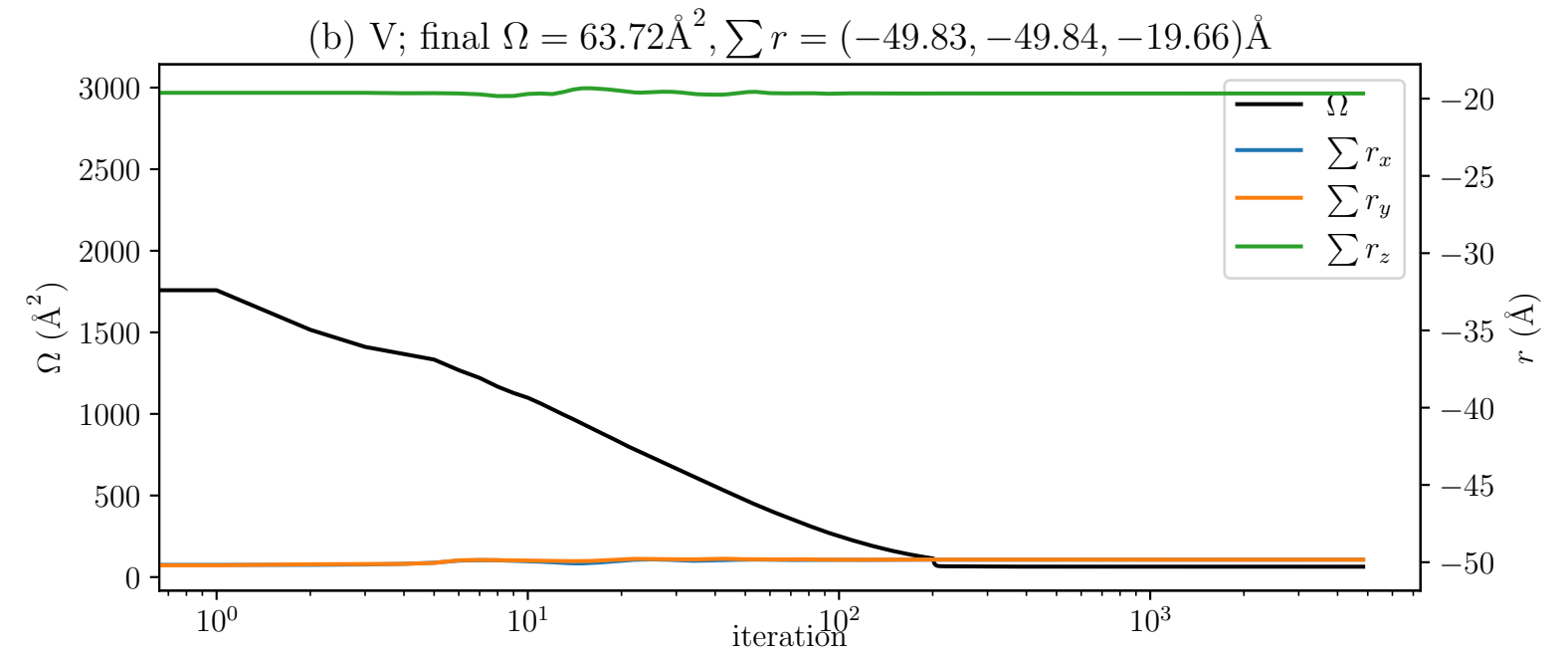
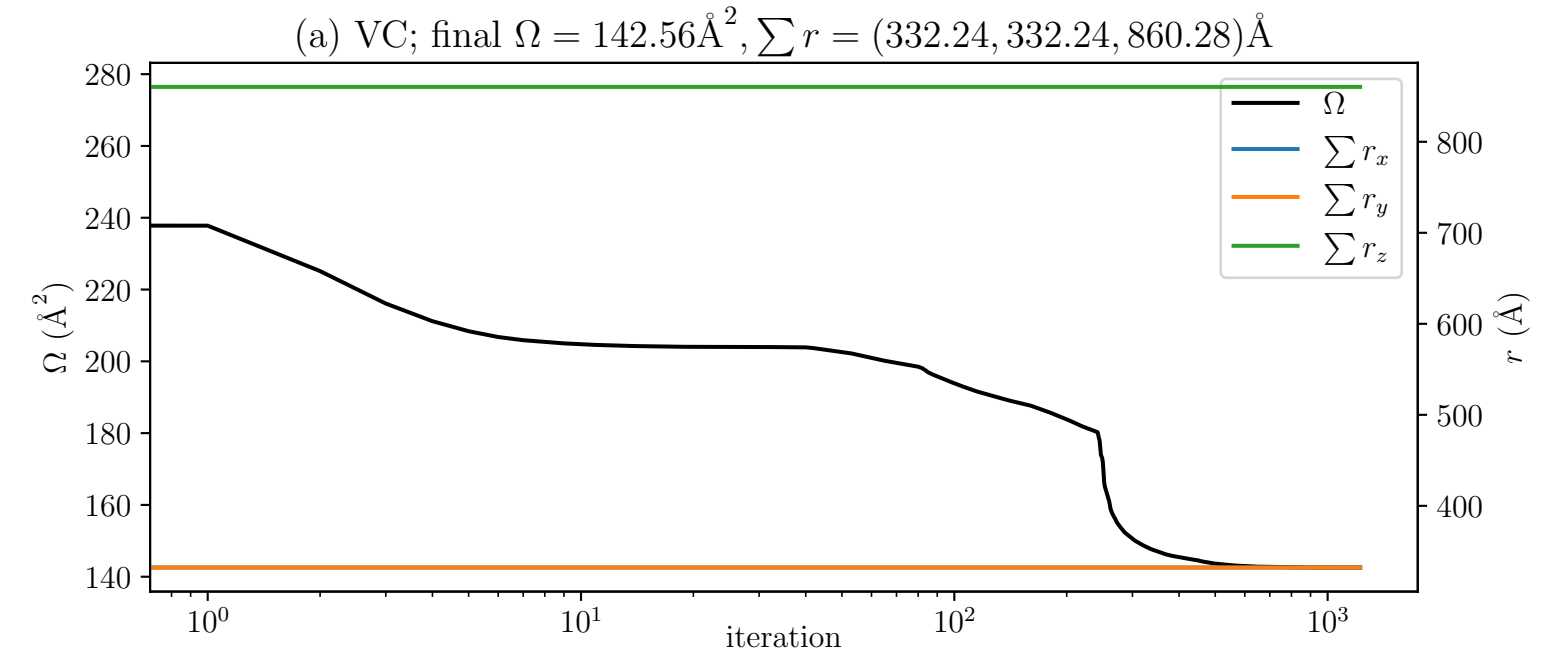


Cu₈O₈Sr₄ (include semicore)
PW AiiDA UUID: 3f4f9280-82e6-45e0-b30c-ae7e23a002e4
W90 AiiDA UUID: 8b9b9bd7-af40-4596-b218-fda0f184e278

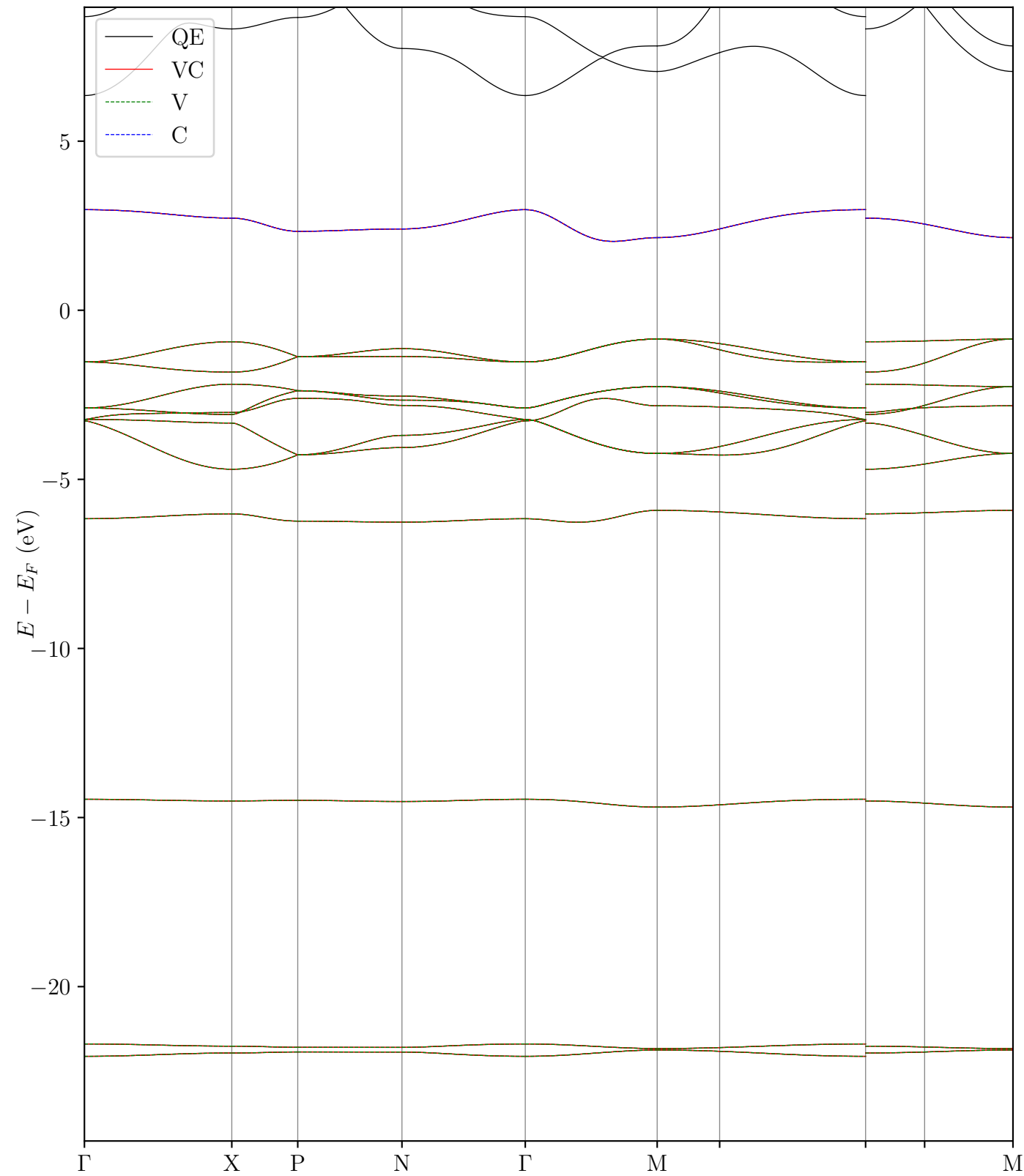


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.2	0.2	0.2	0.2	0.7	0.9	0.6
η_{max}	3.8	3.5	5.9	5.5	3.8	4.2	7.0



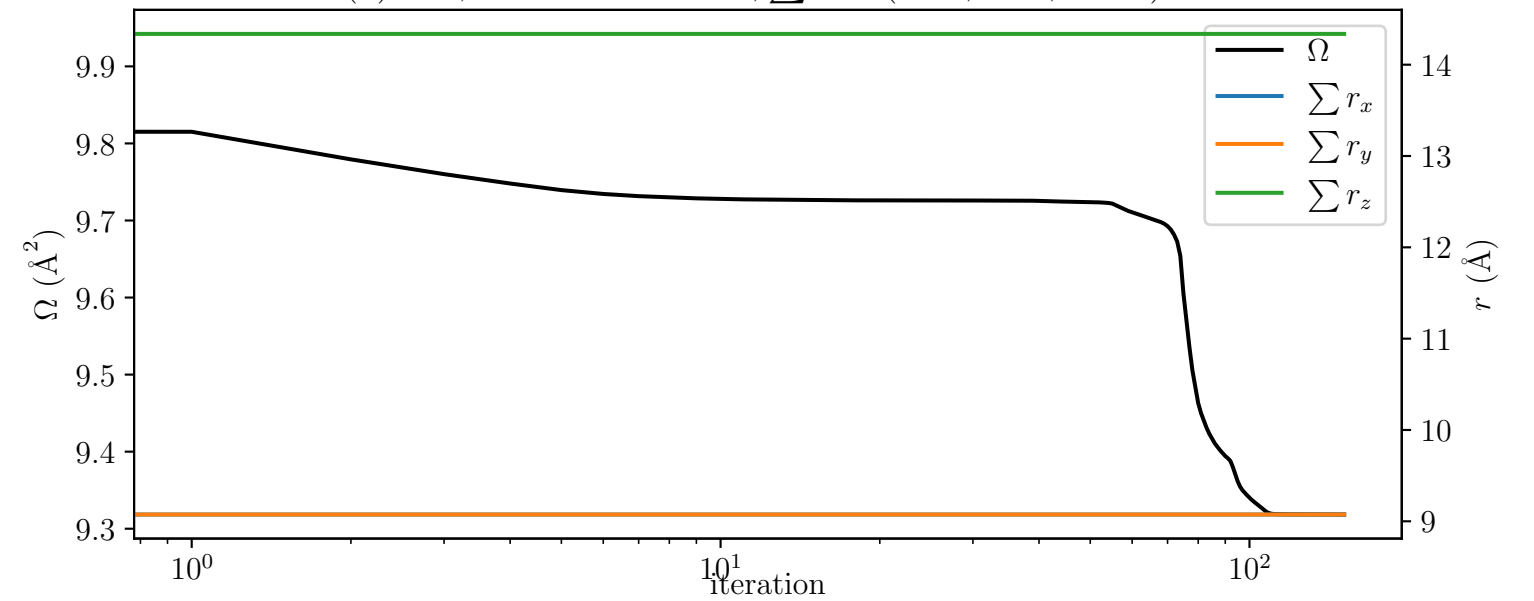
F₂Xe (exclude semicore)
PW AiiDA UUID: 309f6d22-bf64-40b8-937f-2f6144c3bc94
W90 AiiDA UUID: c1550bfe-d299-4239-9a2c-b9d9f1cb81d2



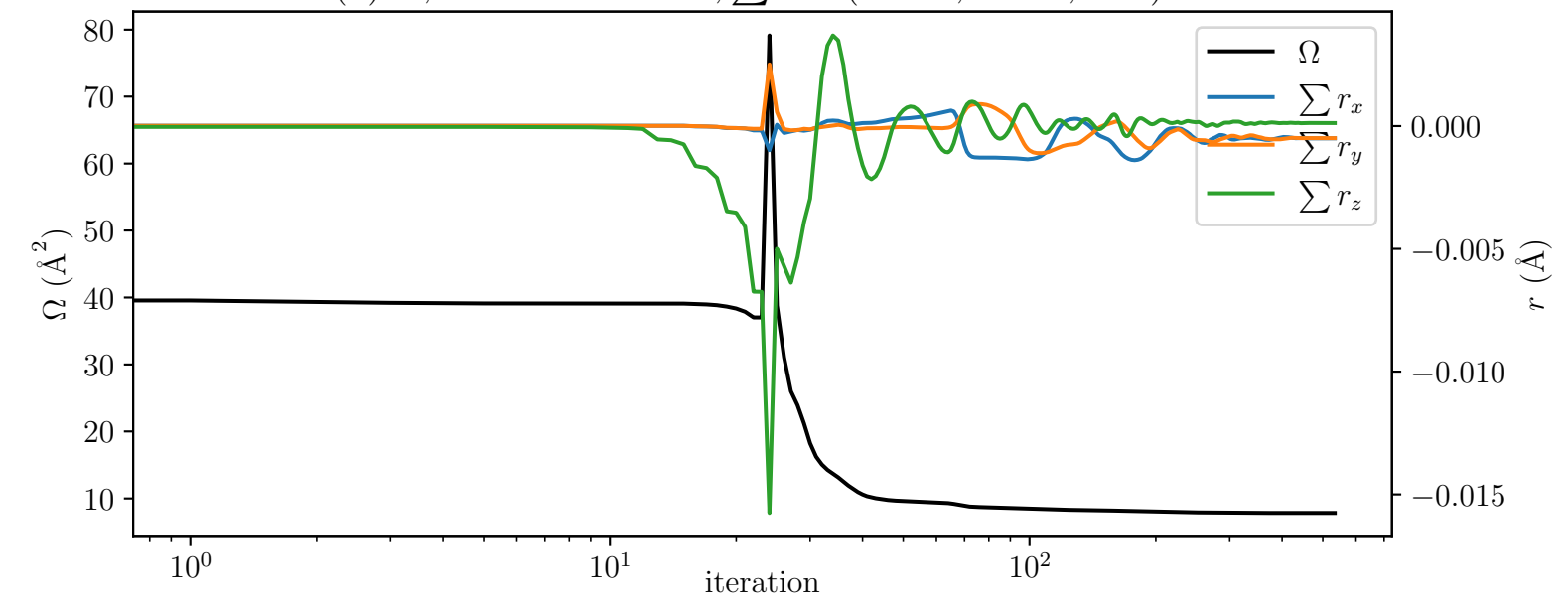
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.0	0.0	0.0	0.0	0.0	0.0	0.0
η_{max}	0.0	0.0	0.0	0.0	0.0	0.0	0.0

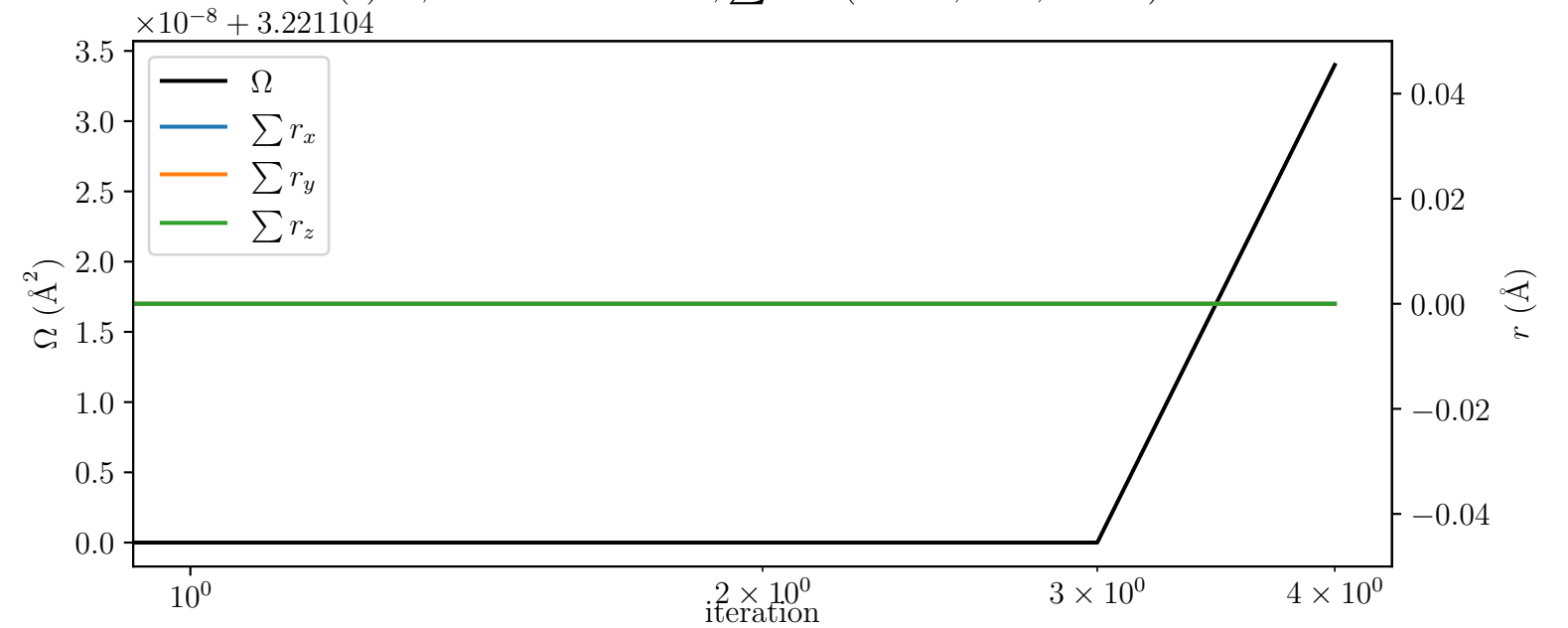
(a) VC; final $\Omega = 9.32 \text{ \AA}^2$, $\sum r = (9.07, 9.07, 14.34) \text{ \AA}$



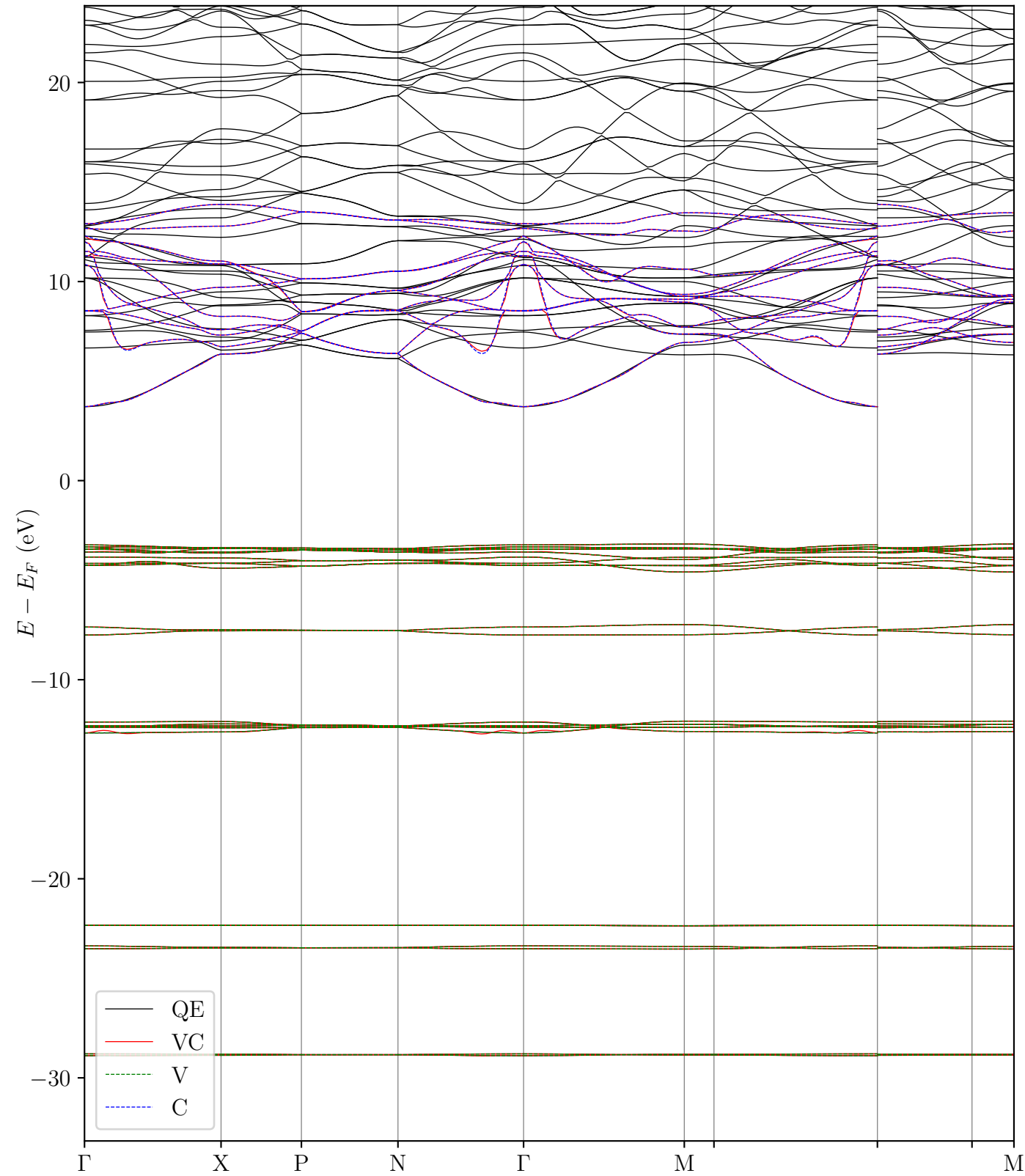
(b) V; final $\Omega = 7.84 \text{ \AA}^2$, $\sum r = (-0.00, -0.00, 0.00) \text{ \AA}$



(c) C; final $\Omega = 3.22 \text{ \AA}^2$, $\sum r = (-0.00, 0.00, -0.00) \text{ \AA}$

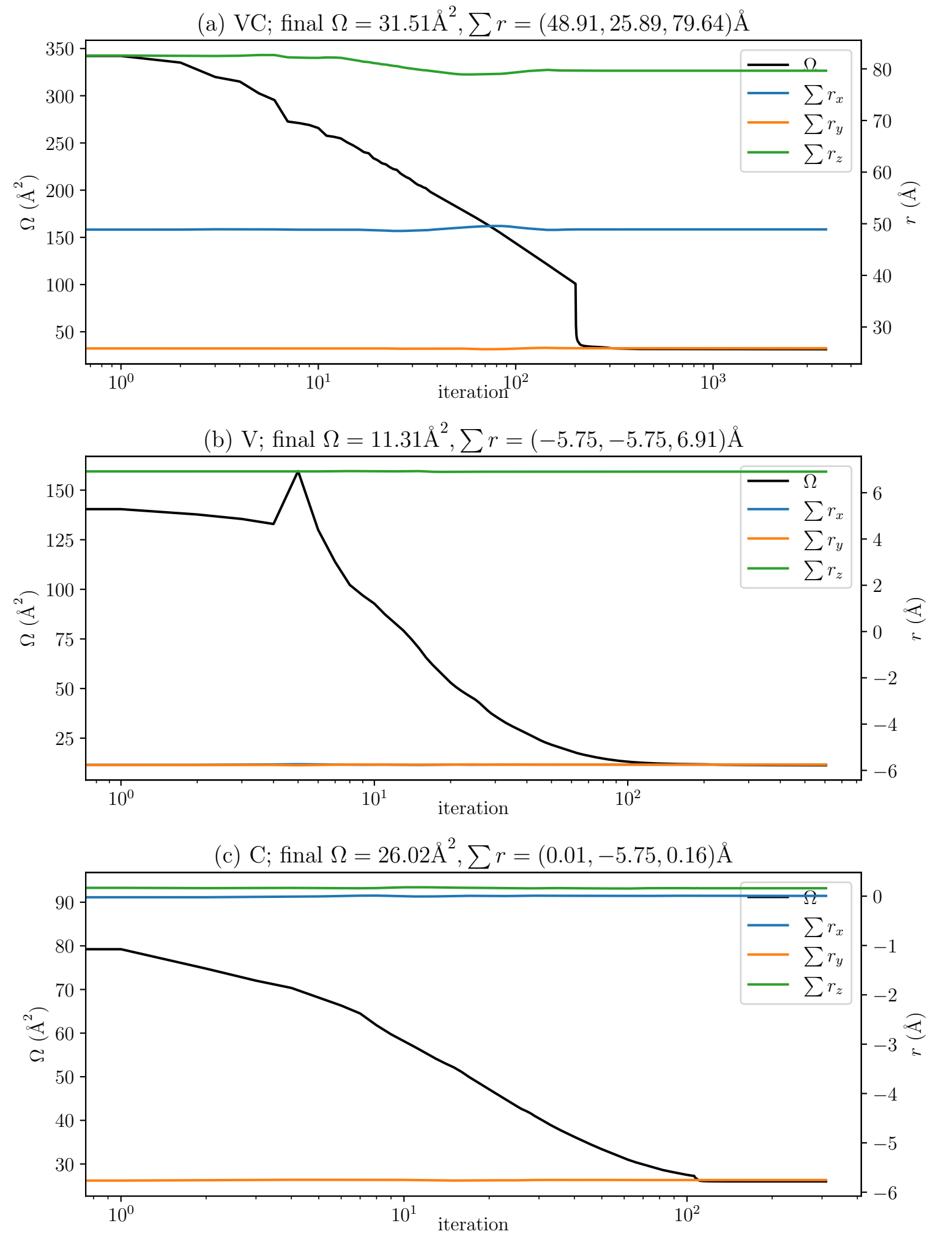


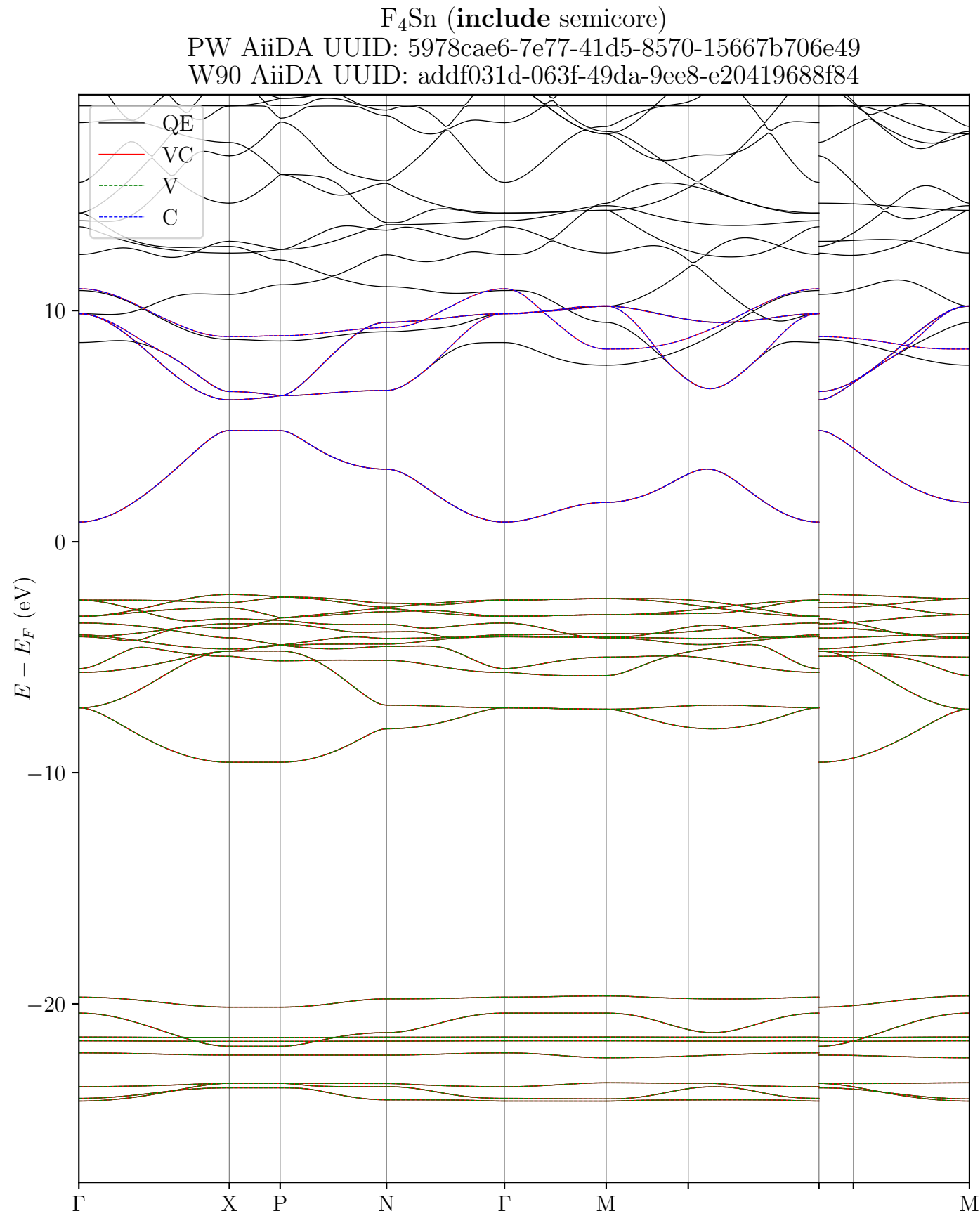
F₄H₂K₂ (**include** semicore)
PW AiiDA UUID: 10b62d5a-ecfe-4dda-ba32-2b0ff042b8de
W90 AiiDA UUID: bdab602c-99a4-492a-ba5c-39aea343992f



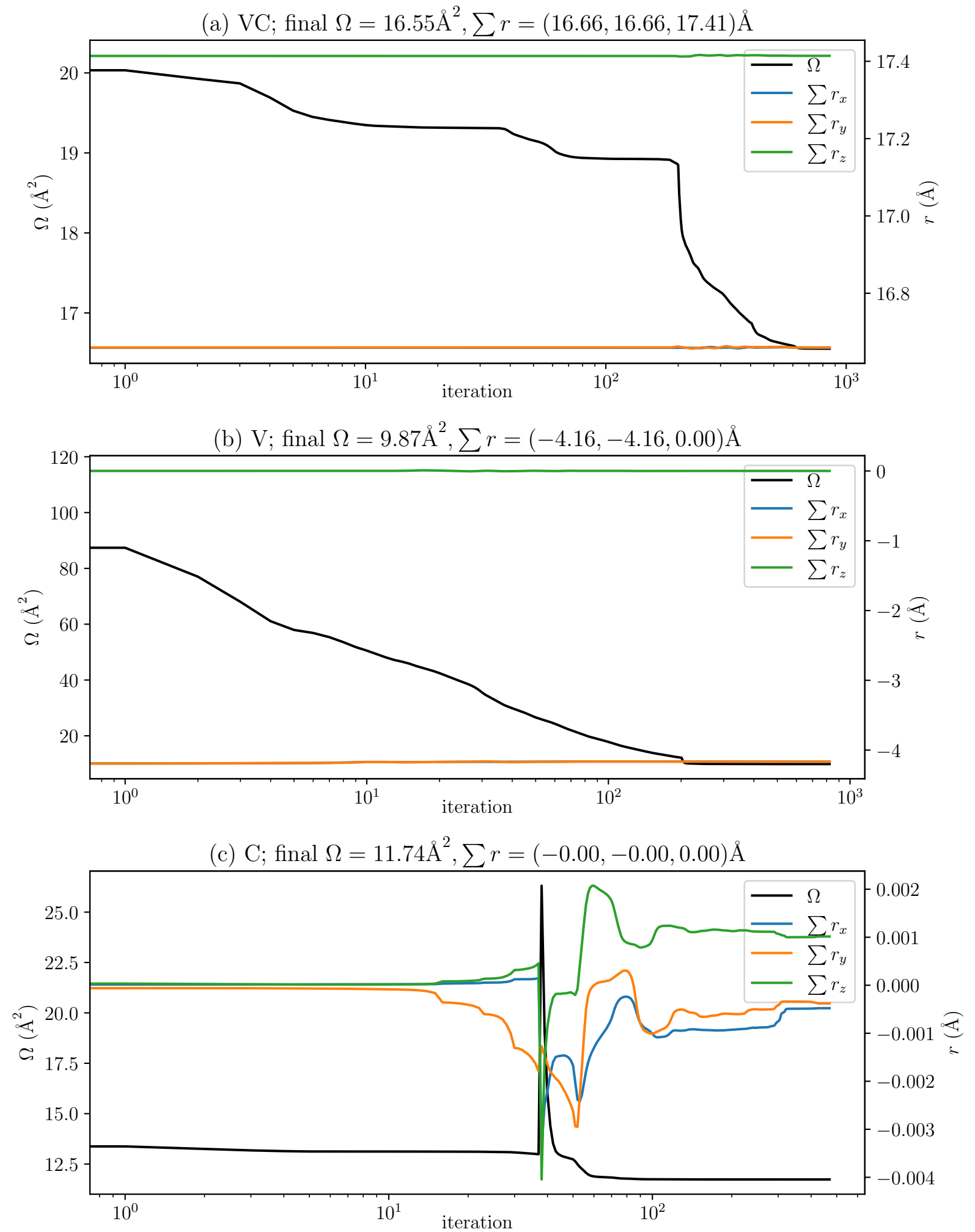
band distance (meV)

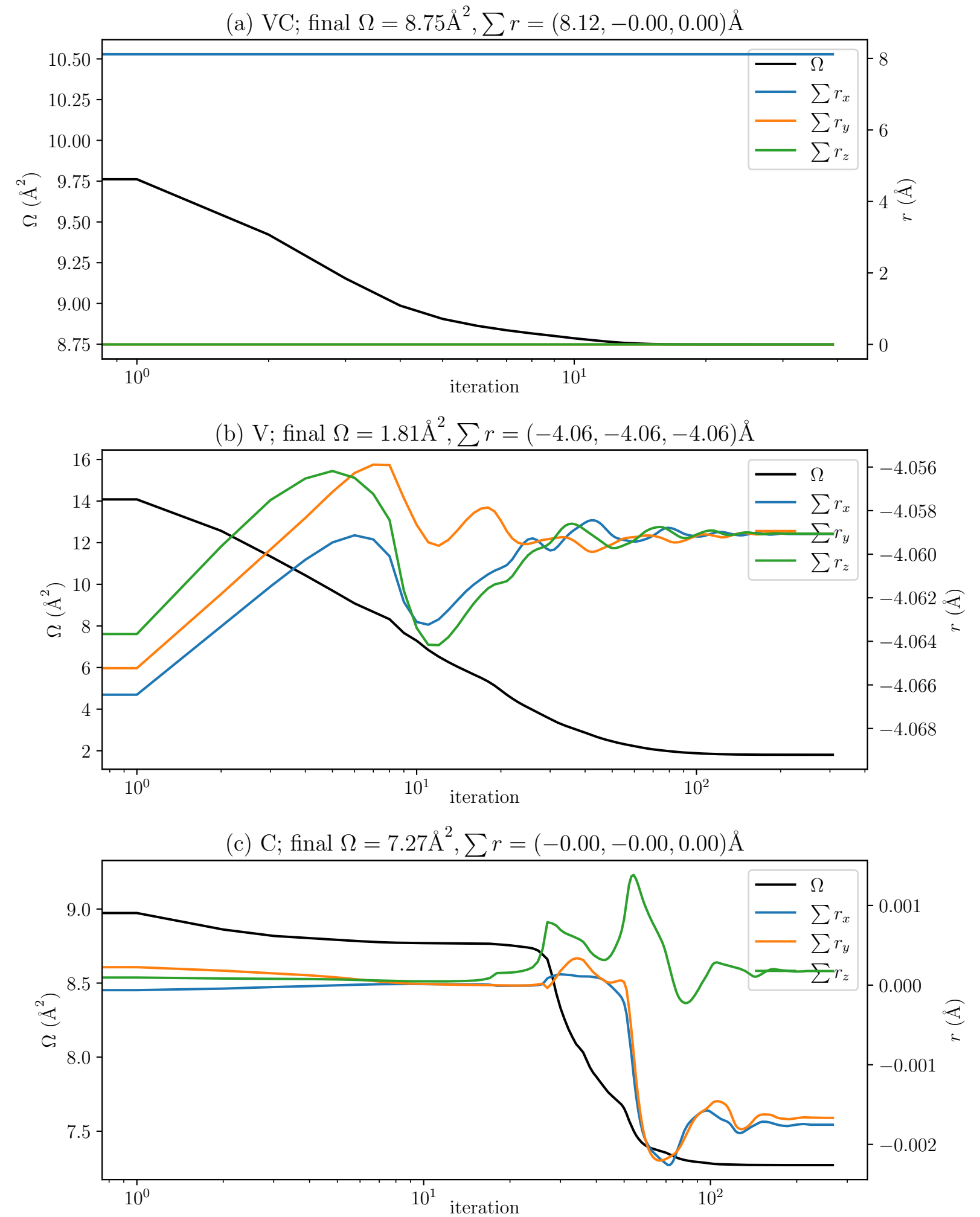
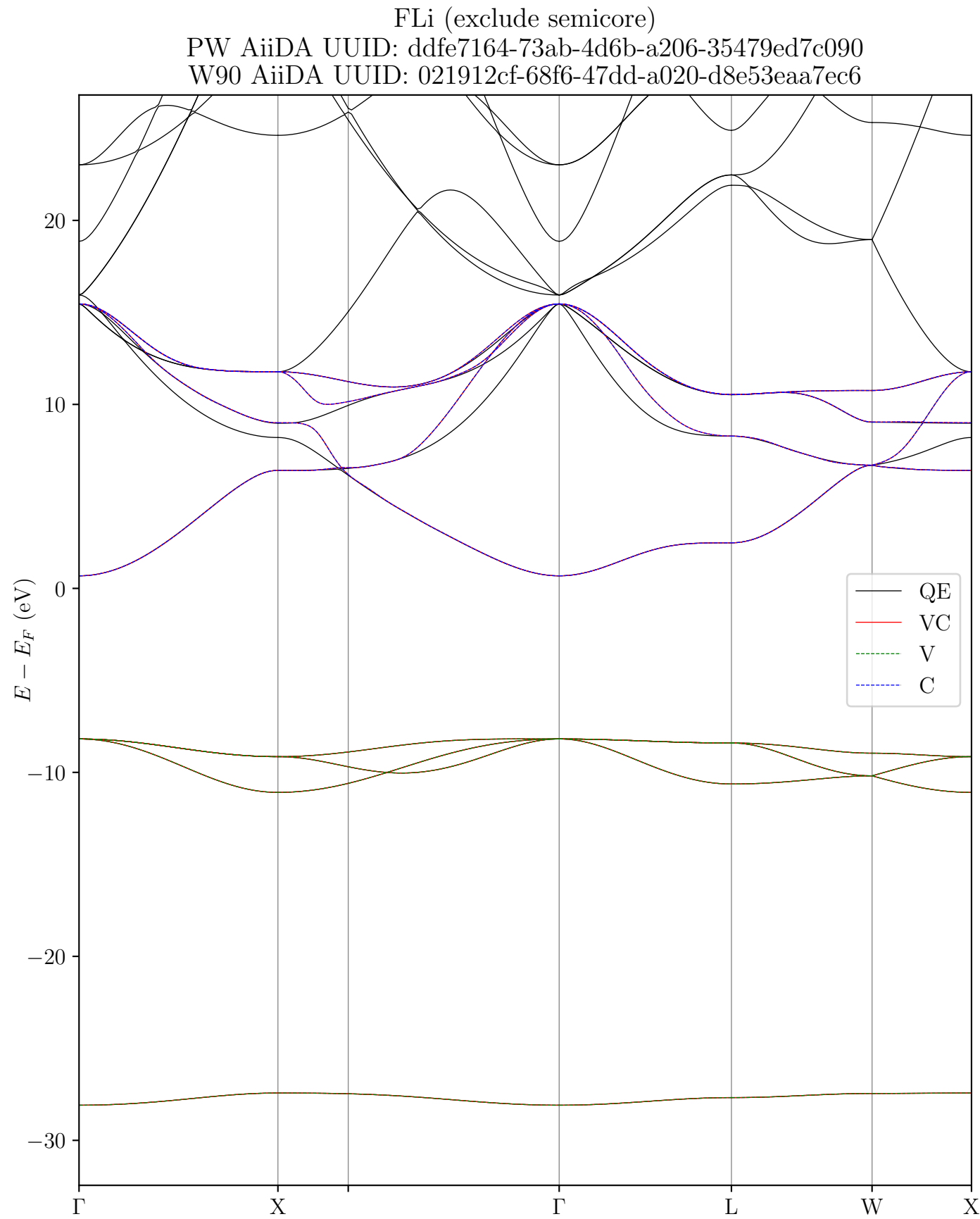
	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	7.3	7.3	0.0	7.3	36.5	36.3	16.0
η_{max}	125.6	125.6	0.0	125.6	0.0	0.0	195.5



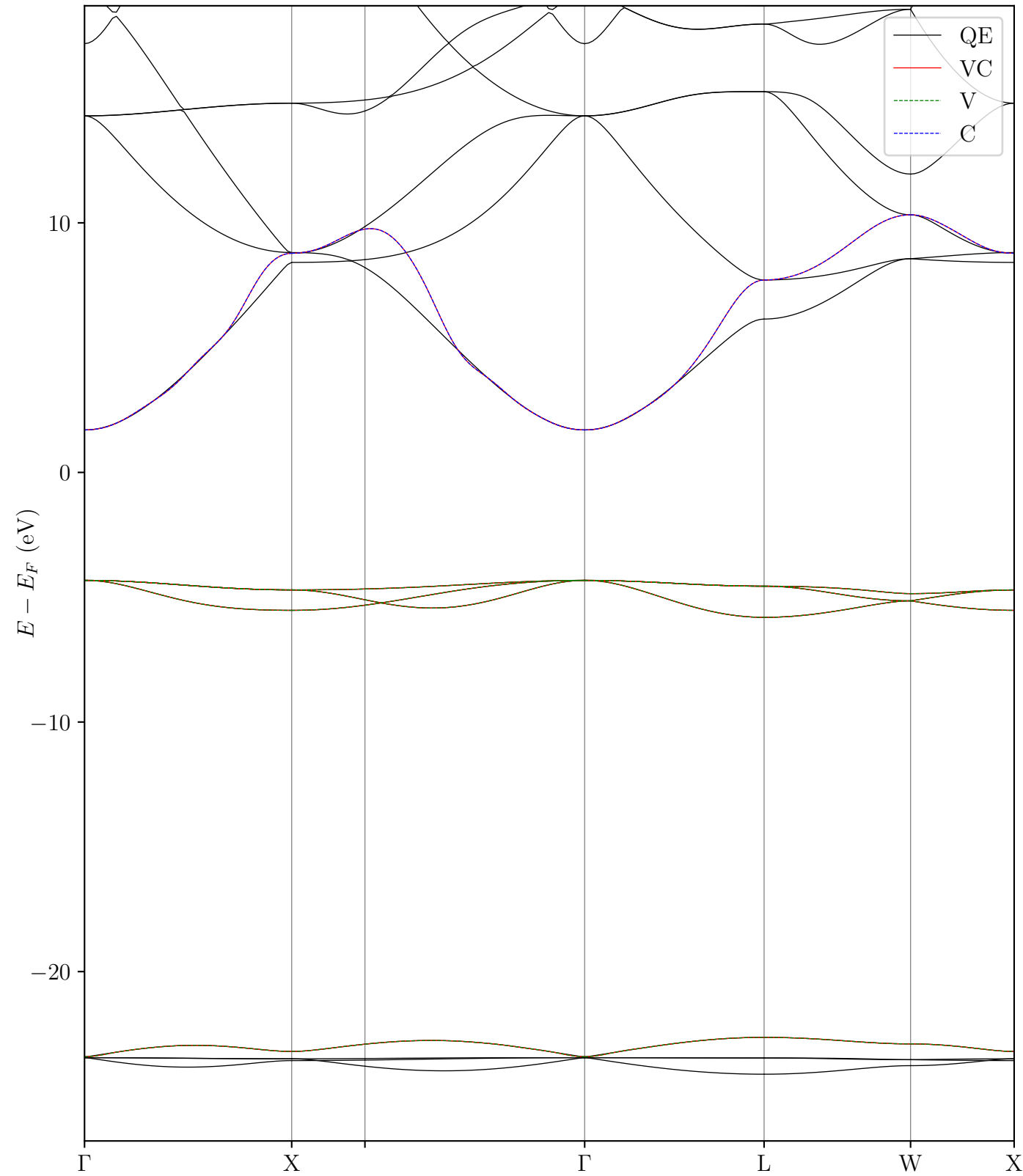


	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.5	0.4	0.0	0.4	1.2	2.6	1.7
η_{max}	3.9	3.9	0.0	3.9	3.1	6.4	5.4





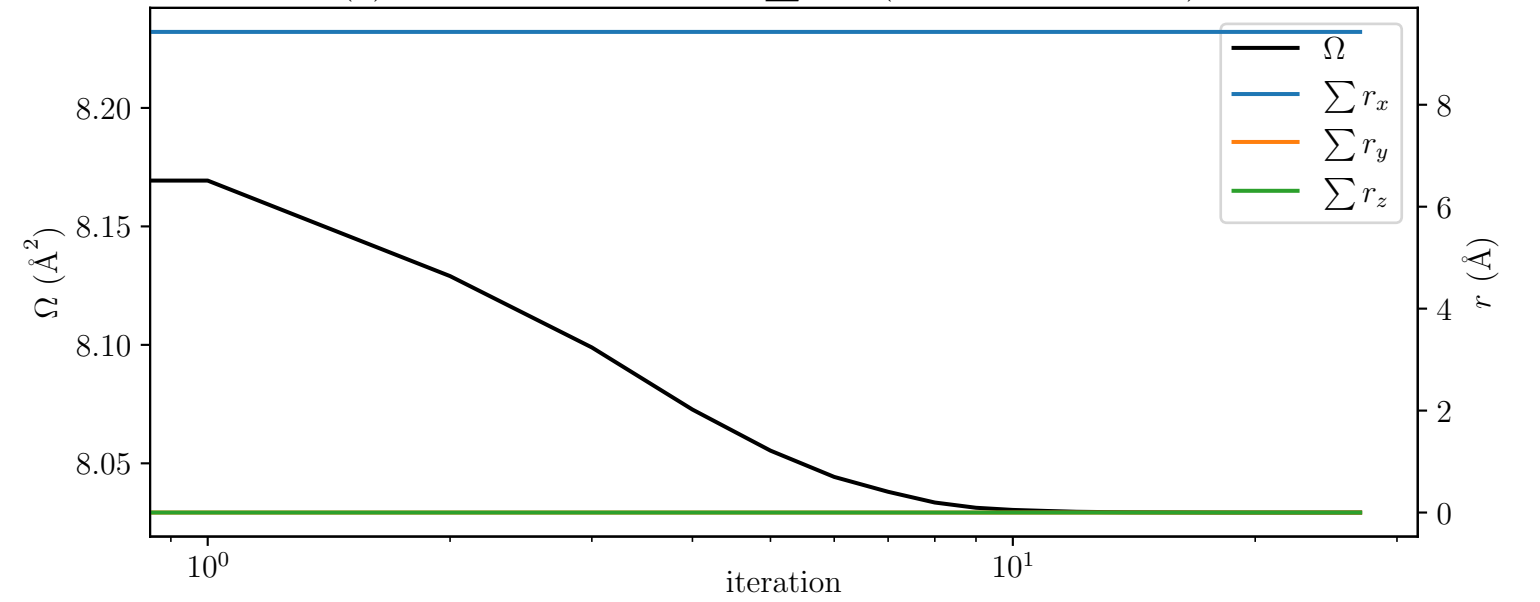
FNa (exclude semicore)
PW AiiDA UUID: ff21f8ae-0282-4fb8-ac27-19c5be4a324b
W90 AiiDA UUID: b9f0b905-b425-4a23-8800-89cc94199e42



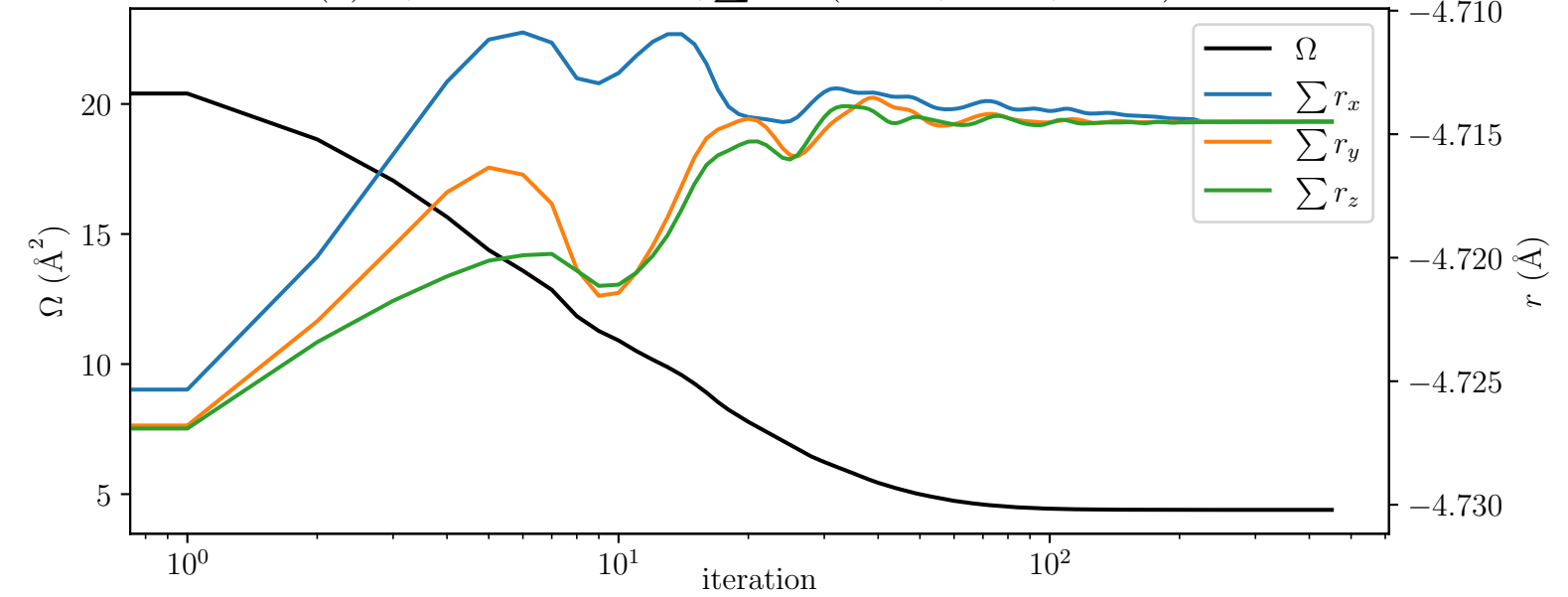
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	2.7	2.5	2.5	0.3	6.0	5.5	0.7
η_{max}	22.5	22.5	22.5	1.6	8.6	7.7	2.3

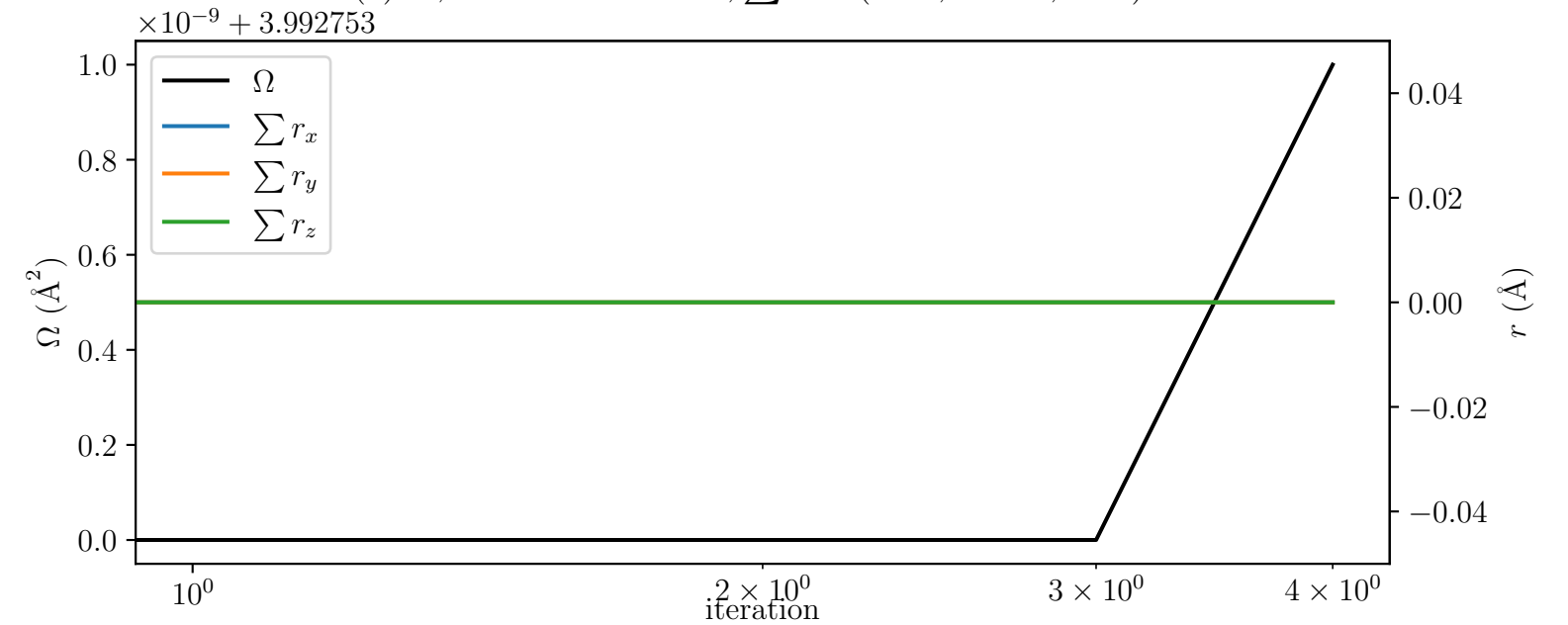
(a) VC; final $\Omega = 8.03 \text{ \AA}^2$, $\sum r = (9.43, -0.00, -0.00) \text{ \AA}$



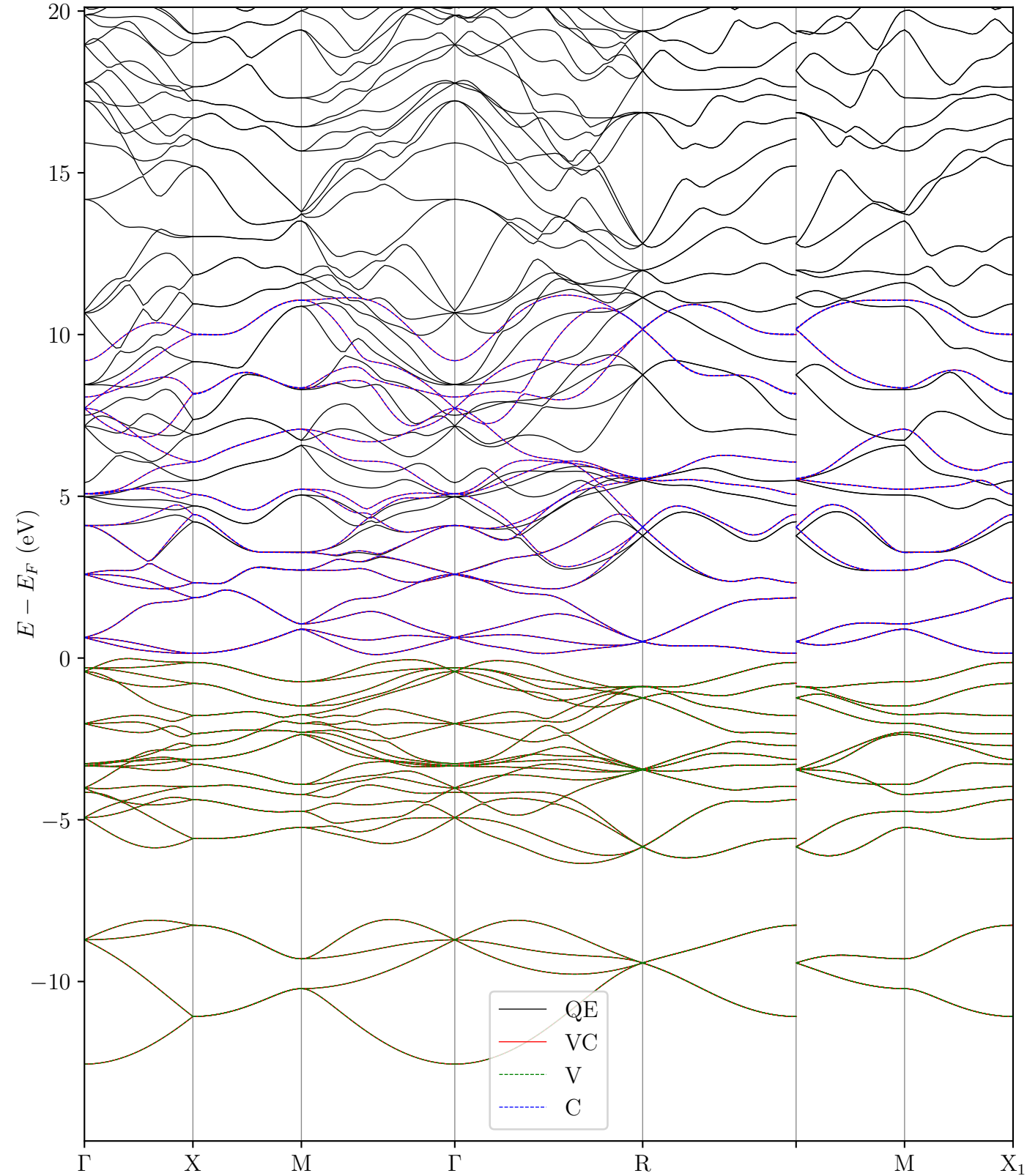
(b) V; final $\Omega = 4.40 \text{ \AA}^2$, $\sum r = (-4.71, -4.71, -4.71) \text{ \AA}$



(c) C; final $\Omega = 3.99 \text{ \AA}^2$, $\sum r = (0.00, -0.00, 0.00) \text{ \AA}$



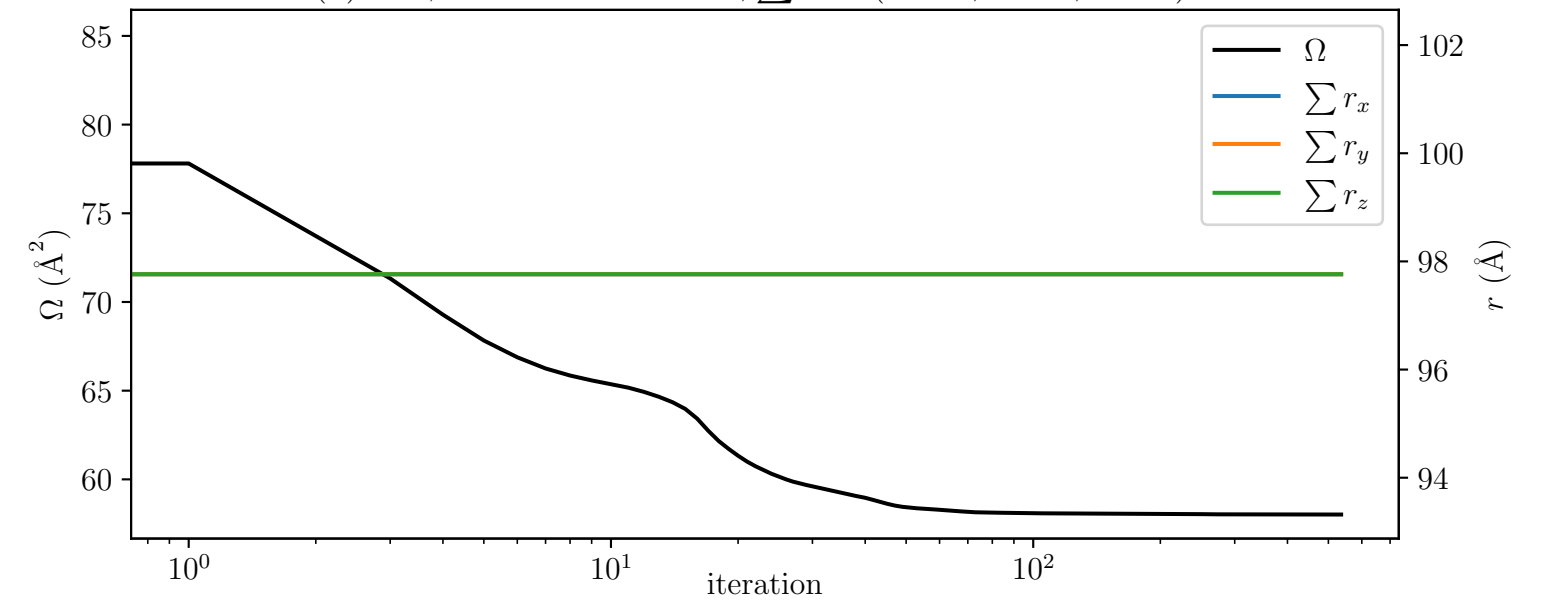
Ge₄Ru₄ (exclude semicore)
PW AiiDA UUID: b6dcbe0f-88ff-43d1-a1a0-981f46306c64
W90 AiiDA UUID: 9e401856-be82-467f-8365-b2fb5abd4d92



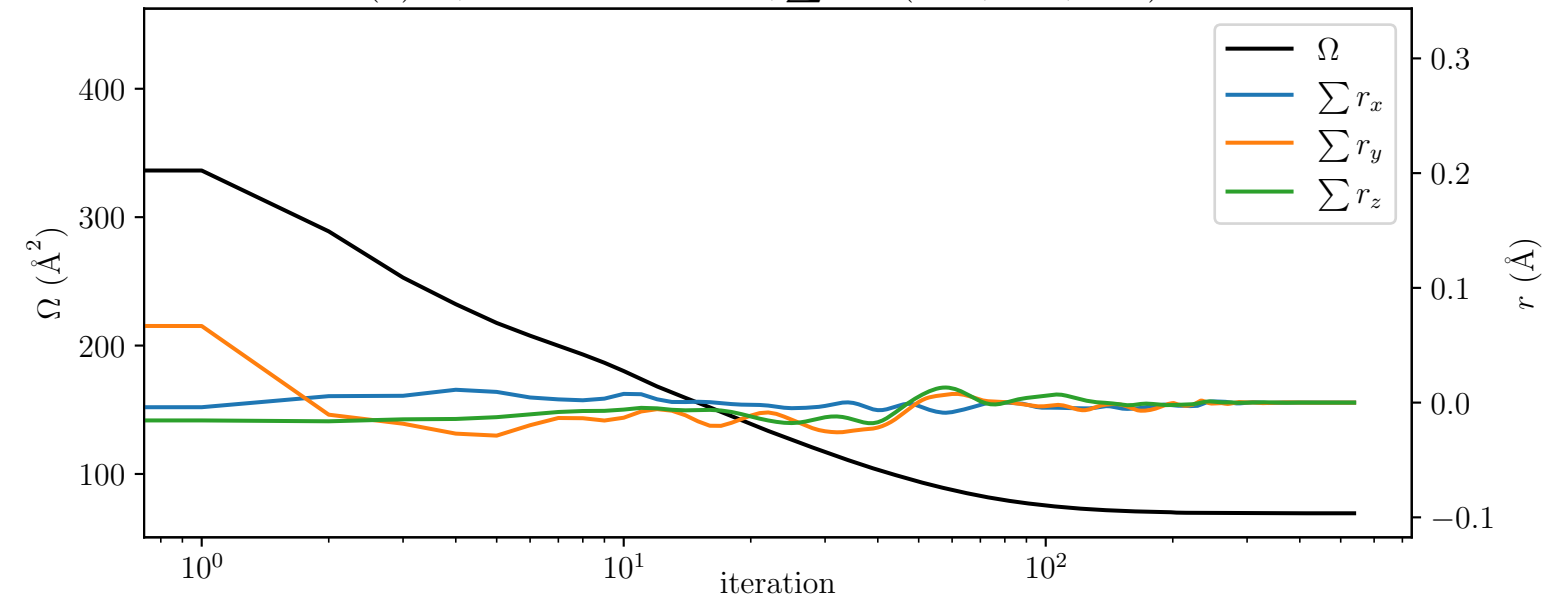
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.5	1.4	1.0	1.7	2.0	4.6	4.8
η_{max}	8.4	8.4	10.1	9.3	6.9	15.4	30.9

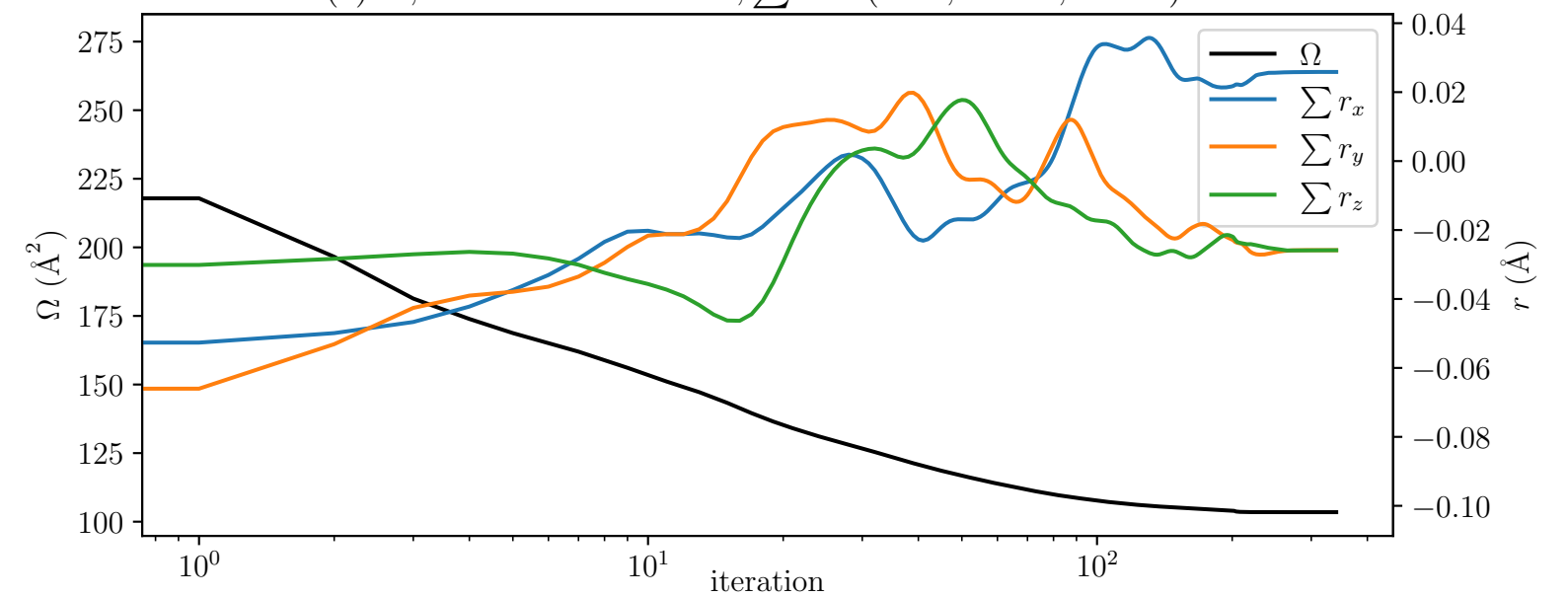
(a) VC; final $\Omega = 58.02 \text{ \AA}^2$, $\sum r = (97.76, 97.76, 97.76) \text{ \AA}$



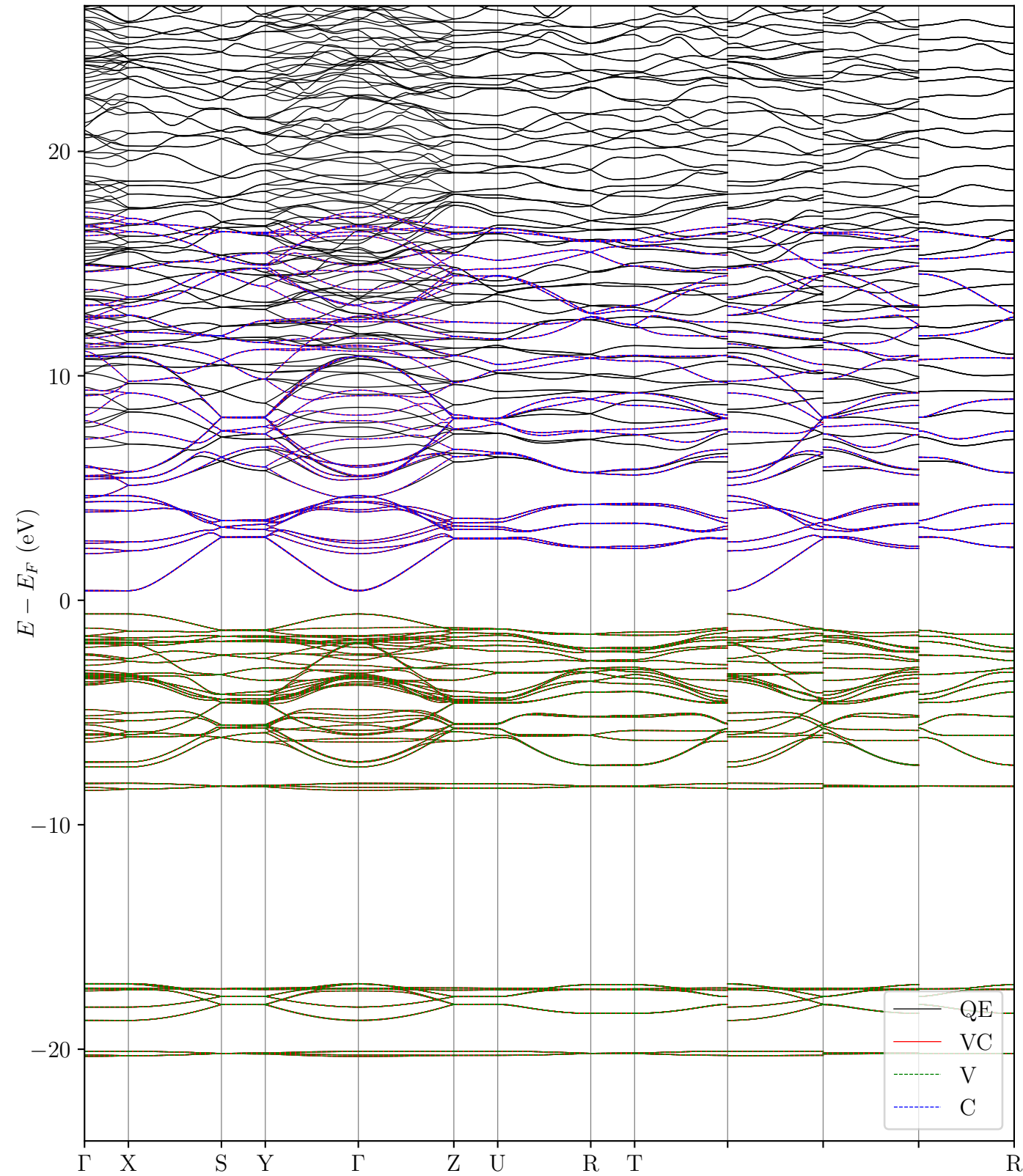
(b) V; final $\Omega = 69.38 \text{ \AA}^2$, $\sum r = (0.00, 0.00, 0.00) \text{ \AA}$



(c) C; final $\Omega = 103.47 \text{ \AA}^2$, $\sum r = (0.03, -0.03, -0.03) \text{ \AA}$



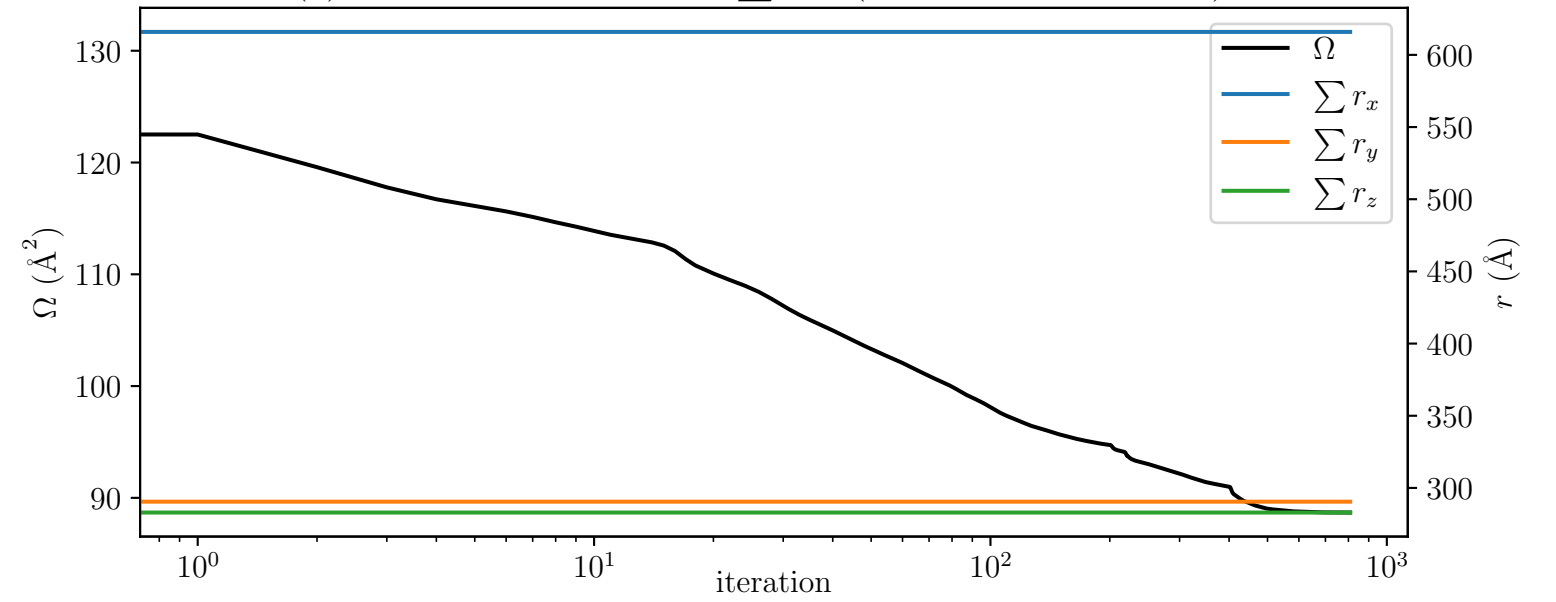
H₈O₁₆W₄ (exclude semicore)
PW AiiDA UUID: 91a86788-d3f7-40a7-9f00-2664287f622a
W90 AiiDA UUID: b61fb27e-33b1-4ecc-ac5d-b49e4db5ad4f



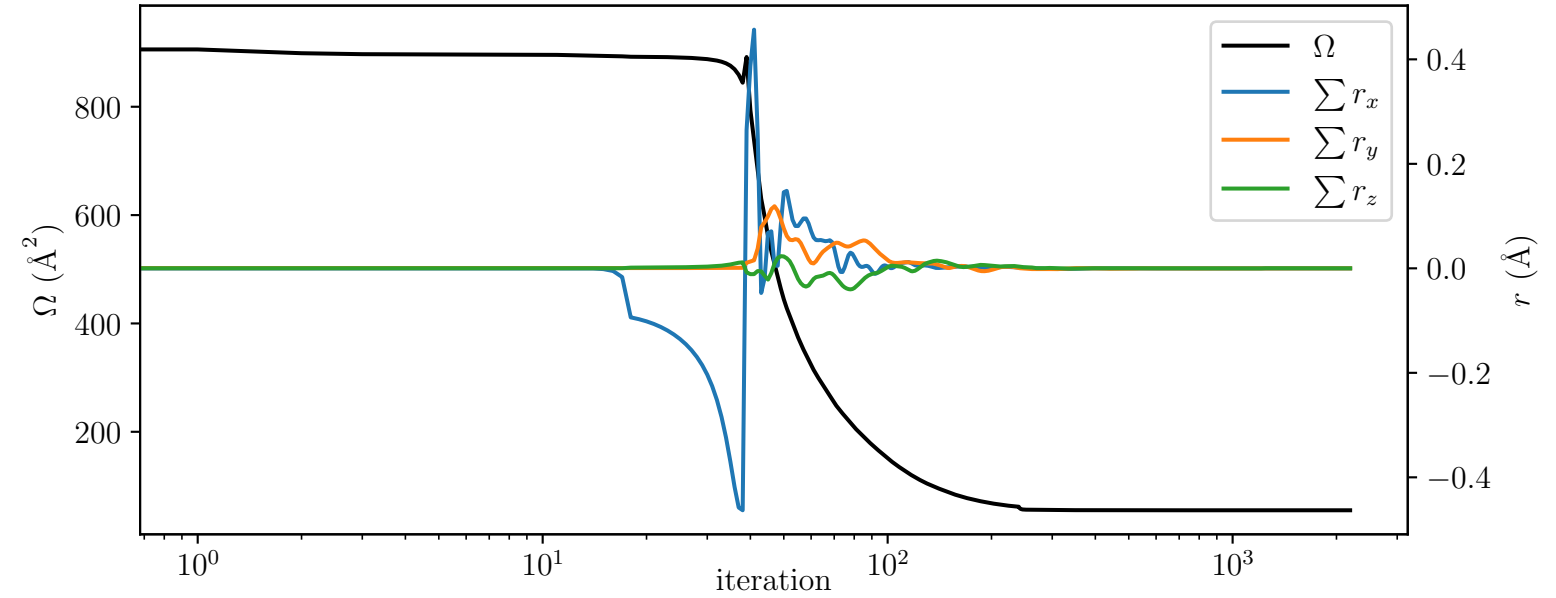
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.2	0.2	0.4	0.4	0.5	2.5	0.9
η_{max}	2.8	2.8	5.8	5.2	2.2	6.5	6.1

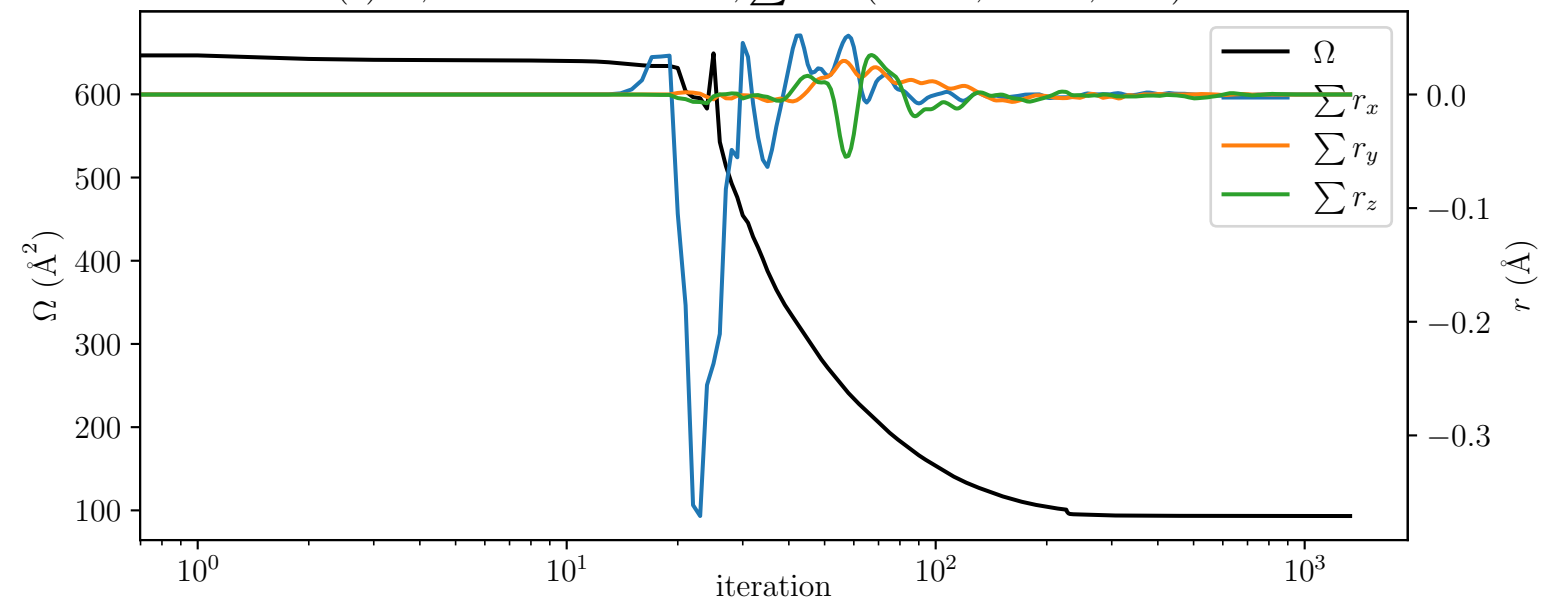
(a) VC; final $\Omega = 88.69 \text{ \AA}^2$, $\sum r = (615.91, 290.46, 282.95) \text{ \AA}$



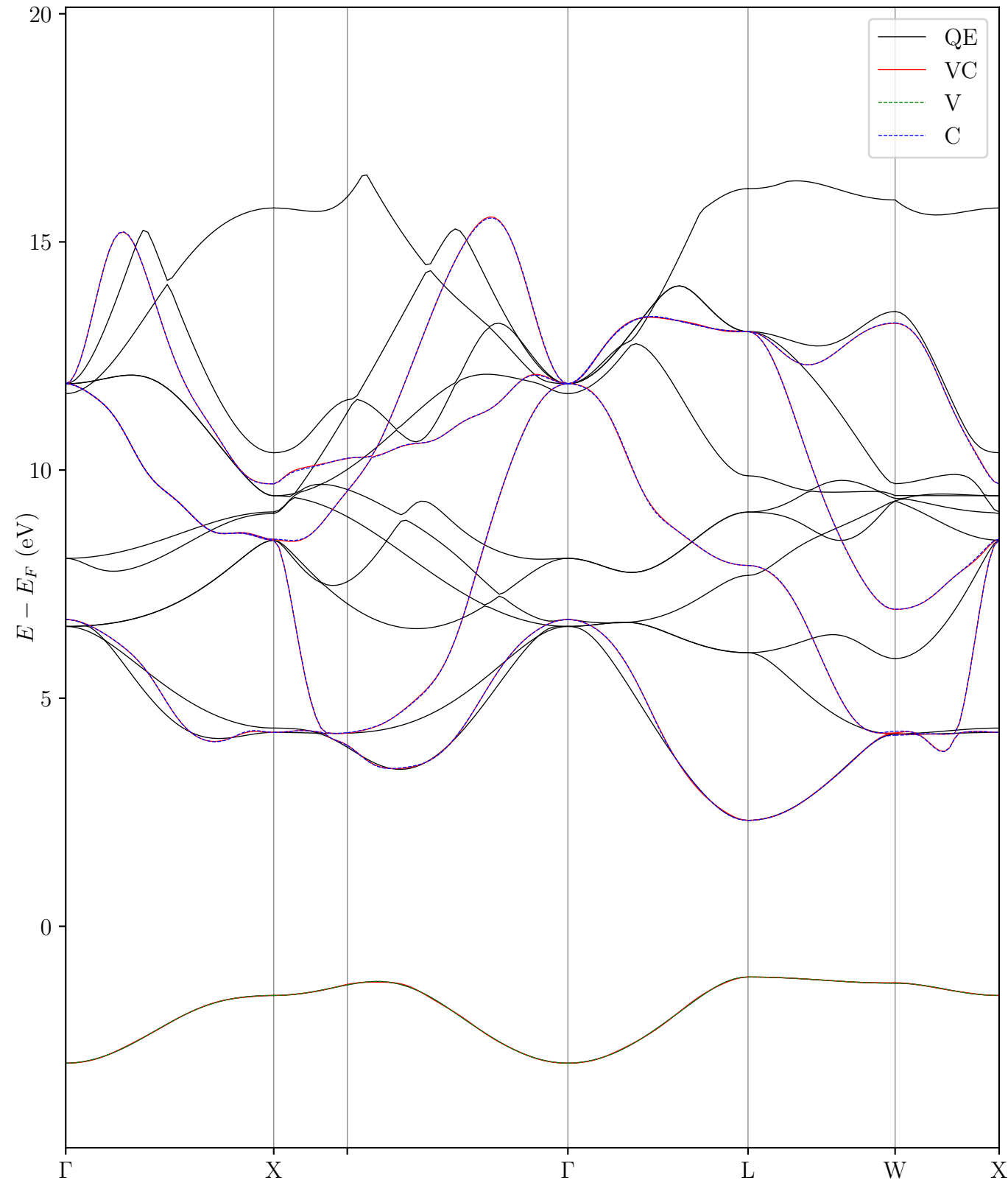
(b) V; final $\Omega = 55.13 \text{ \AA}^2$, $\sum r = (-0.00, -0.00, -0.00) \text{ \AA}$



(c) C; final $\Omega = 93.20 \text{ \AA}^2$, $\sum r = (-0.00, -0.00, 0.00) \text{ \AA}$

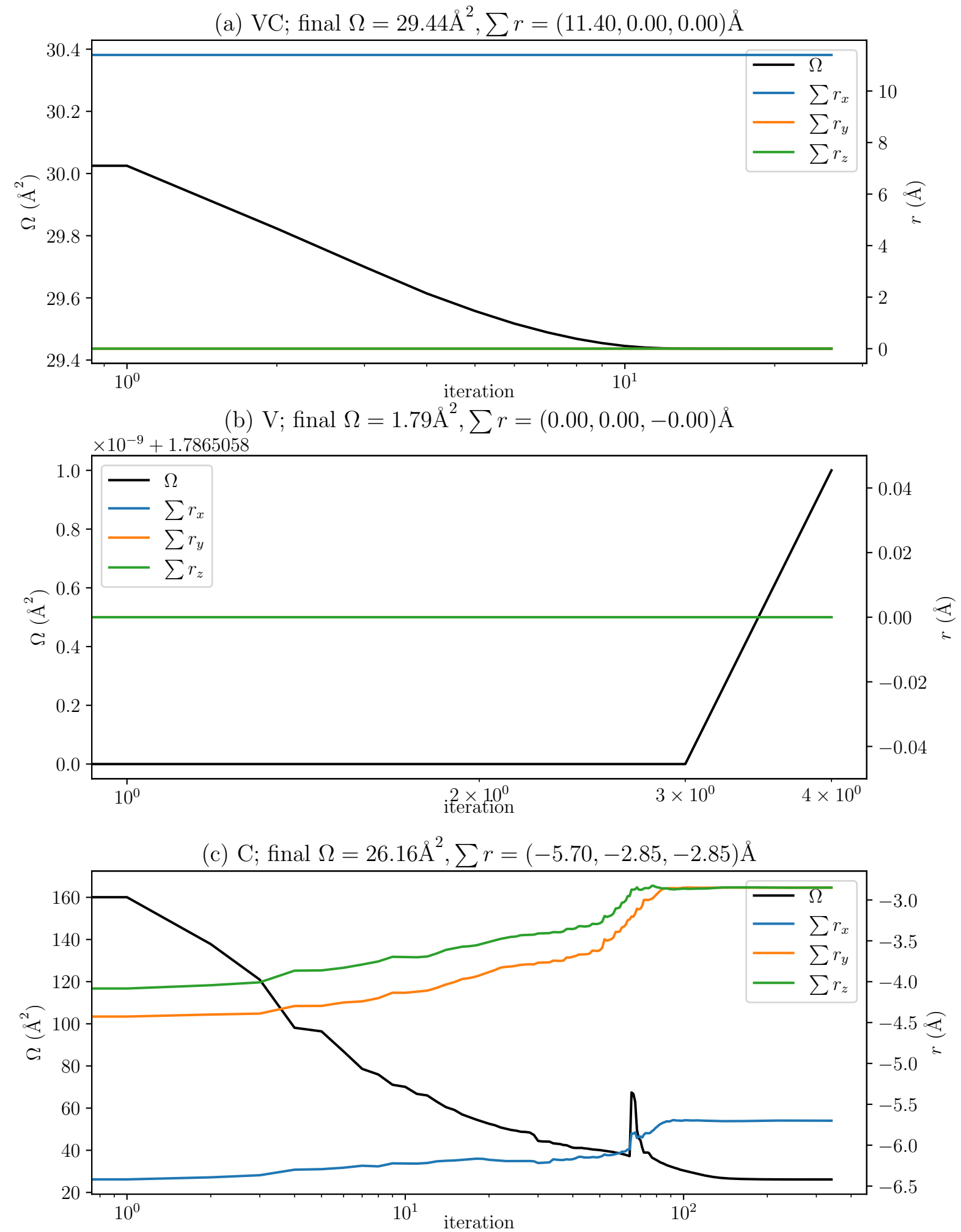


HK (hydrogenic projection, energy disentanglement)
PW AiiDA UUID: 3c529ff0-2261-4d4c-9988-bd1164e97155
W90 AiiDA UUID: ace593e4-8053-4fc4-8585-923b449ddbfb

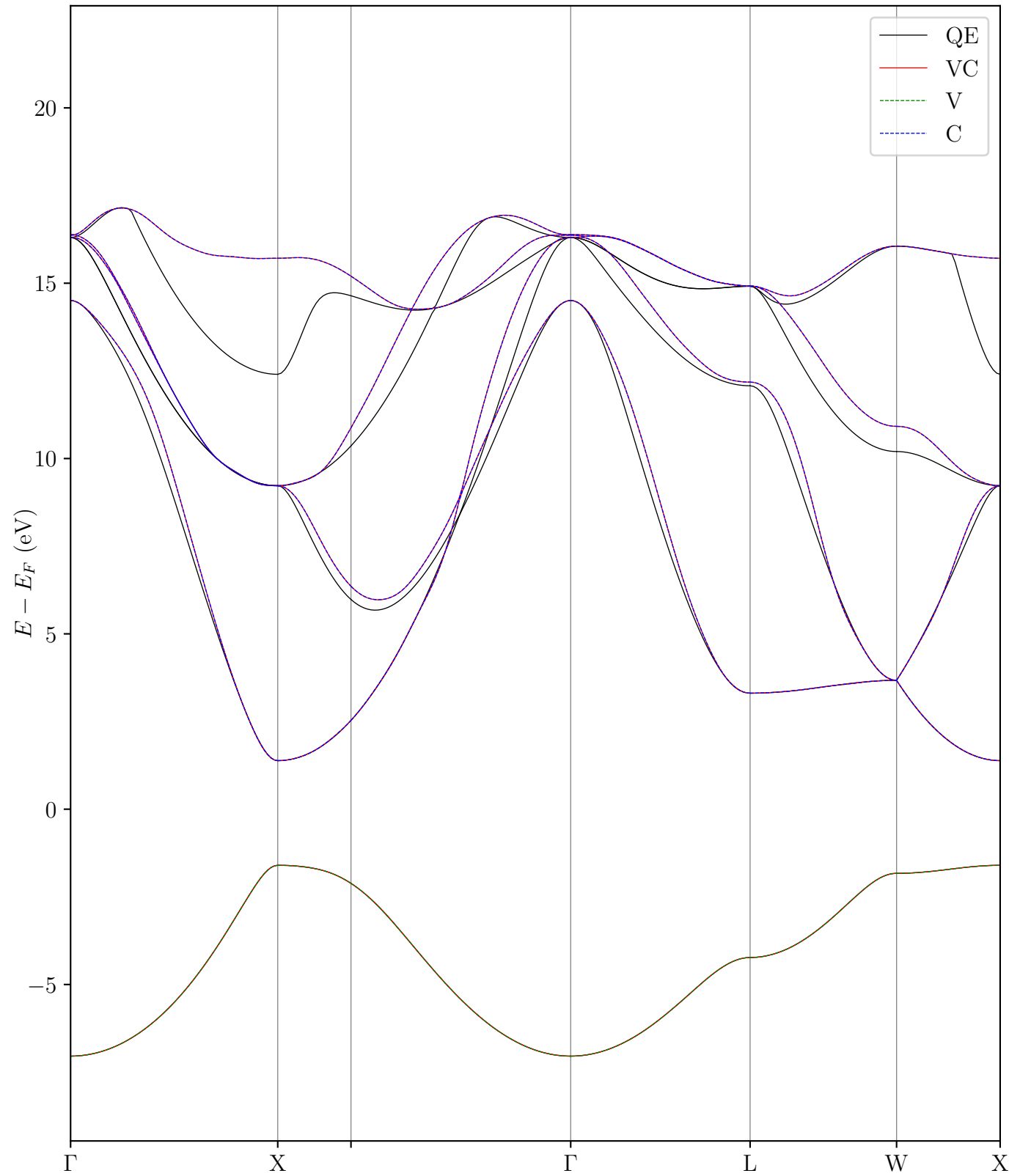


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	6.6	6.6	0.1	6.7	6.7	2.8	9.7
η_{max}	17.5	17.5	0.3	17.5	0.3	0.1	45.7



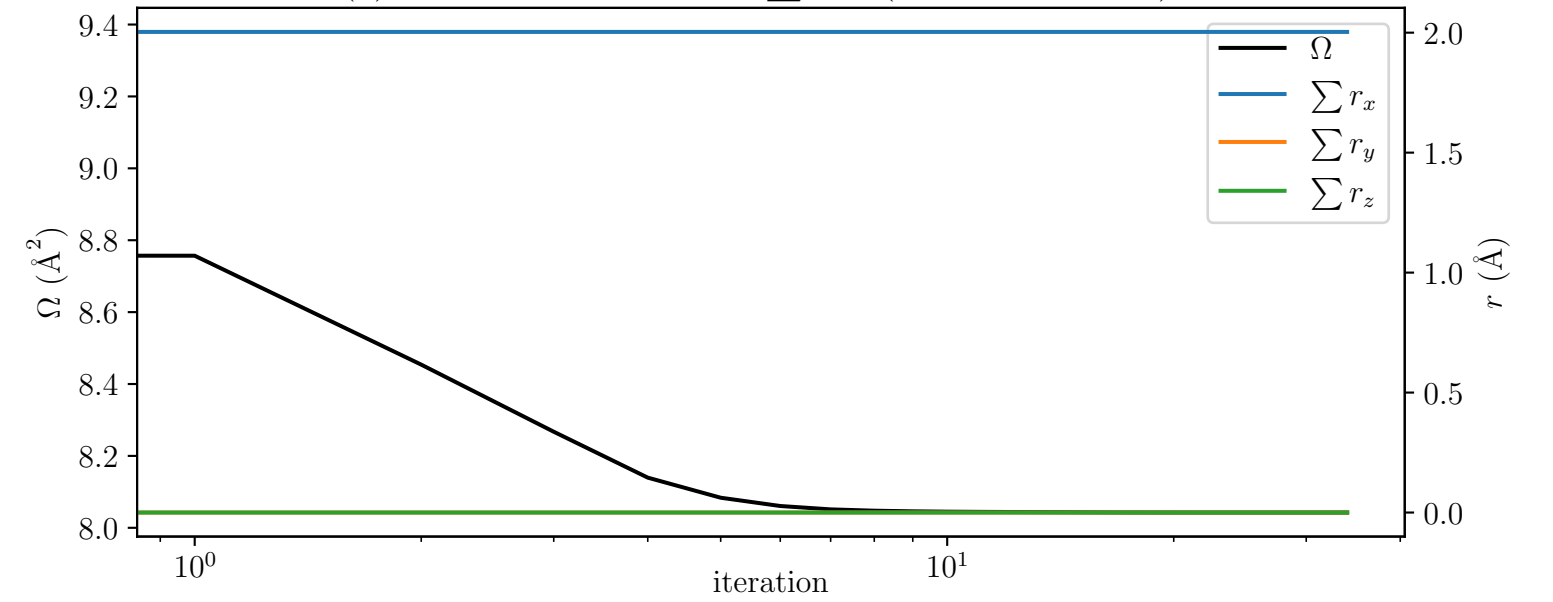
HLi (exclude semicore)
PW AiiDA UUID: 78645328-897b-4ace-bf42-7909b9f99487
W90 AiiDA UUID: e0cff6b3-7ff8-46a9-acb6-5488f95ca3a5



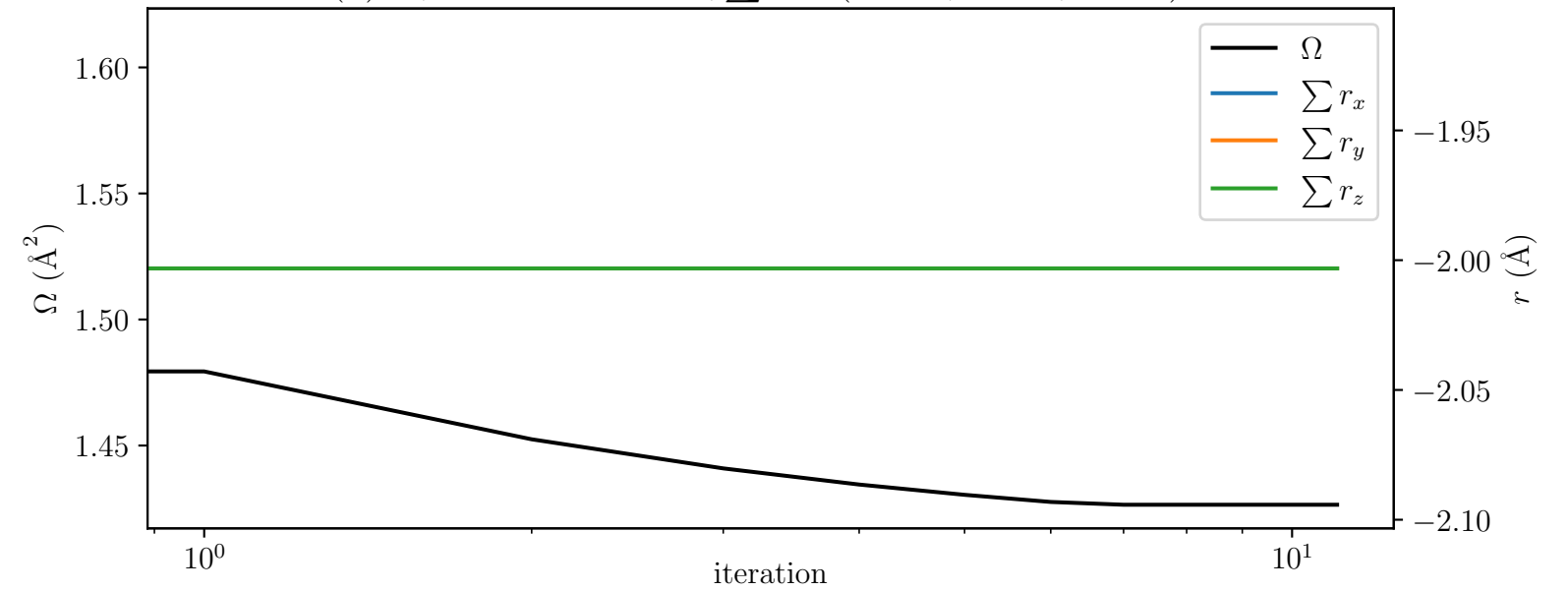
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	2.3	2.0	0.9	2.0	3.8	2.9	1.7
η_{max}	10.7	9.3	4.6	9.1	10.7	6.9	9.4

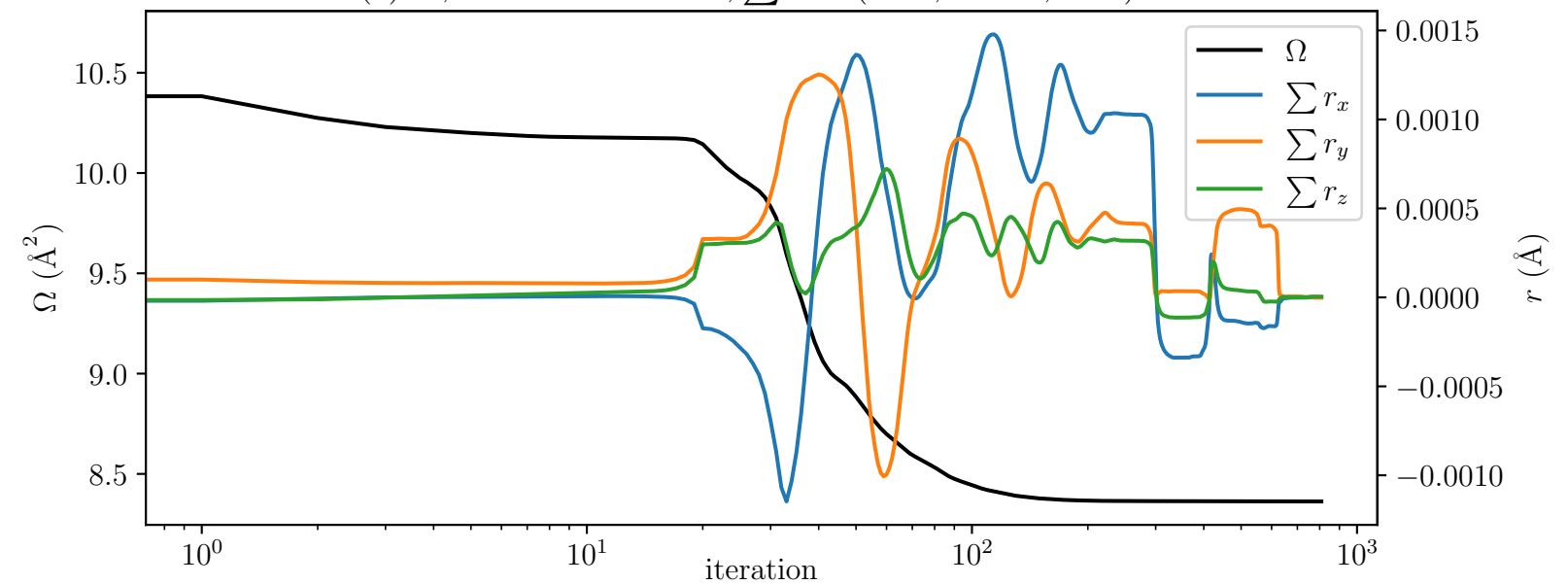
(a) VC; final $\Omega = 8.04 \text{ \AA}^2$, $\sum r = (2.00, -0.00, 0.00) \text{ \AA}$



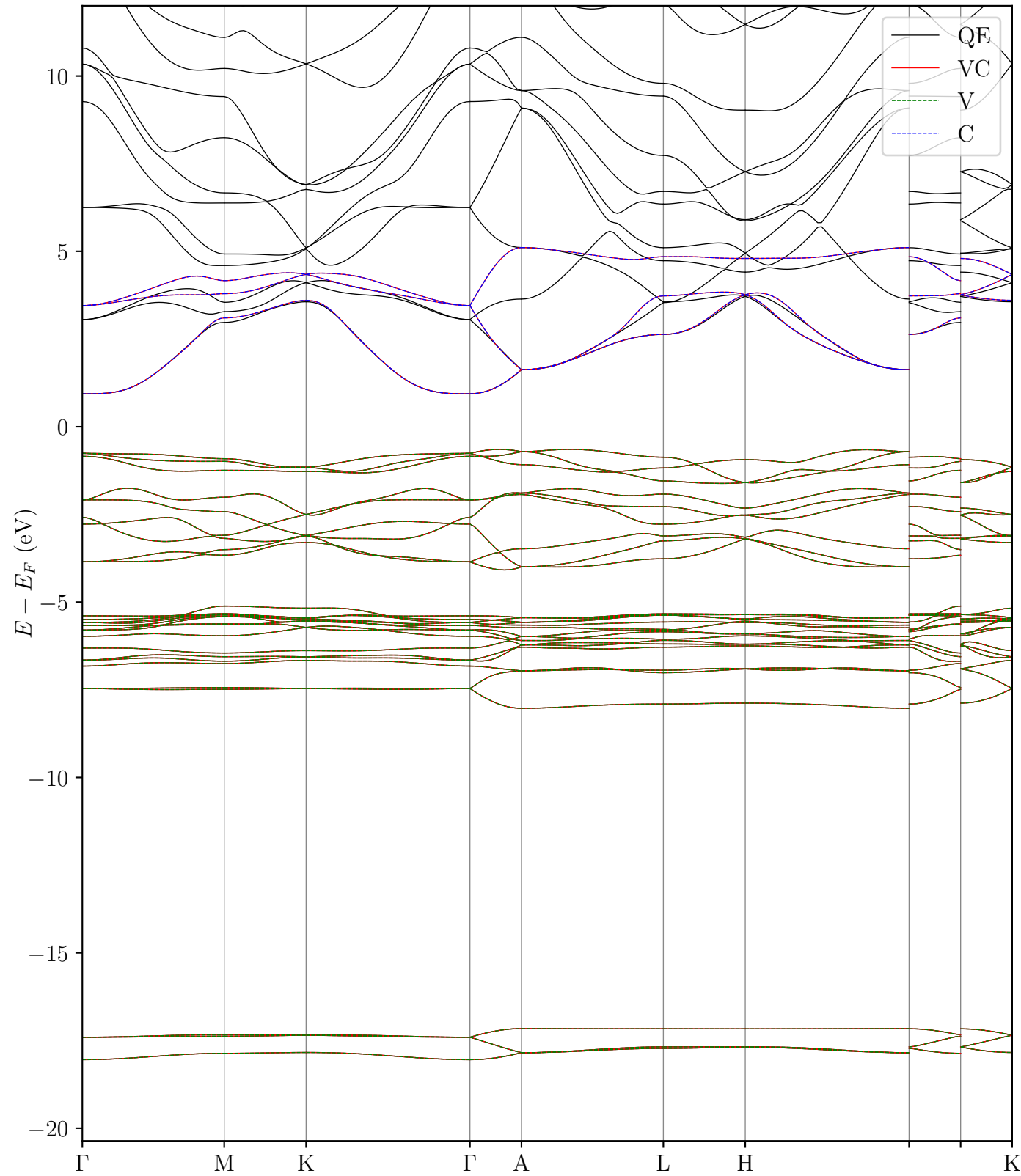
(b) V; final $\Omega = 1.43 \text{ \AA}^2$, $\sum r = (-2.00, -2.00, -2.00) \text{ \AA}$



(c) C; final $\Omega = 8.36 \text{ \AA}^2$, $\sum r = (0.00, -0.00, 0.00) \text{ \AA}$

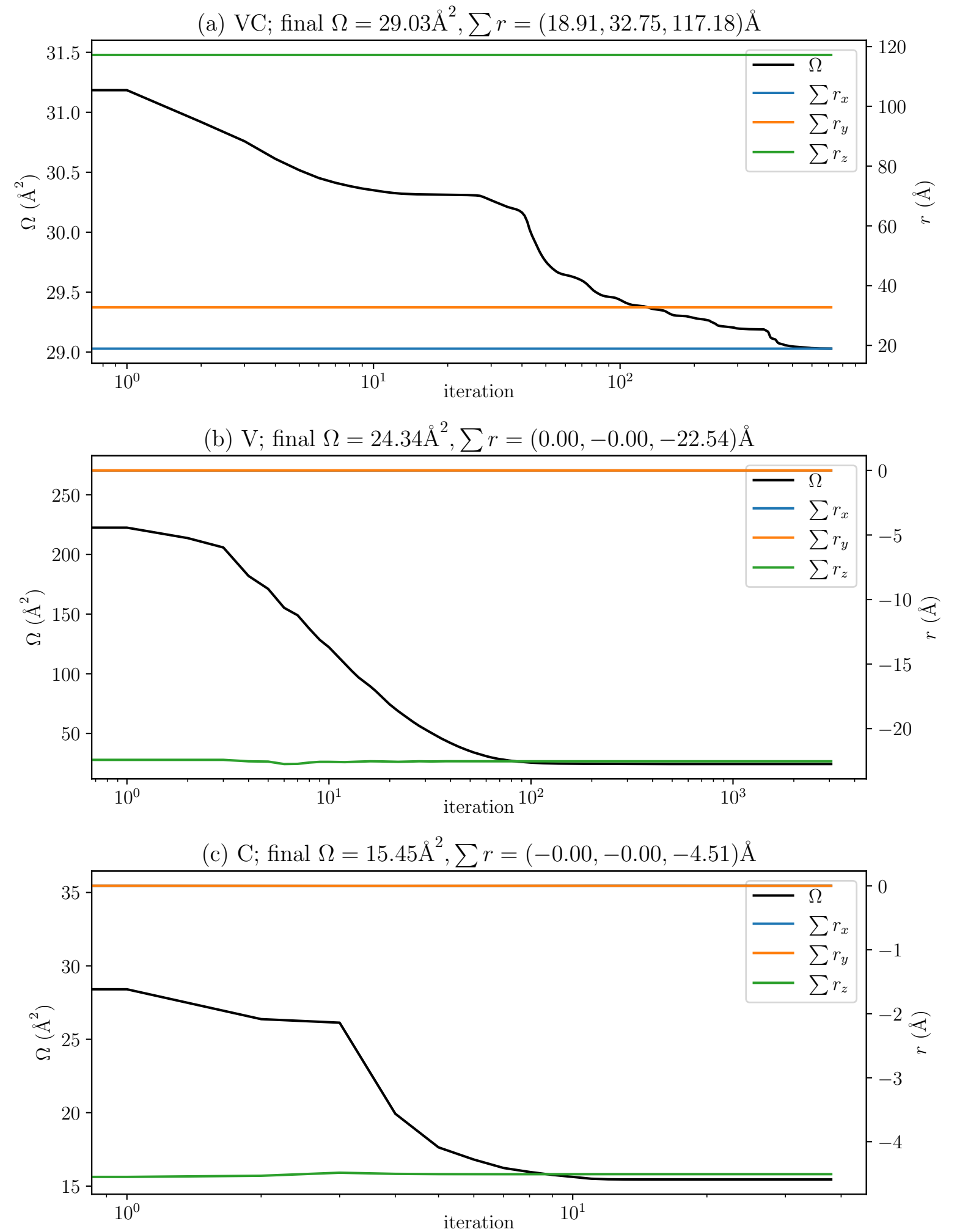


Hg₃O₃ (exclude semicore)
PW AiiDA UUID: f666fd13-4558-4528-9fdb-7d7943dd957c
W90 AiiDA UUID: 12870f30-e20a-4001-8c0d-852a3d82af33

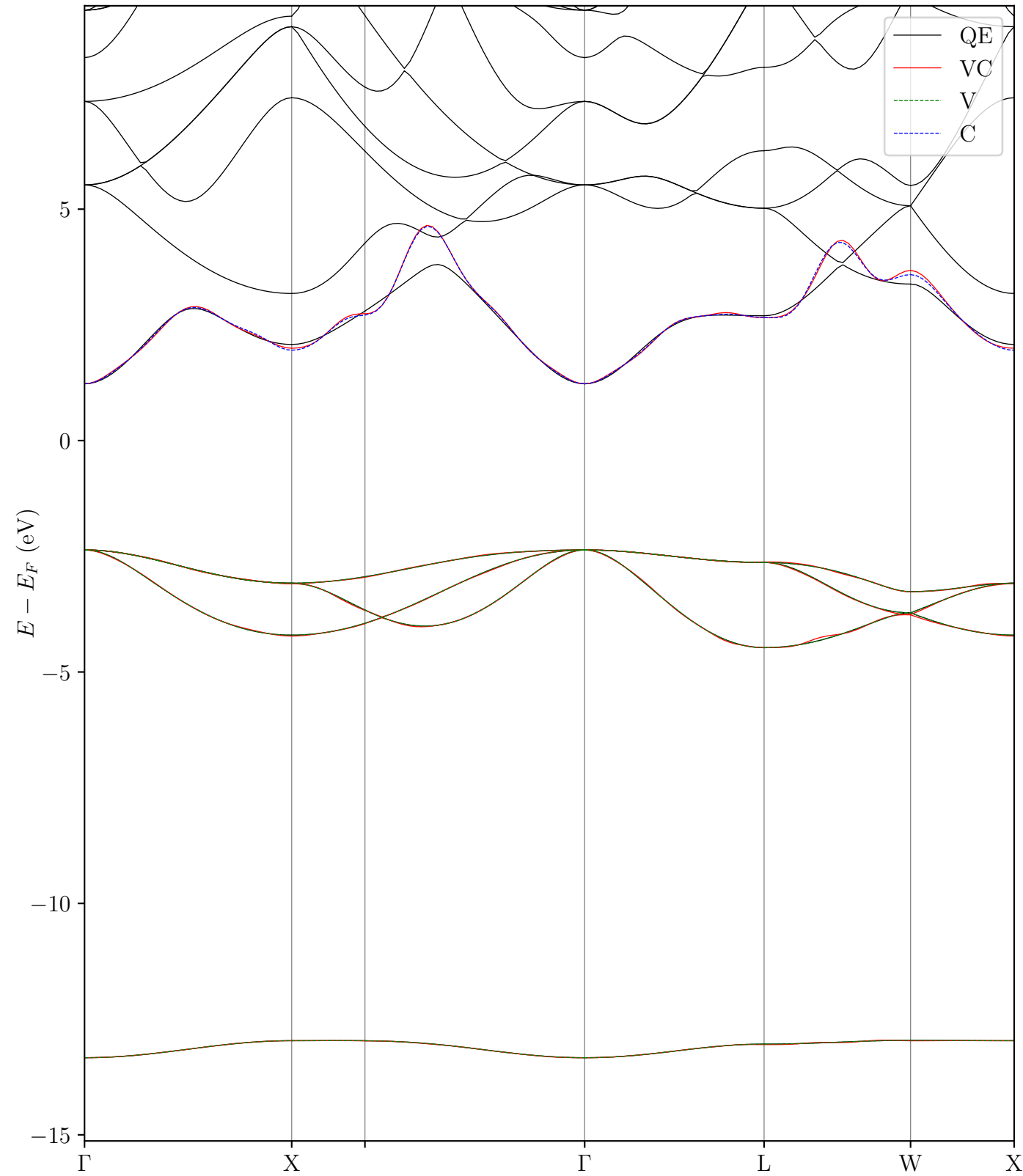


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.6	0.3	0.0	0.3	3.7	3.8	1.0
η_{max}	12.4	2.3	0.3	2.3	12.4	12.4	3.1

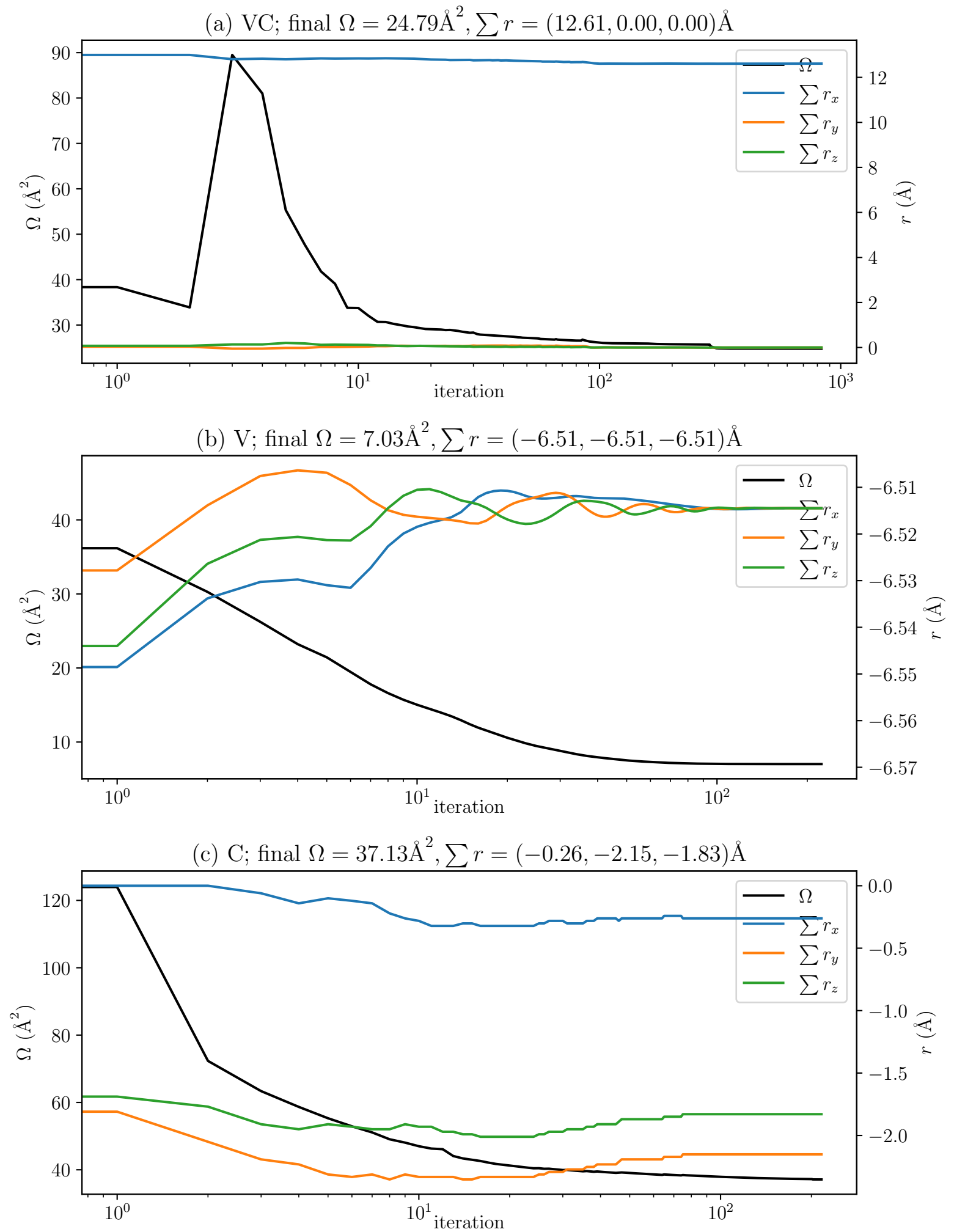


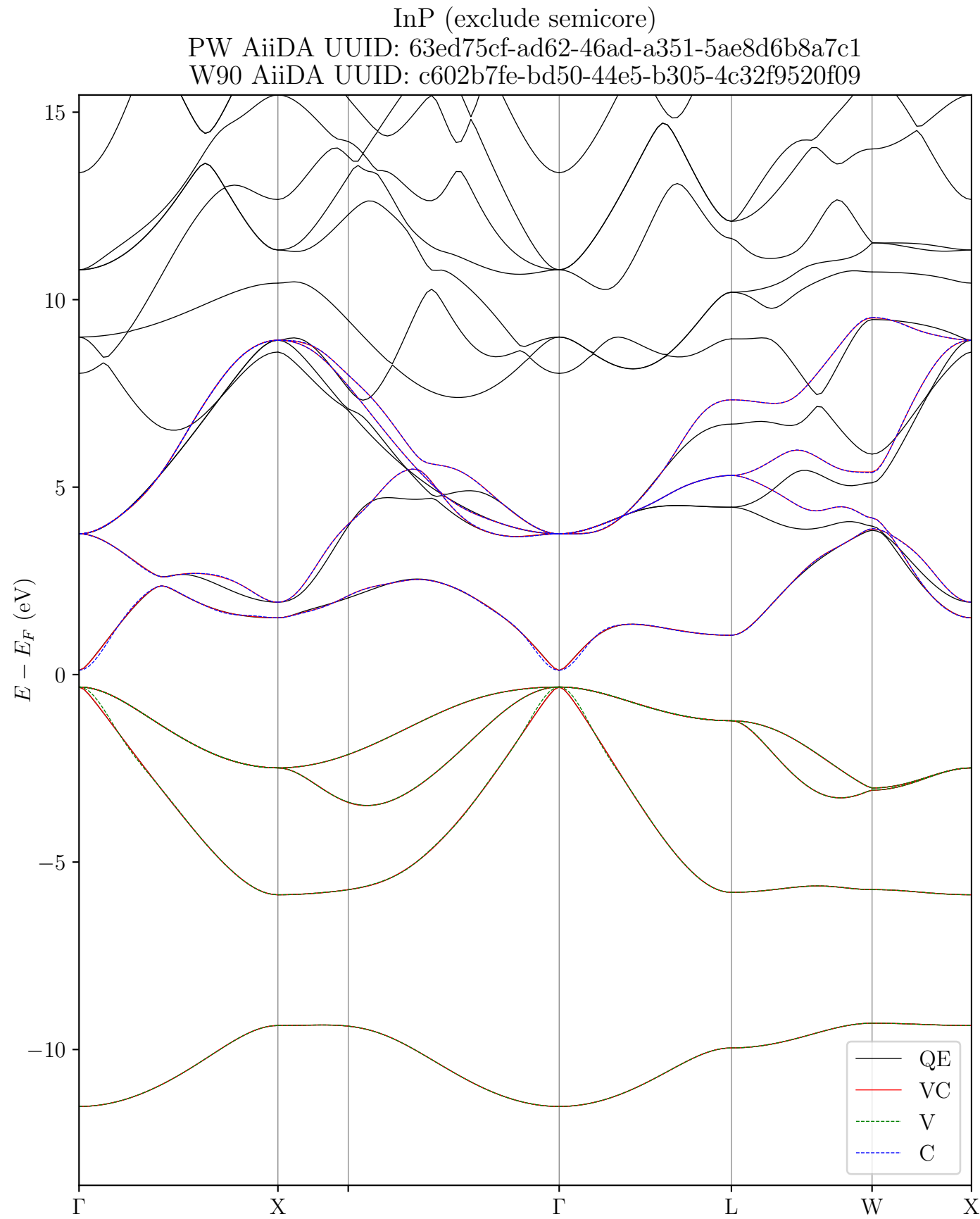
INa (exclude semicore)
PW AiiDA UUID: cf491184-fa7f-4e3f-8418-499494570a68
W90 AiiDA UUID: dc1fa772-ebbc-44bb-9501-482e7412a101



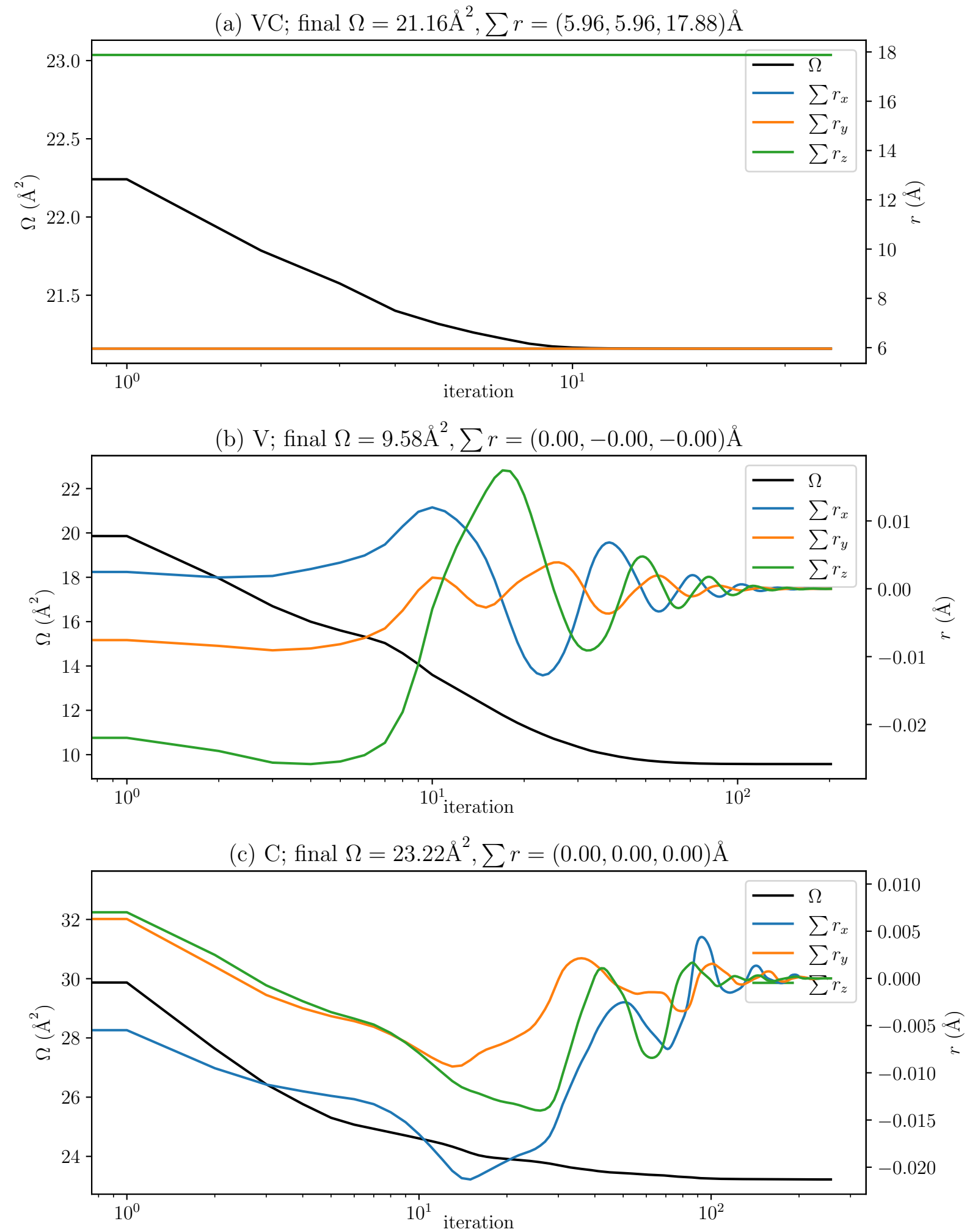
band distance (meV)

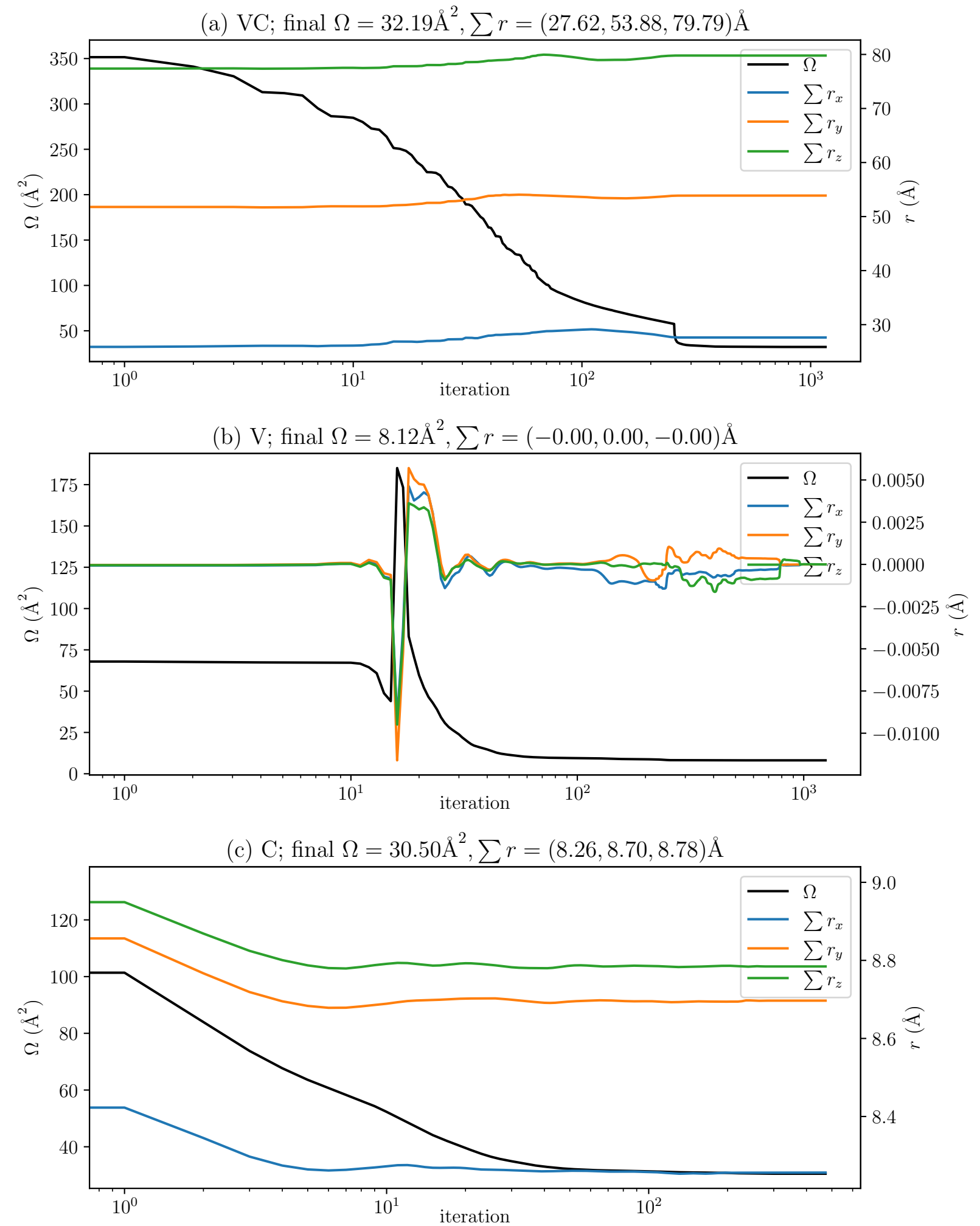
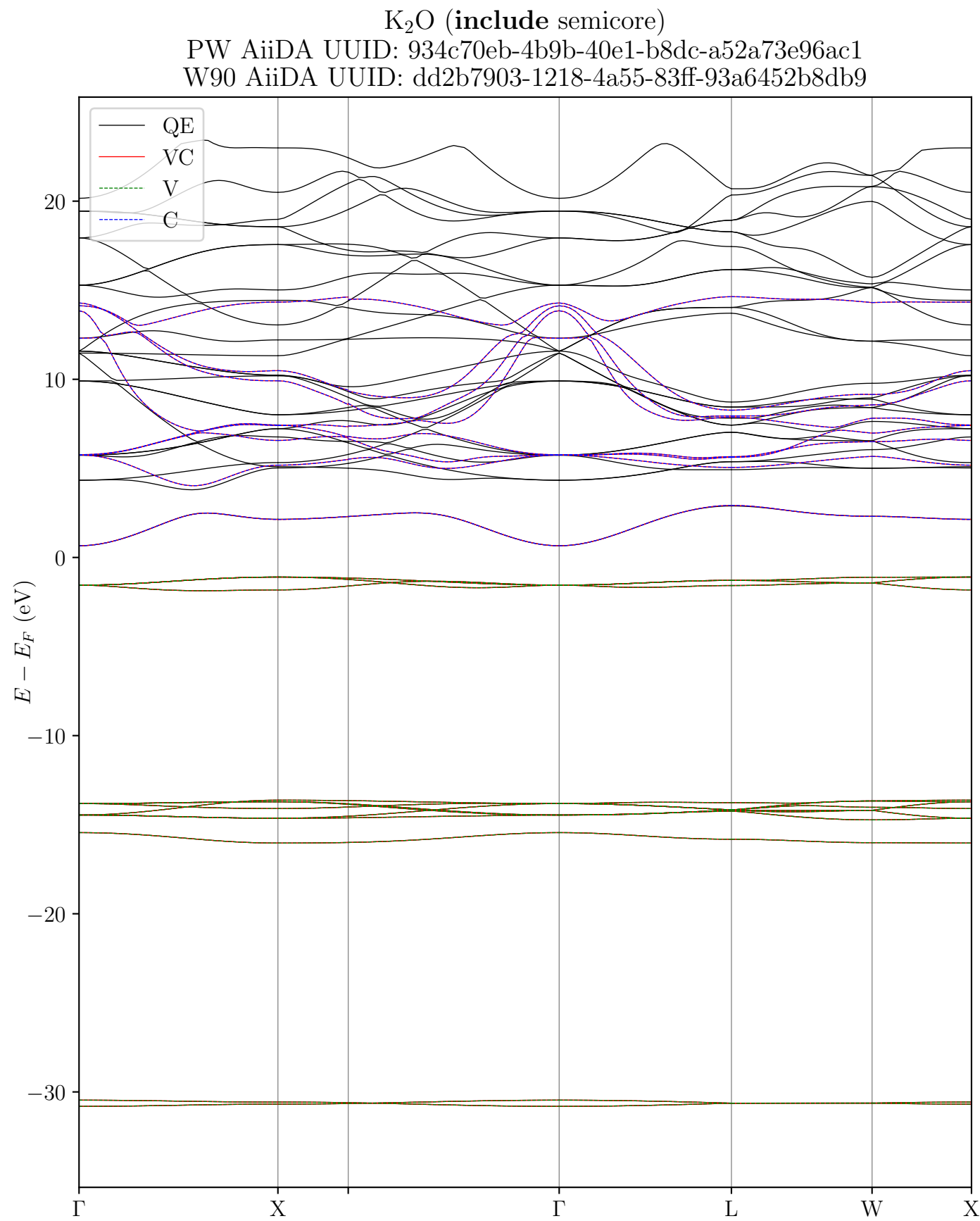
	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	12.8	9.8	0.2	9.8	37.5	41.7	25.2
η_{max}	61.4	61.4	0.9	61.5	44.8	55.3	91.6



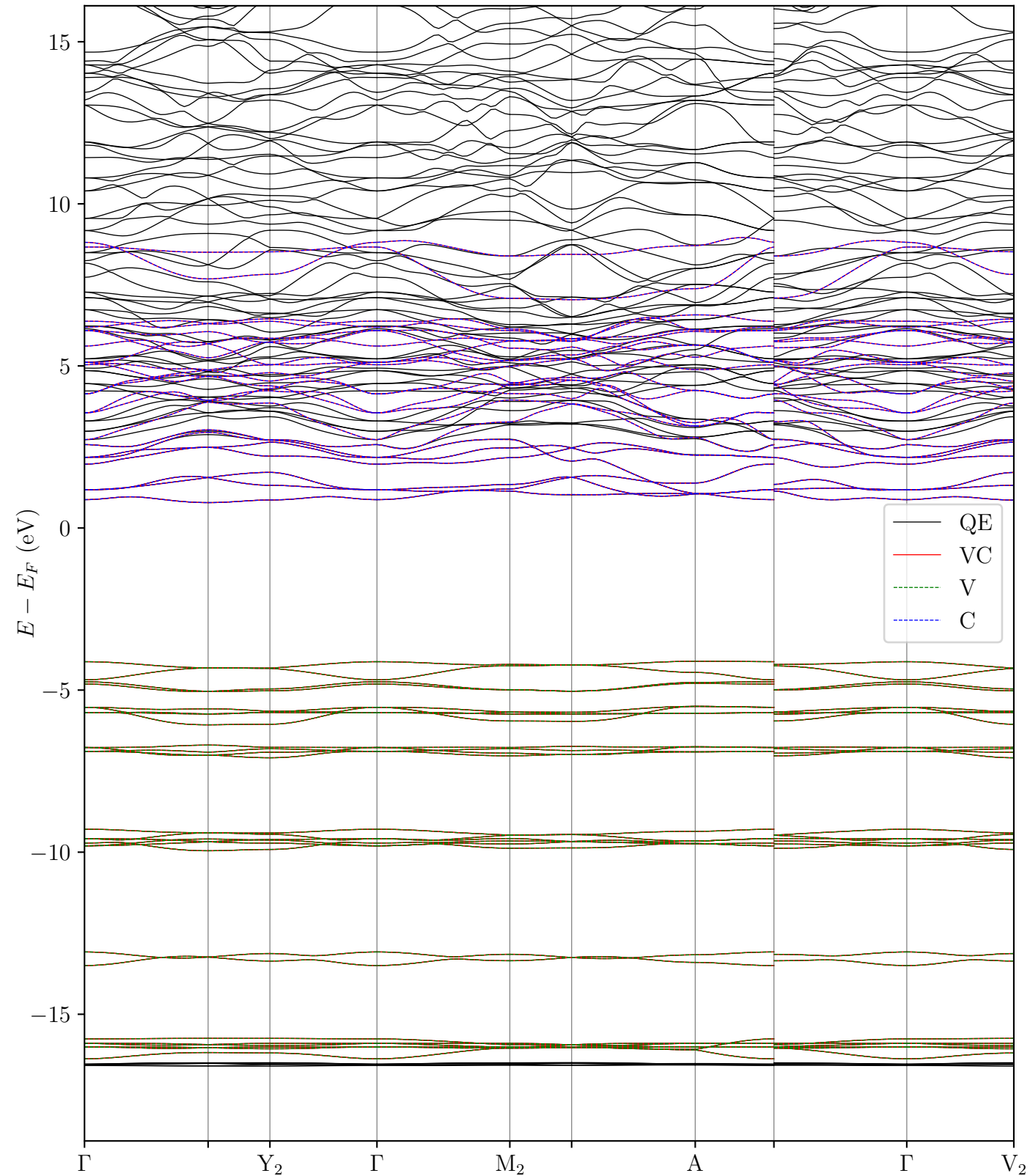


	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	9.0	2.0	15.5	14.8	23.6	42.3	13.7
η_{max}	43.7	9.8	129.9	122.4	43.7	123.8	112.3





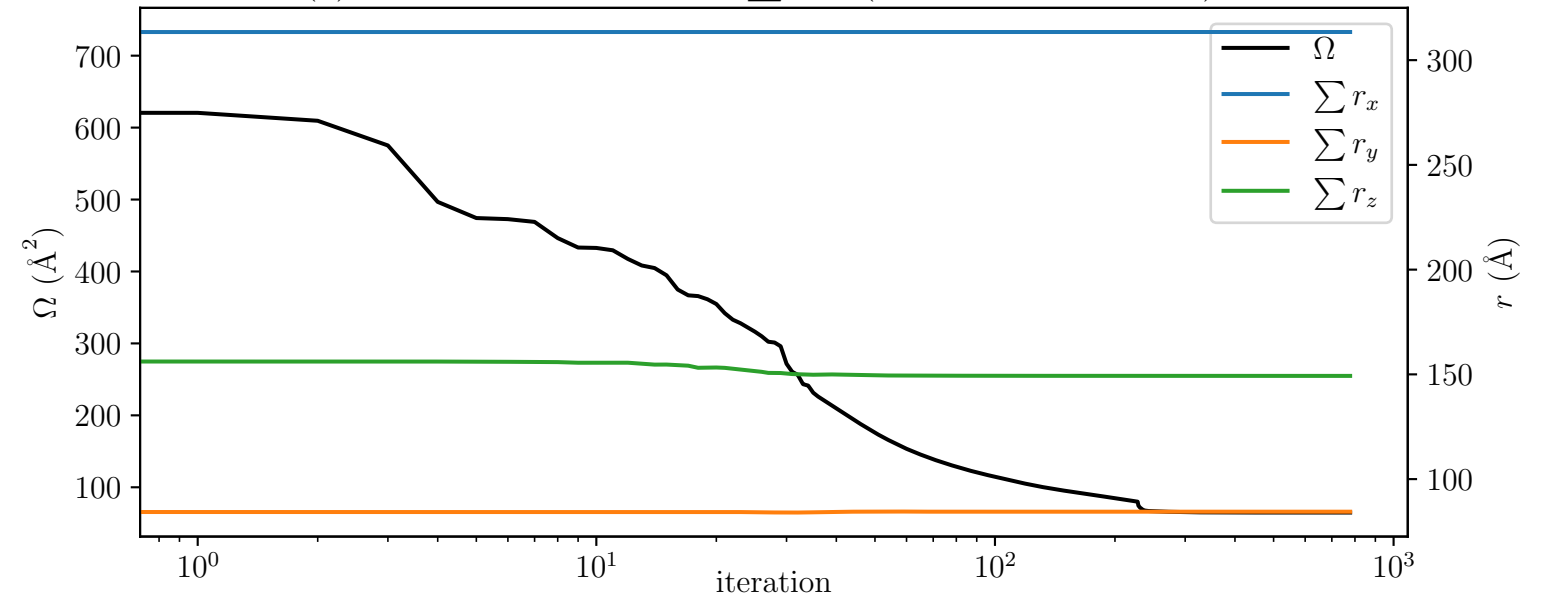
K₄O₆S₂ (exclude semicore)
PW AiiDA UUID: 93c6e920-2925-47b7-a56c-a32fdbd3335e
W90 AiiDA UUID: 52e5580d-02b7-4dc9-9c83-ff01e728699f



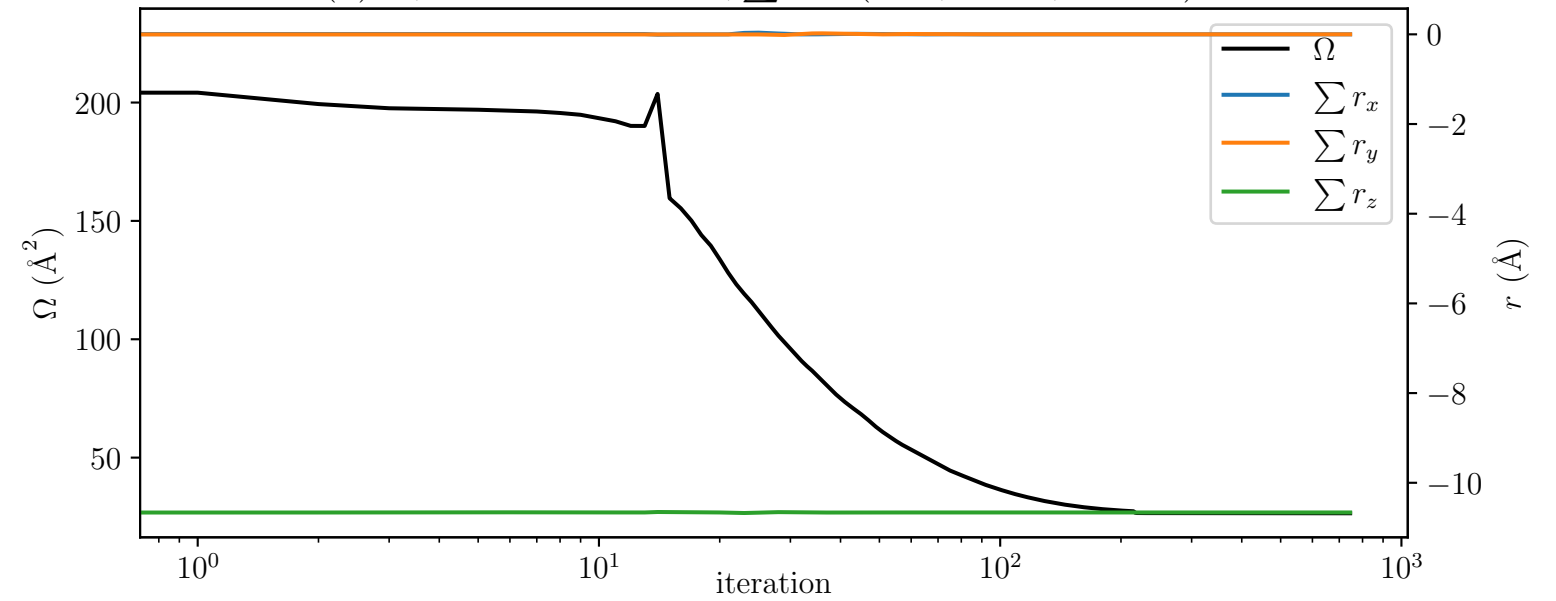
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.8	0.4	0.0	0.4	2.3	2.5	0.7
η_{max}	9.0	3.4	0.1	3.4	9.0	9.8	4.4

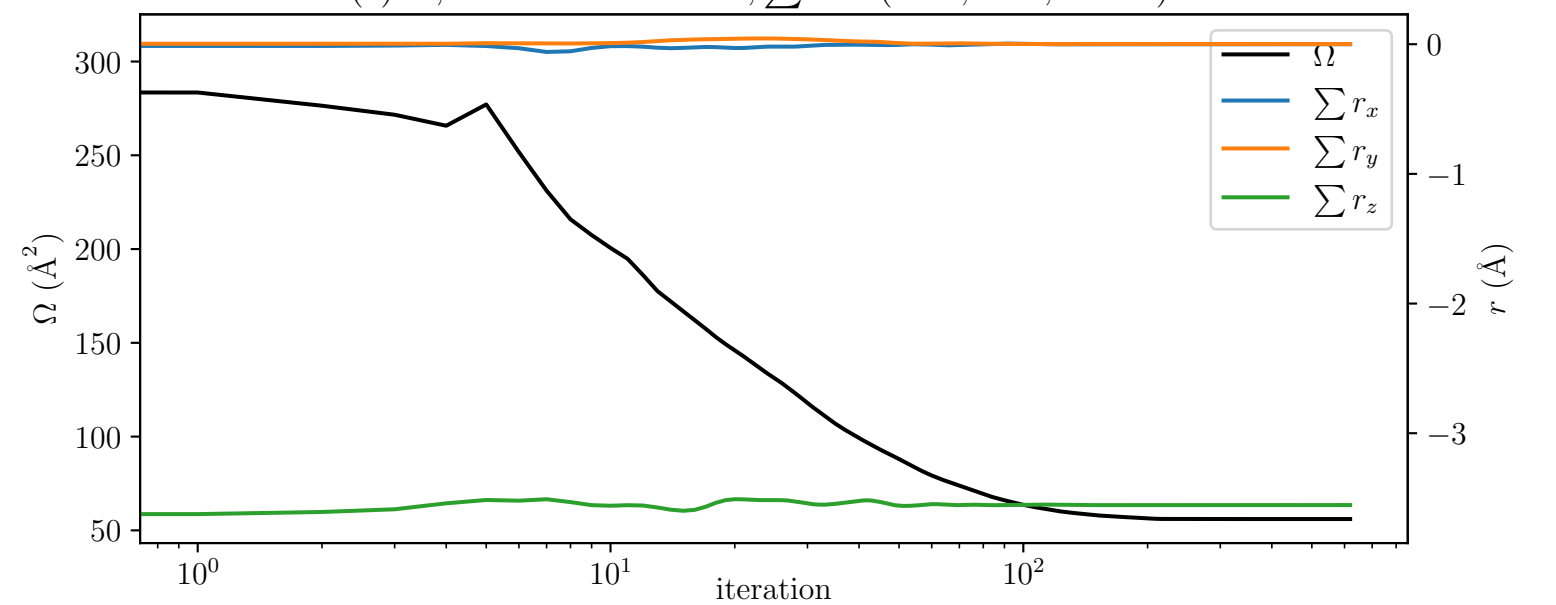
(a) VC; final $\Omega = 64.89 \text{ \AA}^2$, $\sum r = (313.44, 84.45, 149.27) \text{ \AA}$



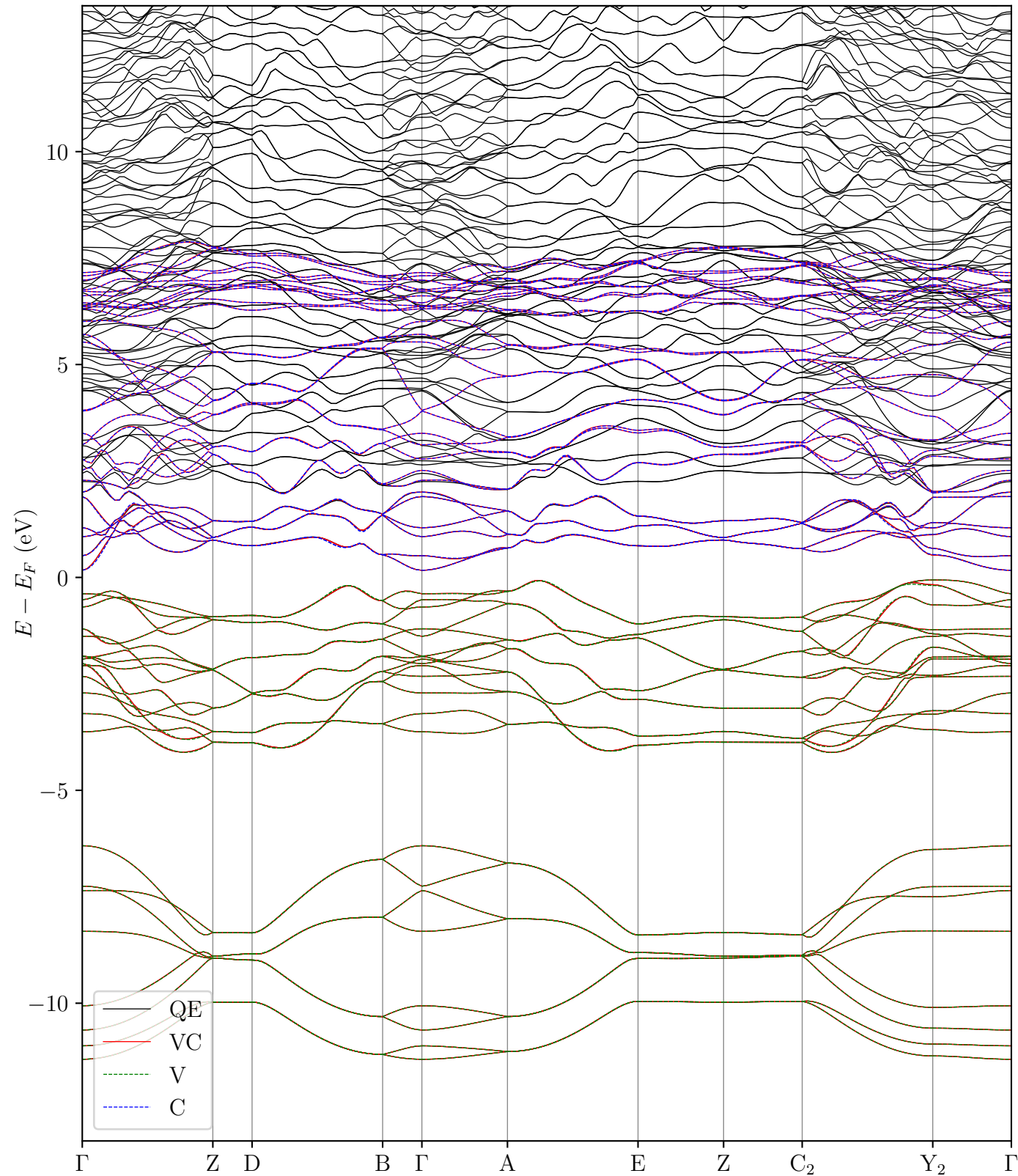
(b) V; final $\Omega = 26.49 \text{ \AA}^2$, $\sum r = (0.00, -0.00, -10.66) \text{ \AA}$



(c) C; final $\Omega = 56.05 \text{ \AA}^2$, $\sum r = (0.00, 0.00, -3.55) \text{ \AA}$



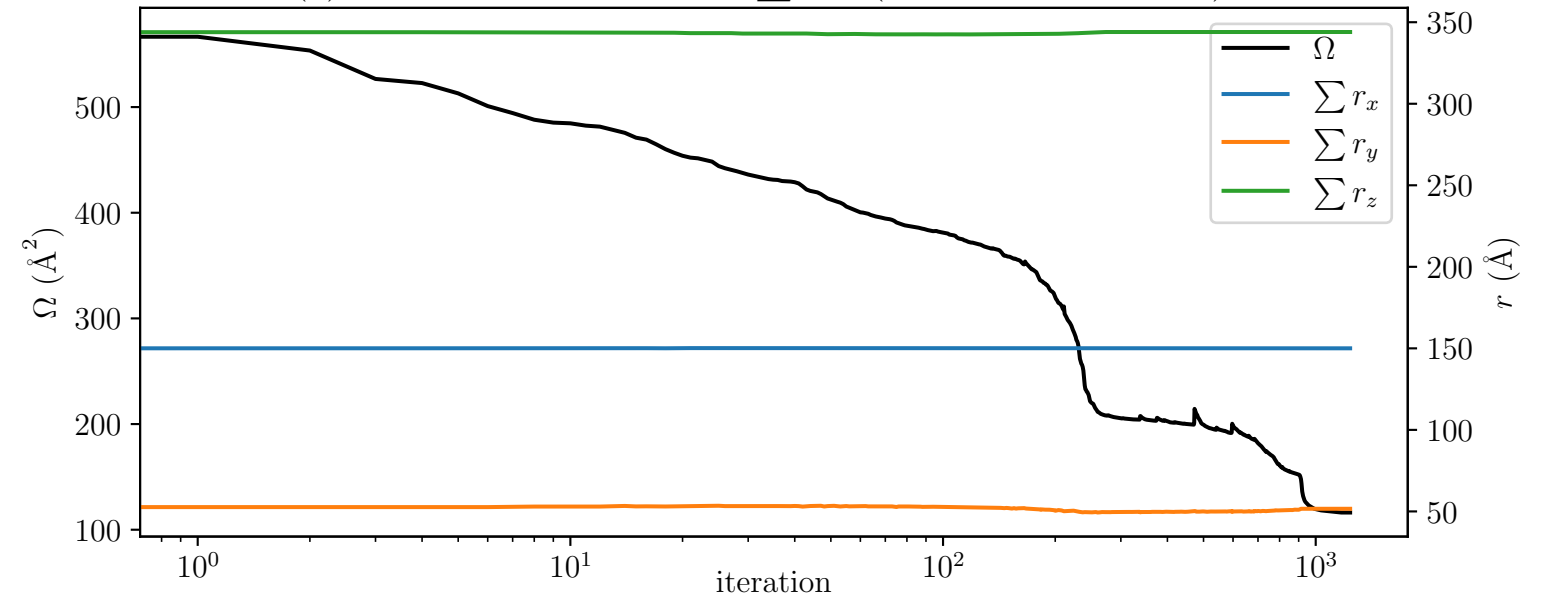
K₄Sb₈ (exclude semicore)
PW AiiDA UUID: 0a63d021-f01c-4fdb-9801-d53dbf058fc0
W90 AiiDA UUID: ab50f875-7717-4256-a2da-69b48af52cb0



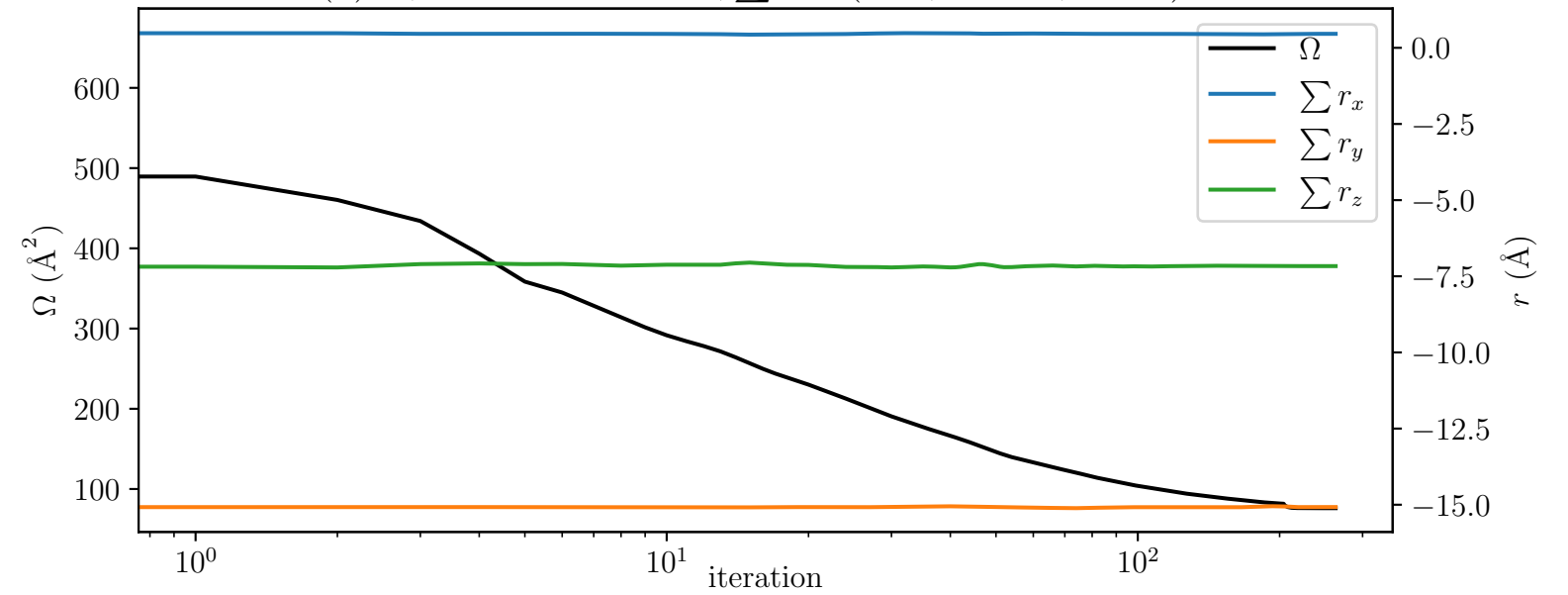
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	6.3	1.6	5.5	5.5	13.3	15.3	4.7
η_{max}	31.9	9.6	44.5	45.3	31.9	65.7	50.1

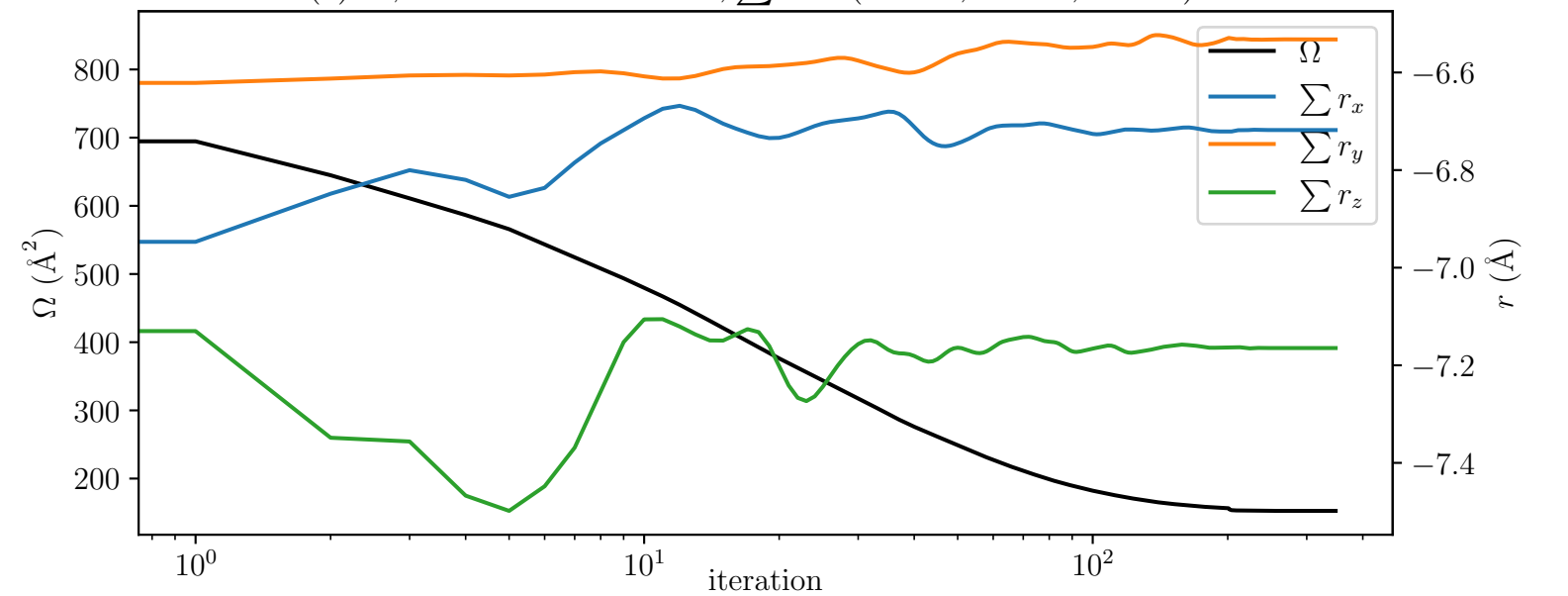
(a) VC; final $\Omega = 116.27 \text{\AA}^2$, $\sum r = (150.02, 51.62, 344.00) \text{\AA}$



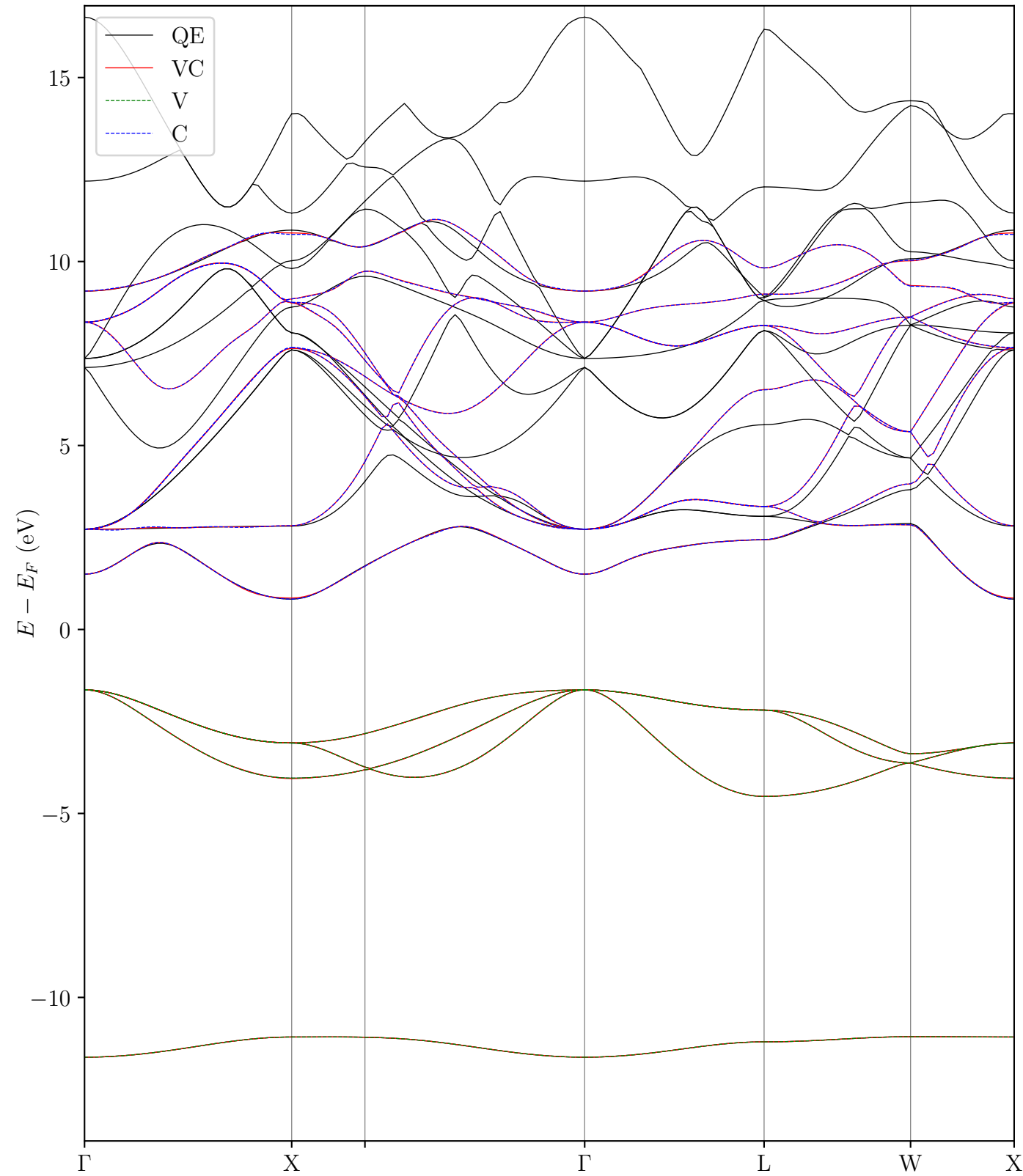
(b) V; final $\Omega = 76.13 \text{\AA}^2$, $\sum r = (0.46, -15.08, -7.17) \text{\AA}$



(c) C; final $\Omega = 152.59 \text{\AA}^2$, $\sum r = (-6.72, -6.53, -7.16) \text{\AA}$



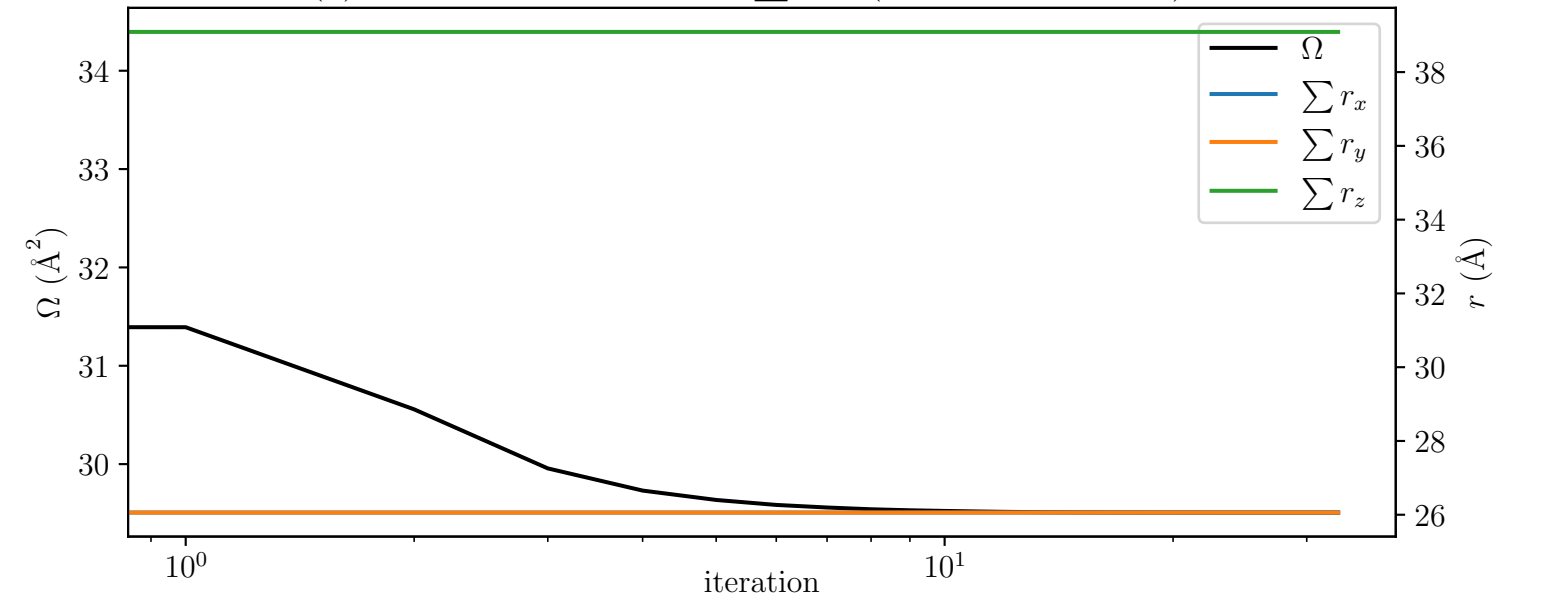
Li₂Te (exclude semicore)
PW AiiDA UUID: 611562b4-f890-4543-939b-25fa2ca665c5
W90 AiiDA UUID: fa610525-6bed-4cd0-ace4-d0beb6eb6403



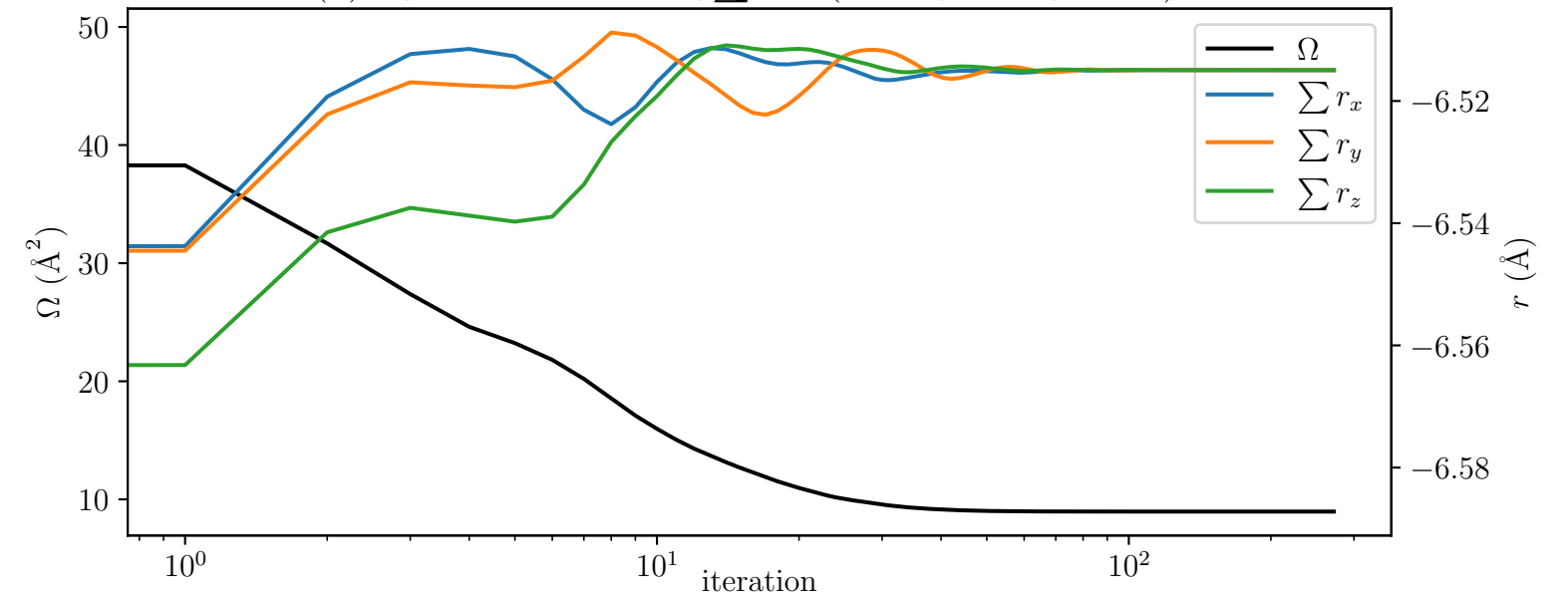
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	5.0	2.6	0.7	2.5	13.8	6.7	7.7
η_{max}	31.2	9.9	3.3	10.9	31.2	13.6	39.3

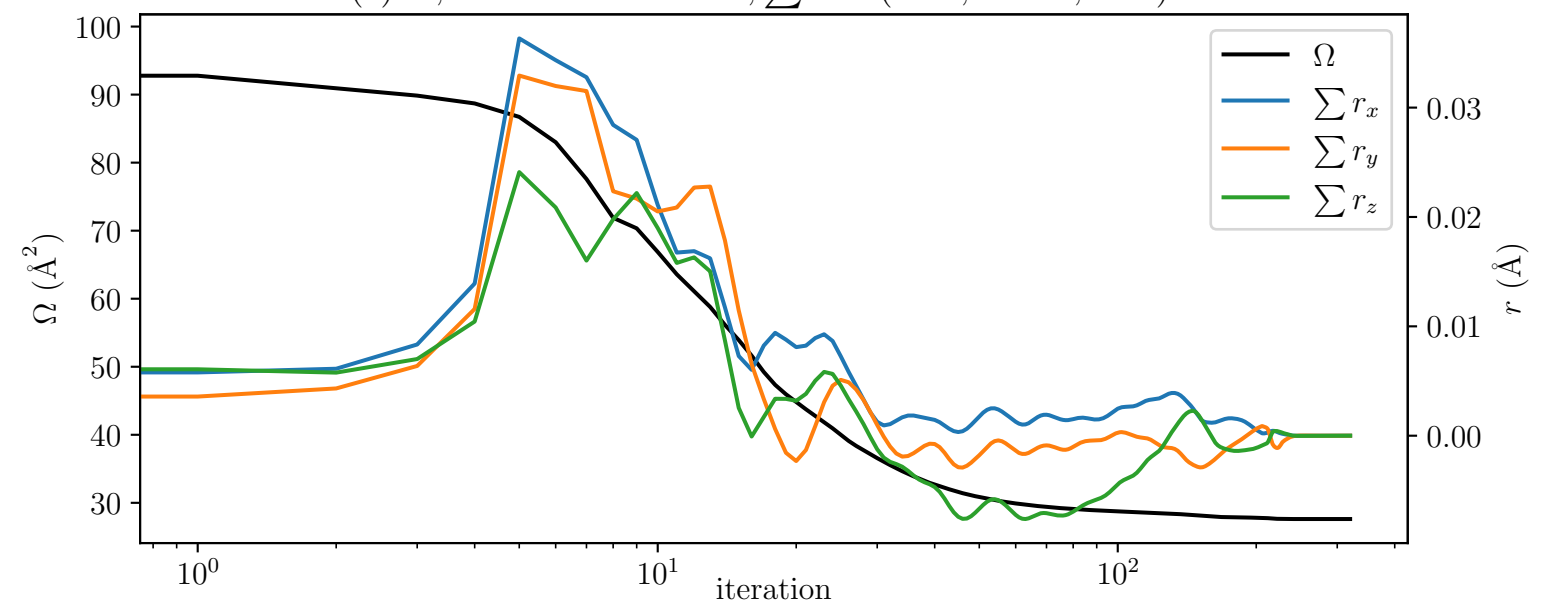
(a) VC; final $\Omega = 29.51 \text{ \AA}^2$, $\sum r = (26.06, 26.06, 39.09) \text{ \AA}$



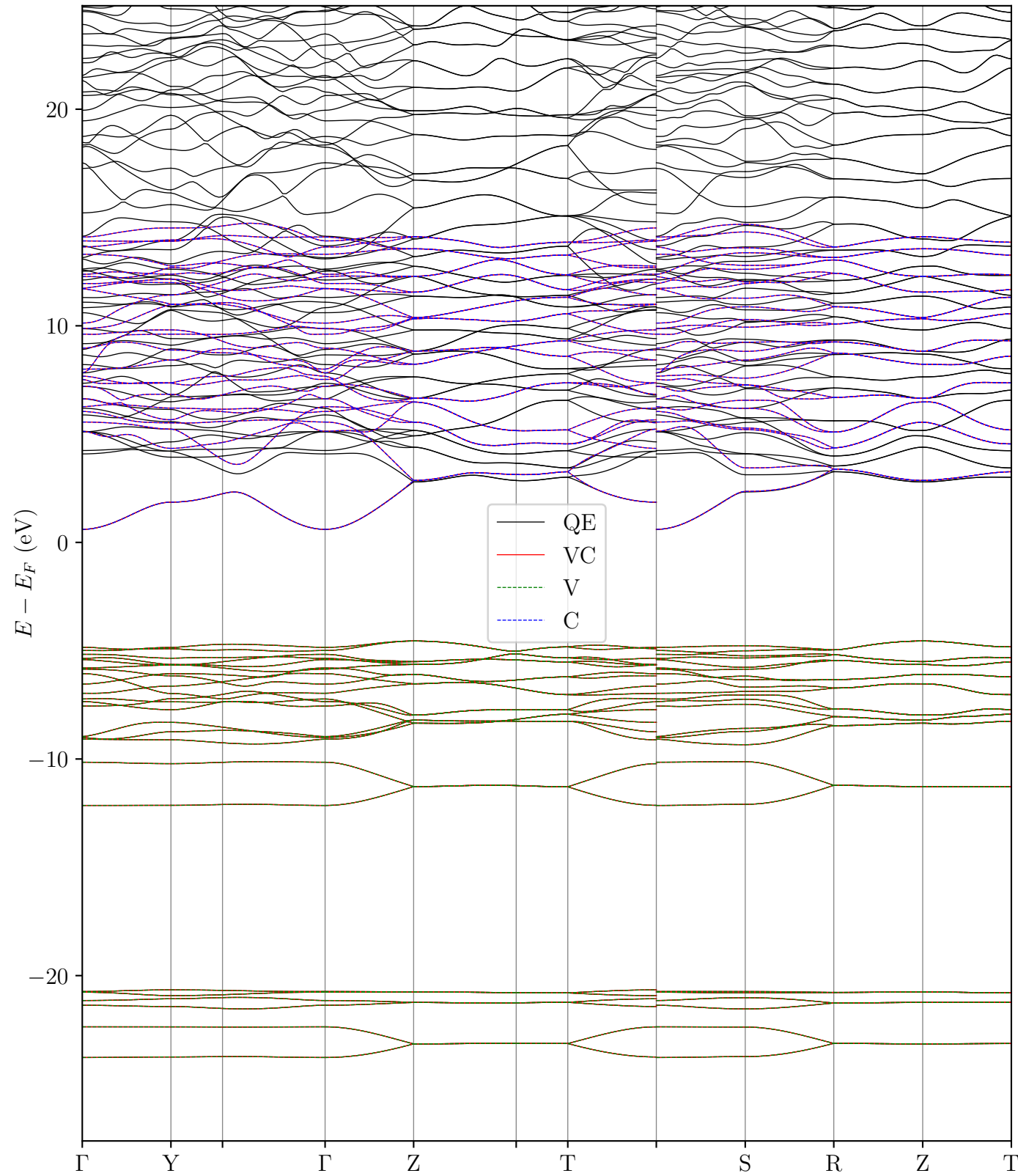
(b) V; final $\Omega = 8.97 \text{ \AA}^2$, $\sum r = (-6.51, -6.51, -6.51) \text{ \AA}$



(c) C; final $\Omega = 27.62 \text{ \AA}^2$, $\sum r = (0.00, -0.00, 0.00) \text{ \AA}$

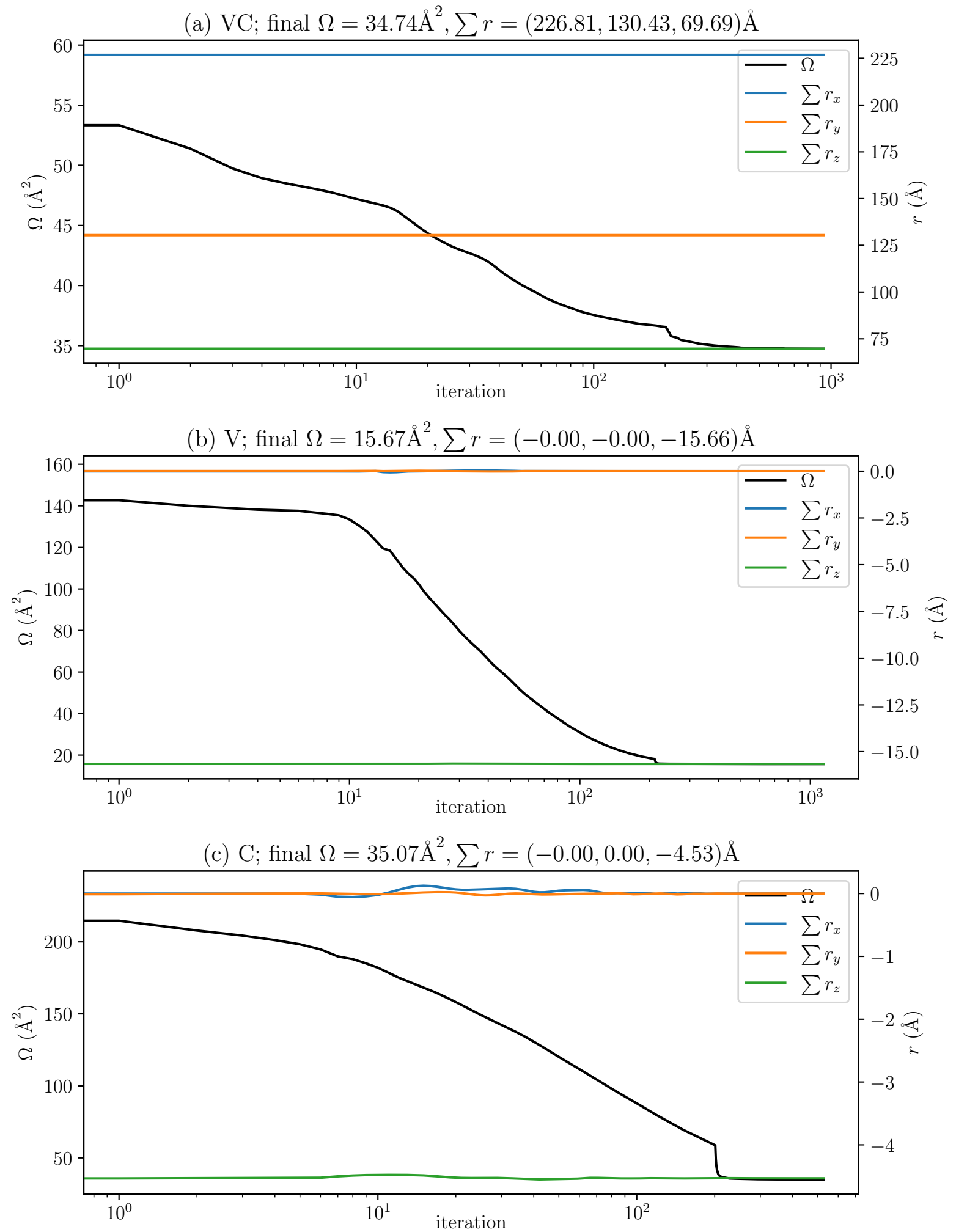


Li₄O₆Si₂ (exclude semicore)
PW AiiDA UUID: 4a3ddaef-df7f-455f-a452-bbee53c5be62
W90 AiiDA UUID: dc5bd4dc-07e5-4330-9b1a-01efb15aeb9e

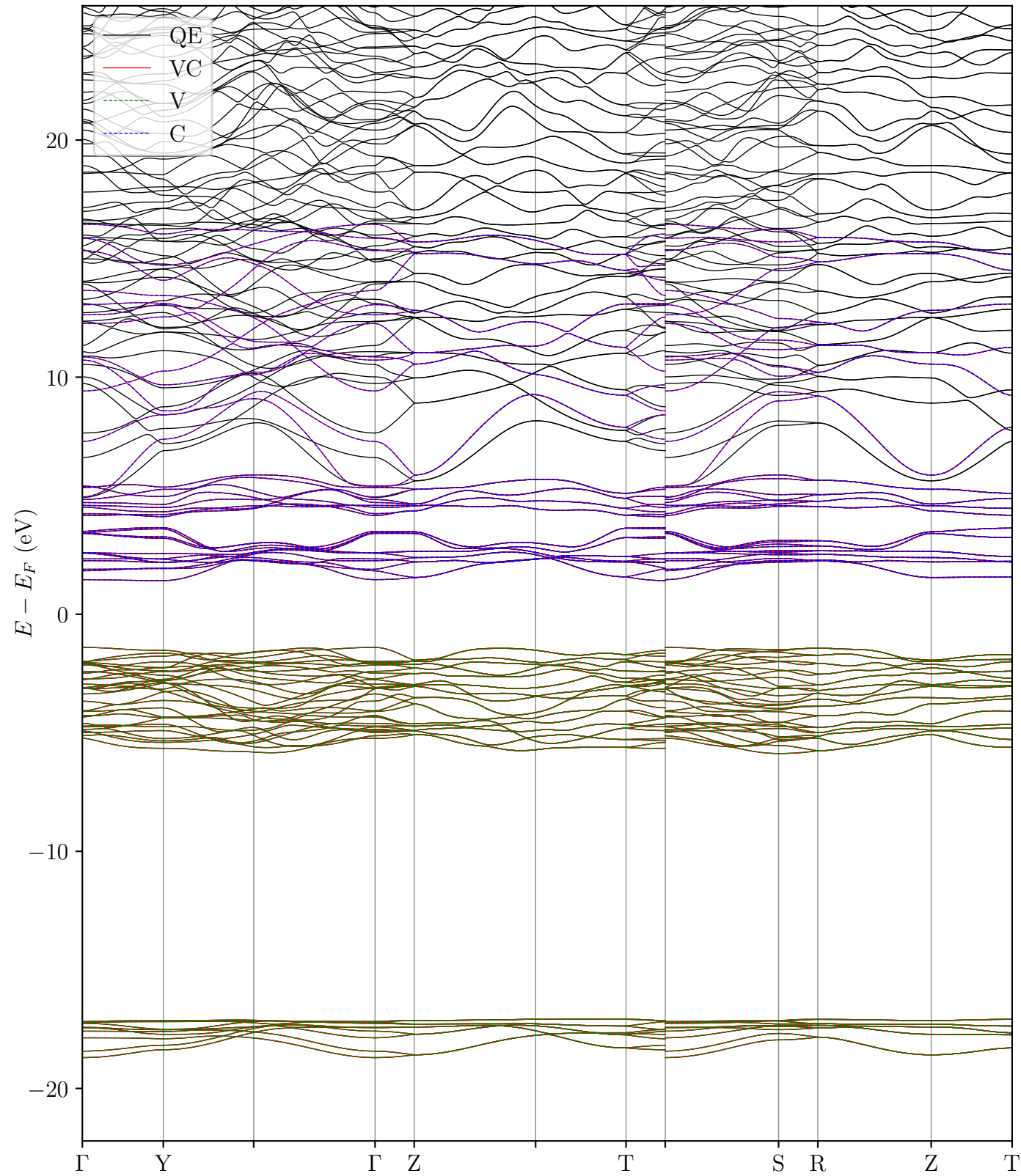


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.9	0.7	0.0	0.7	3.7	3.5	1.3
η_{max}	12.0	6.2	0.0	6.2	12.0	11.0	6.8



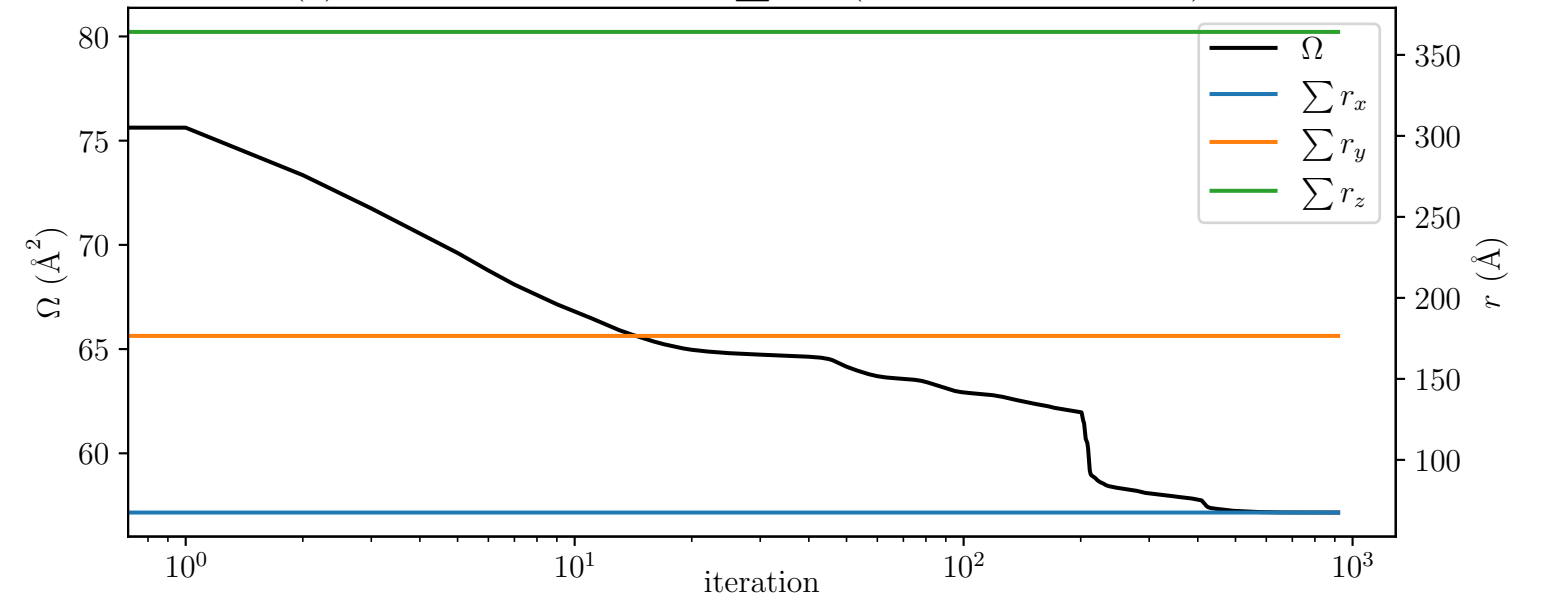
Mg₂O₁₀Ti₄ (exclude semicore)
PW AiiDA UUID: 4c369ec9-4f19-48c7-b0f8-2f23ae39d381
W90 AiiDA UUID: ad1f26f8-ed06-42ad-b03f-a2bc94ba4800



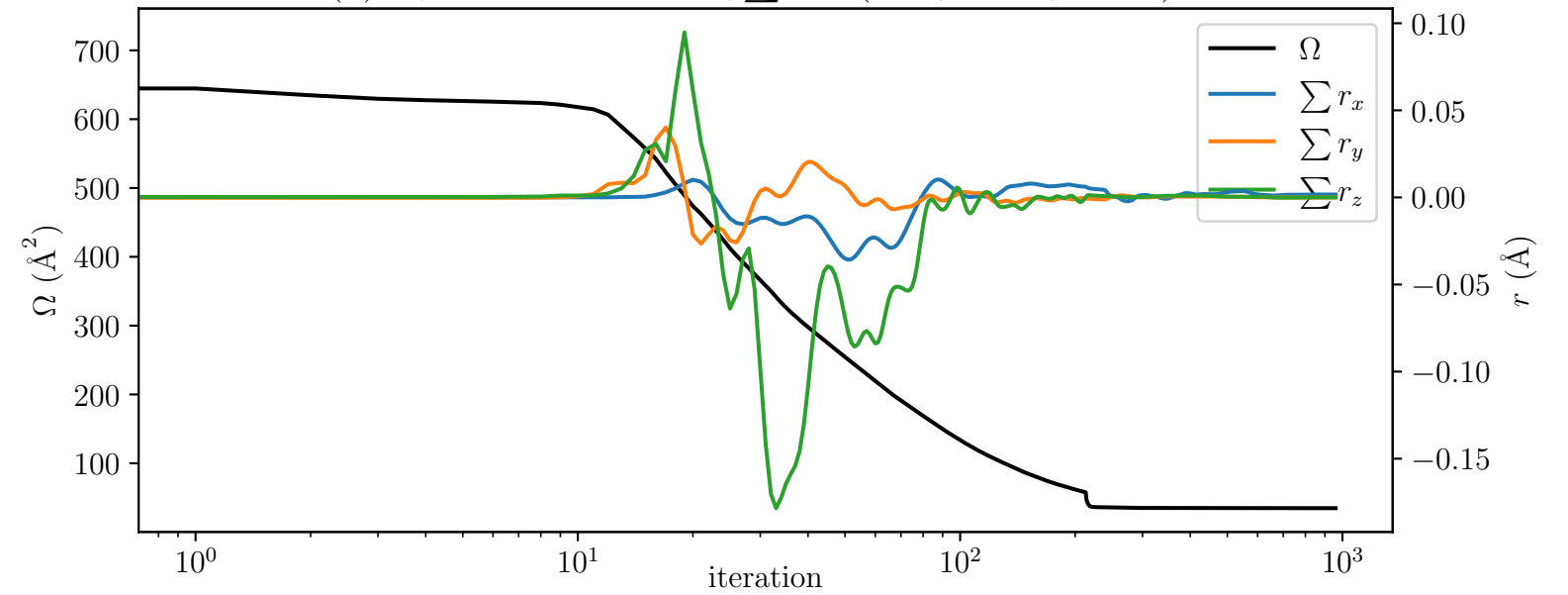
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.1	0.1	0.0	0.1	0.1	0.1	0.3
η_{max}	1.9	1.9	0.3	1.9	0.1	0.1	3.5

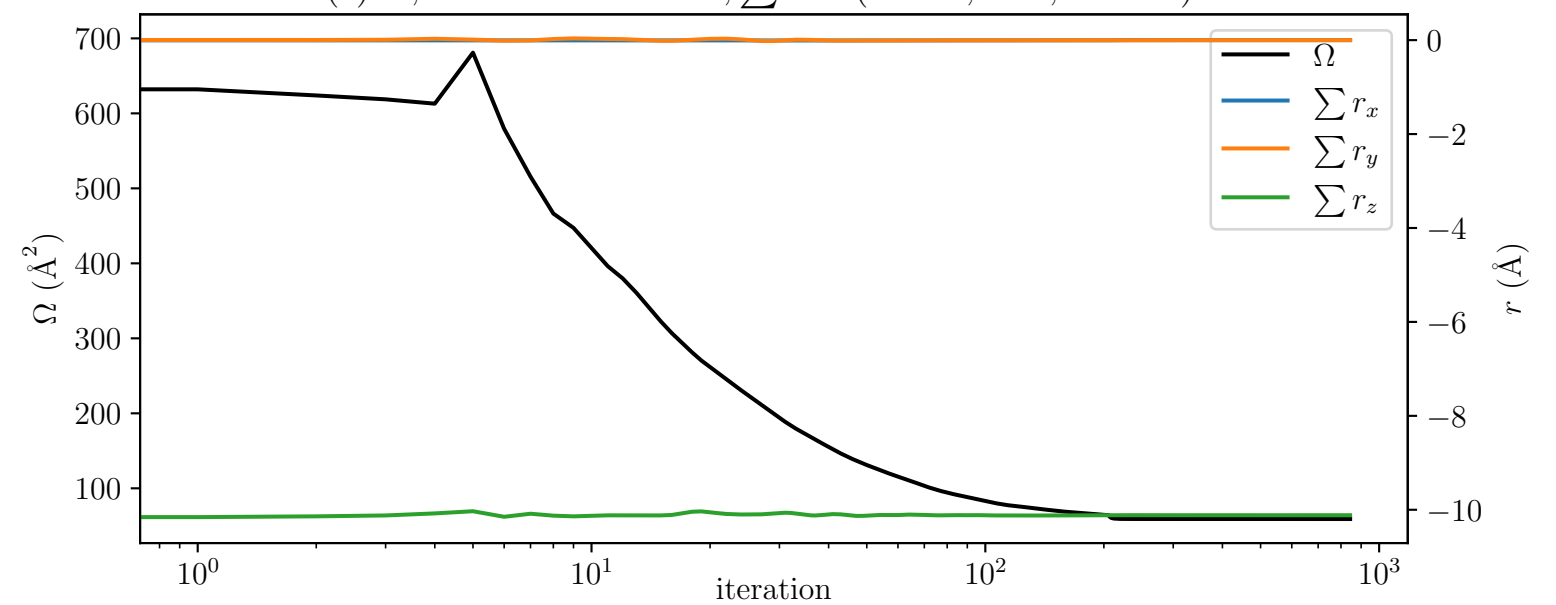
(a) VC; final $\Omega = 57.16 \text{\AA}^2$, $\sum r = (67.49, 176.53, 364.19) \text{\AA}$



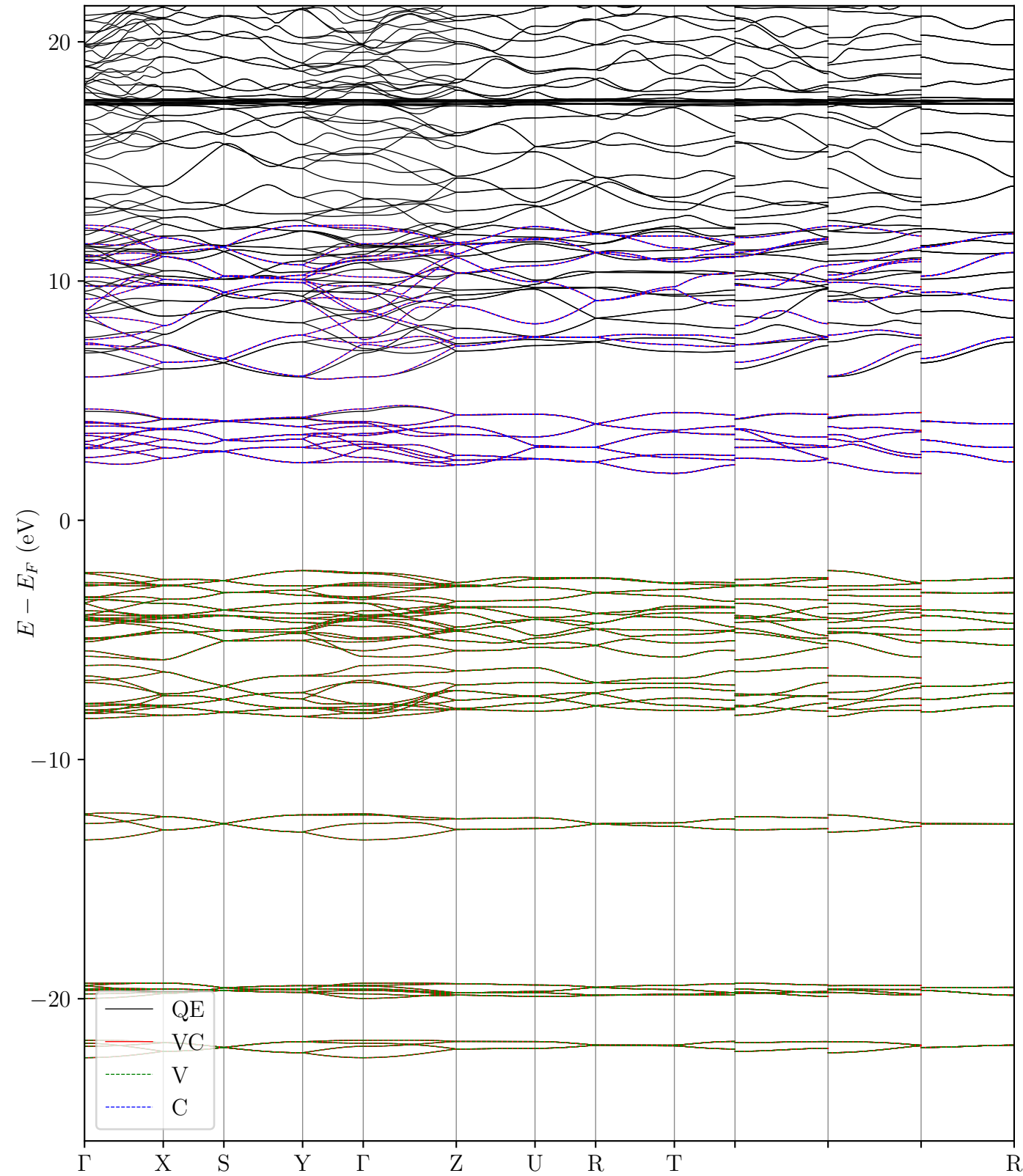
(b) V; final $\Omega = 34.79 \text{\AA}^2$, $\sum r = (0.00, -0.00, -0.00) \text{\AA}$



(c) C; final $\Omega = 59.04 \text{\AA}^2$, $\sum r = (-0.00, 0.00, -10.12) \text{\AA}$

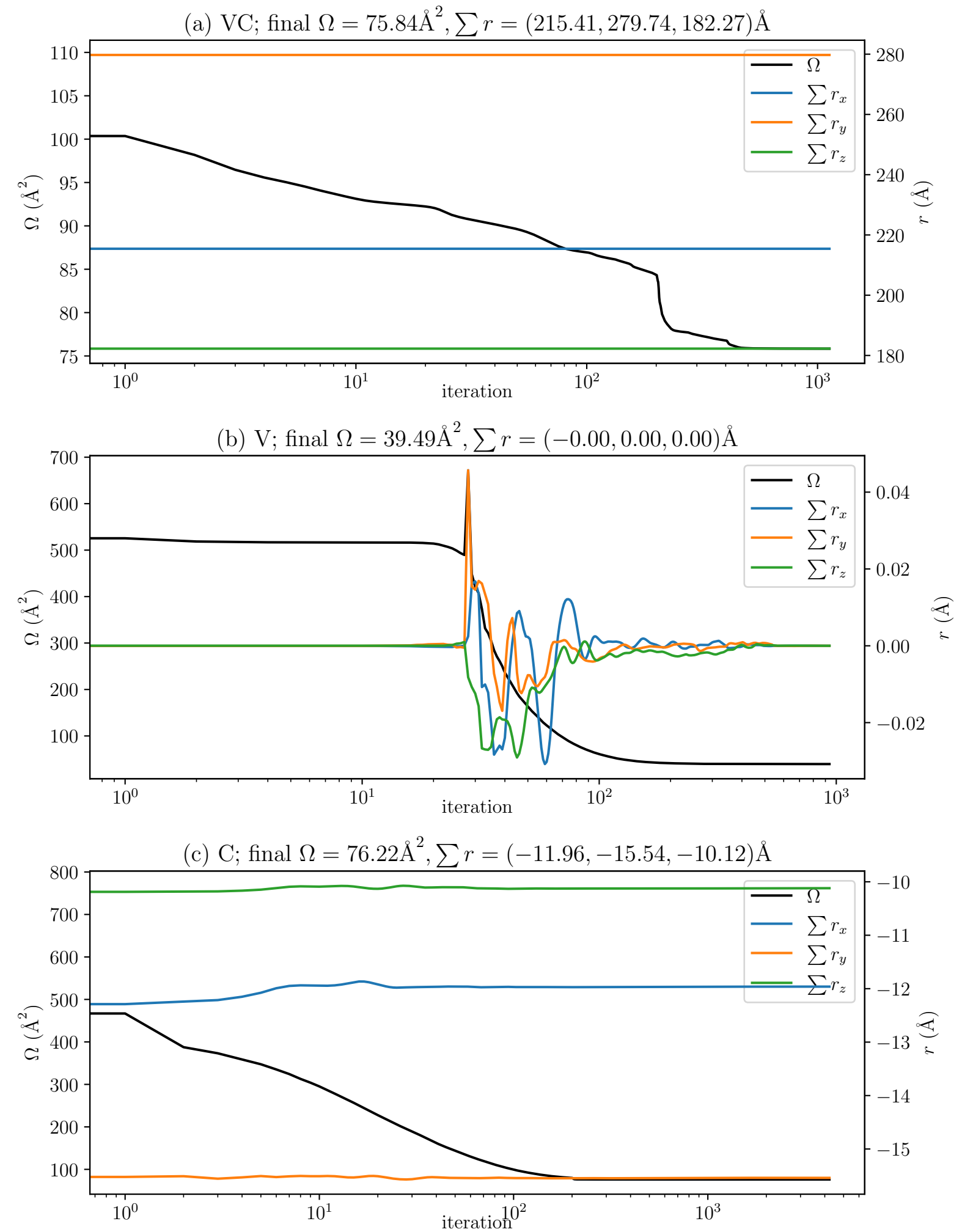


Mg₄O₁₂Se₄ (exclude semicore)
PW AiiDA UUID: cf4e1389-52b4-4e47-8219-53977d66d595
W90 AiiDA UUID: 642be8ed-b5eb-4299-aeef-74ead356407a

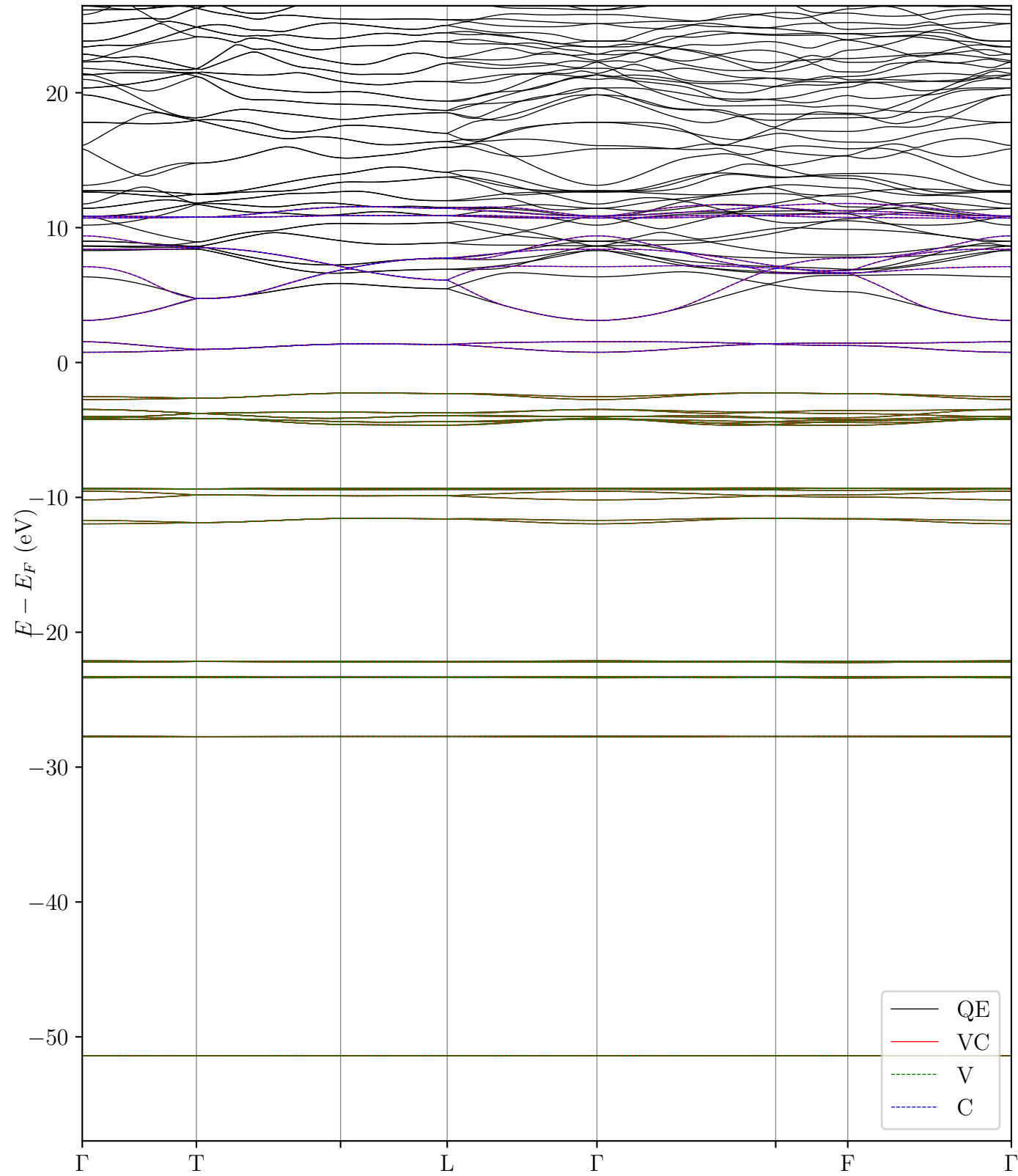


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.1	0.1	0.0	0.1	0.7	0.9	0.5
η_{max}	1.1	1.1	0.0	1.1	0.8	0.9	3.5

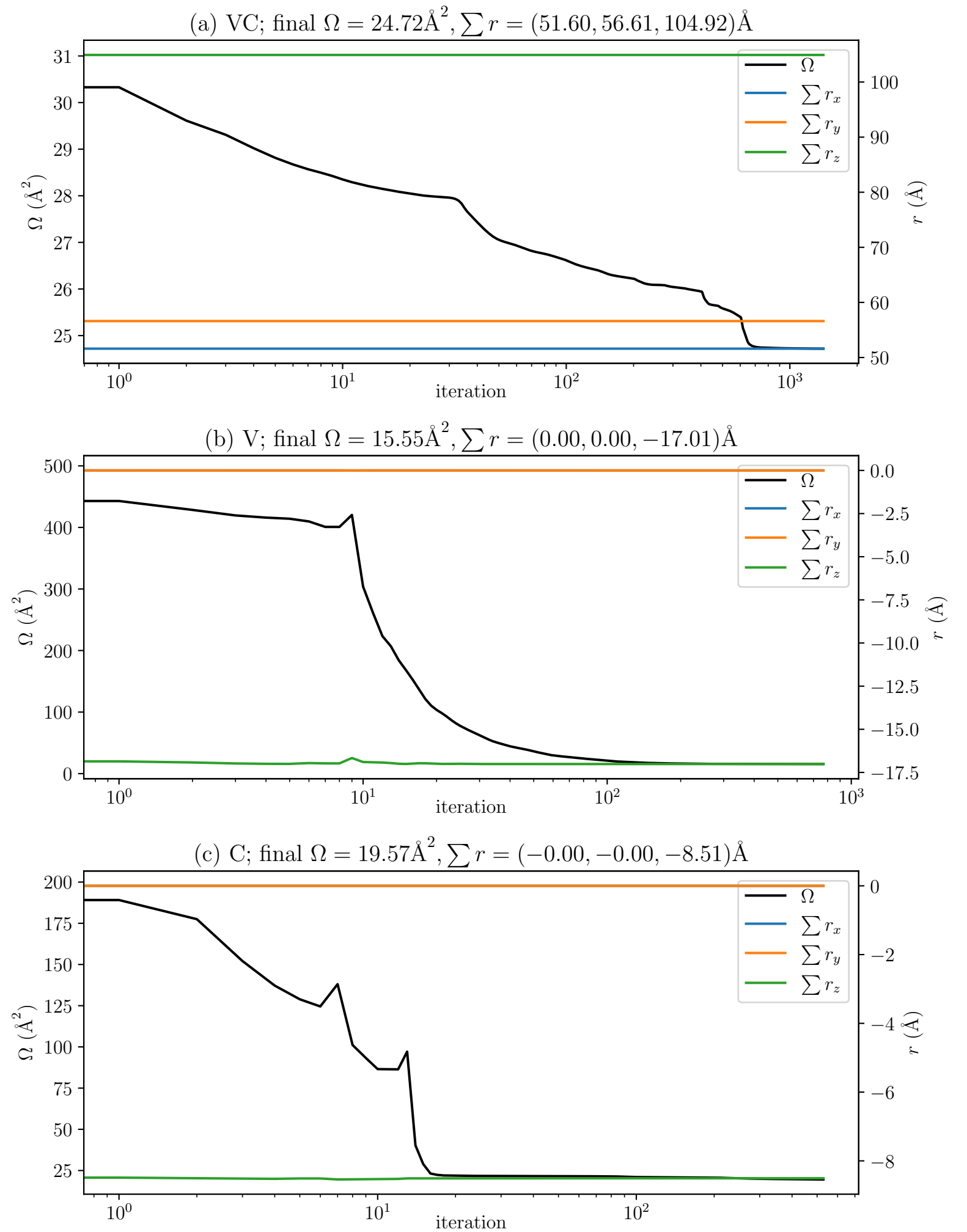


N₂Na₂O₆ (**include** semicore)
PW AiiDA UUID: 43cad09a-030f-41cf-a7c8-a871f7941b9d
W90 AiiDA UUID: 36fea661-dd3b-459a-8d6c-adeb861dbaa9

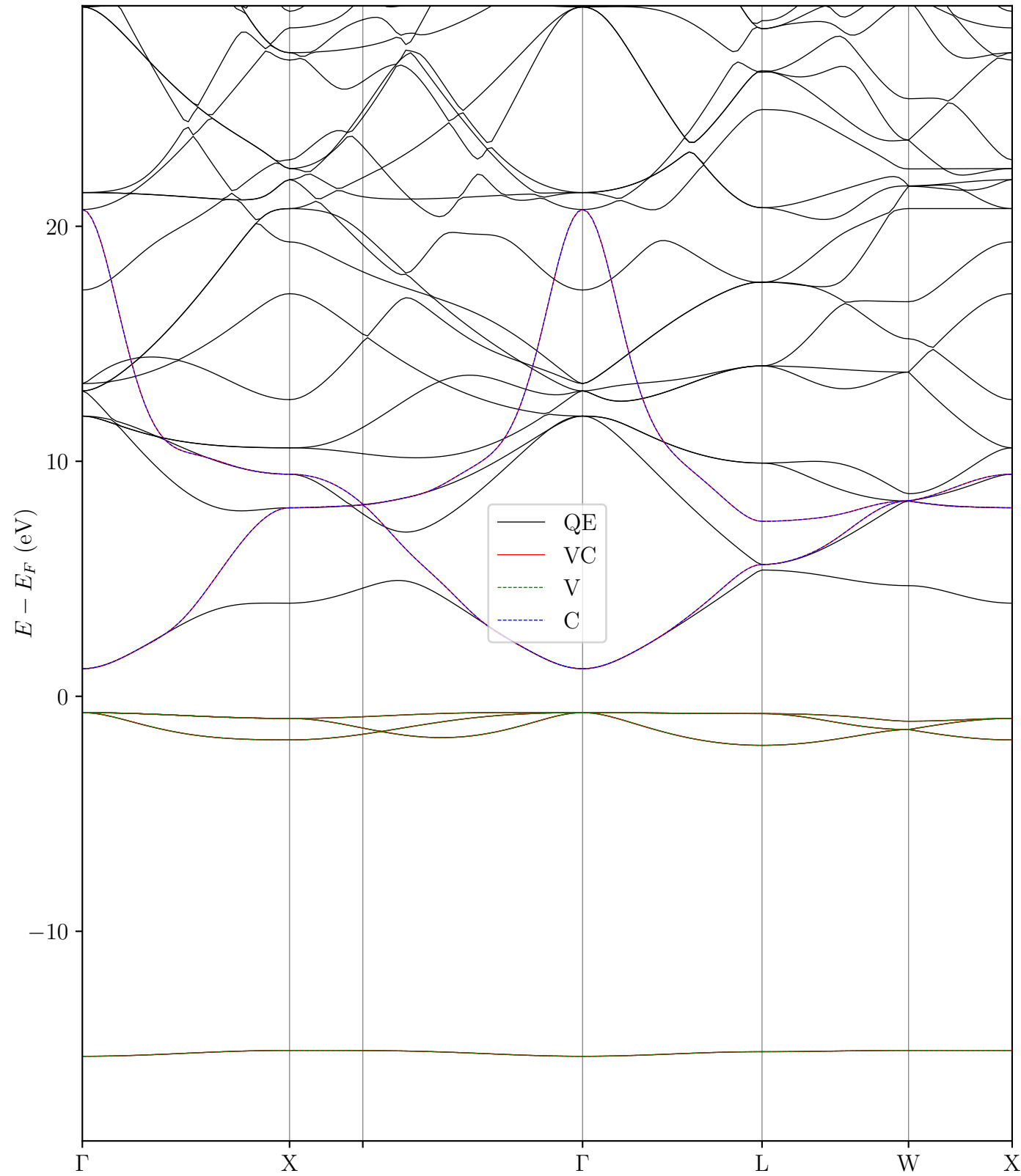


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.2	0.2	0.0	0.2	0.3	0.2	1.1
η_{max}	1.4	1.3	0.2	1.3	1.4	0.7	7.7

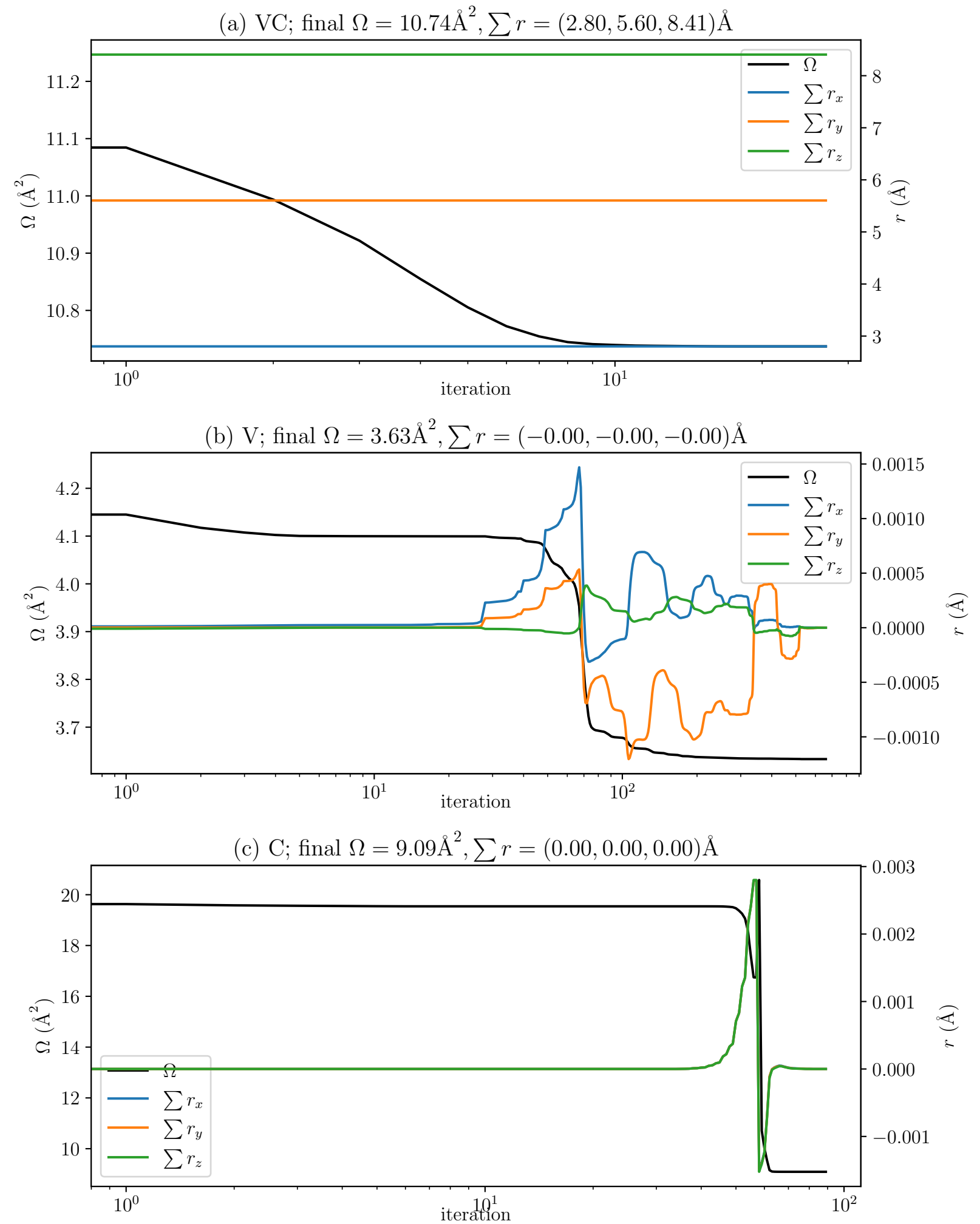


Na₂O (exclude semicore)
PW AiiDA UUID: 6ef089fa-e43b-4f04-a94a-a769473447c1
W90 AiiDA UUID: 71f01603-390a-47e5-89a7-2800d5b783f3

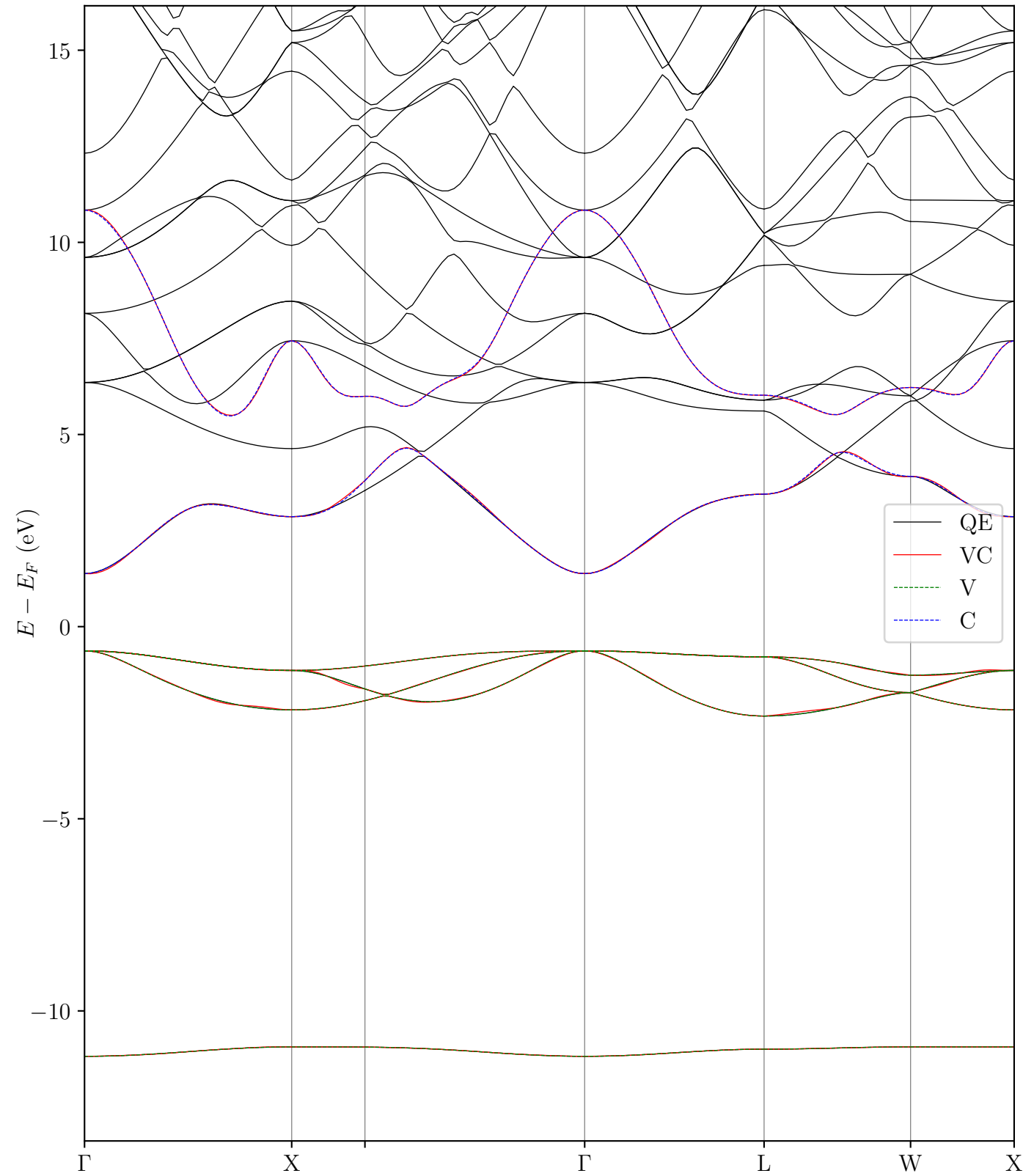


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.6	0.3	0.3	0.3	2.7	2.8	0.6
η_{max}	4.7	1.4	1.9	1.3	4.7	4.3	2.0



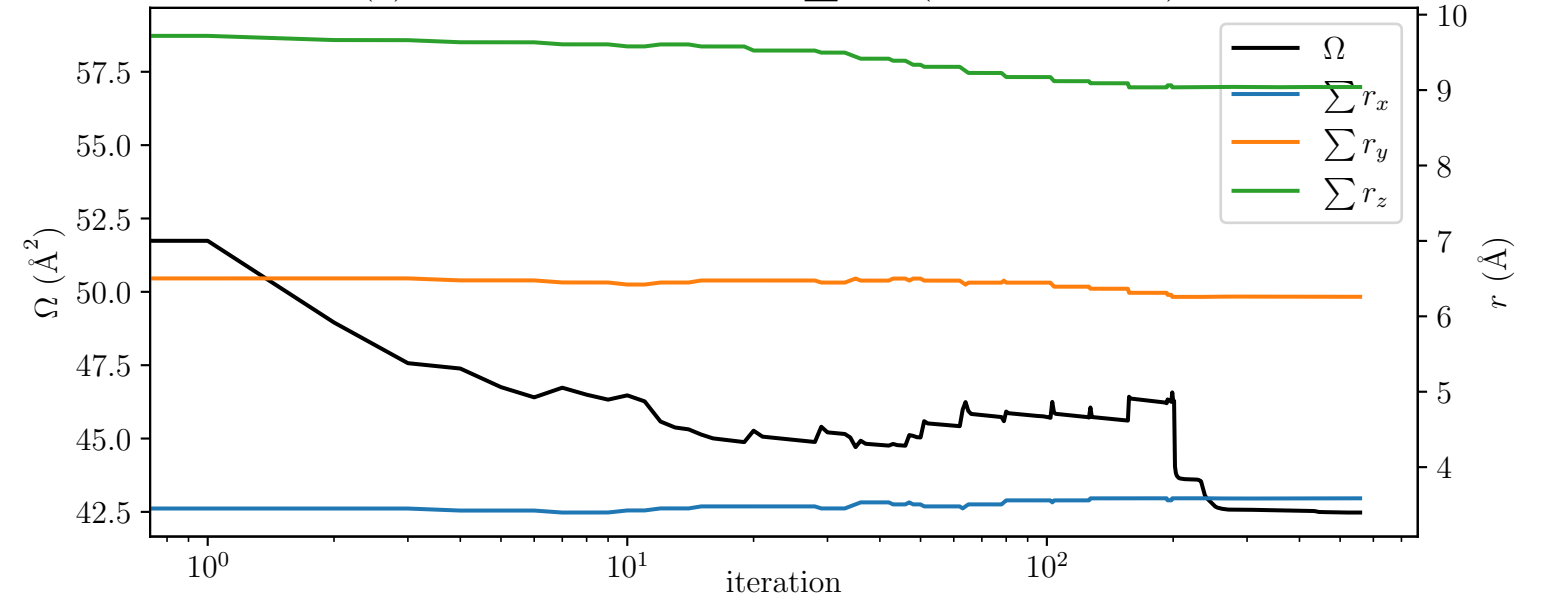
Na₂Se (exclude semicore)
PW AiiDA UUID: 70d62af4-5dbf-4d7d-a607-8d7658ebf866
W90 AiiDA UUID: 5df55b78-7e08-4588-873a-f1850b674019



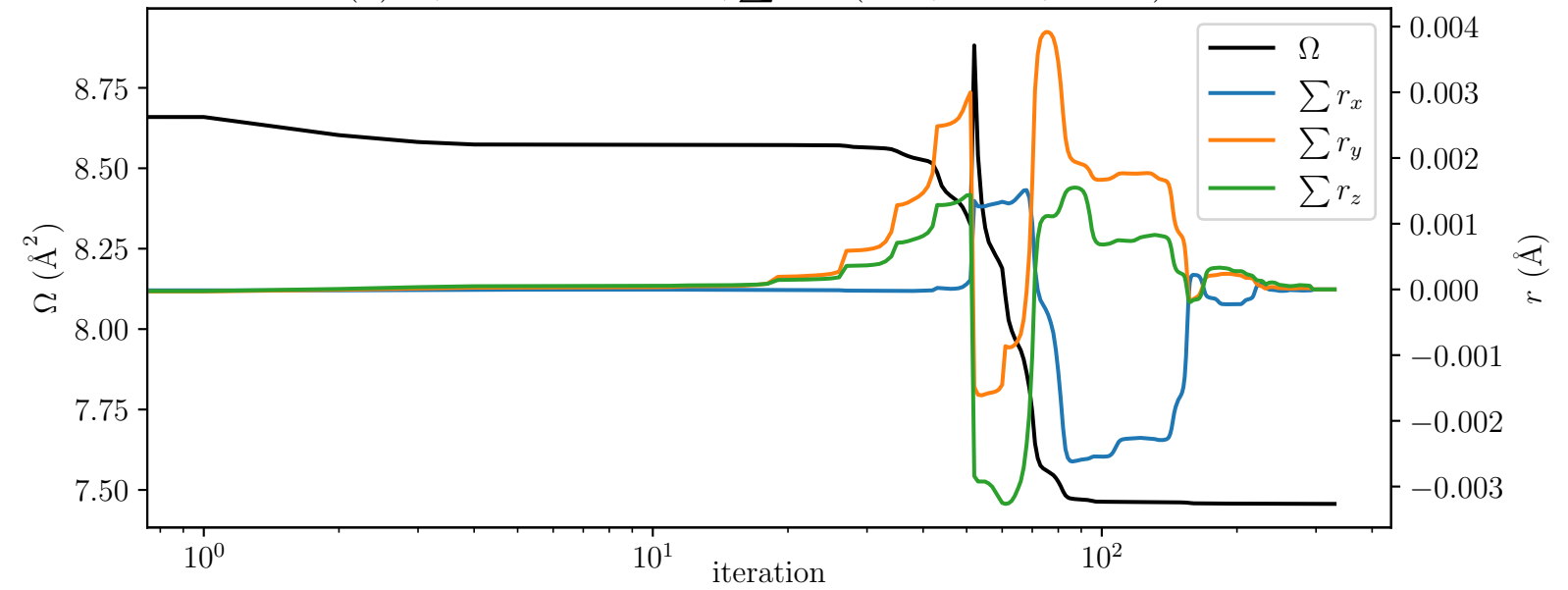
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	9.8	9.4	0.8	9.6	17.3	3.0	14.6
η_{max}	52.5	52.5	5.1	52.3	40.6	6.4	50.3

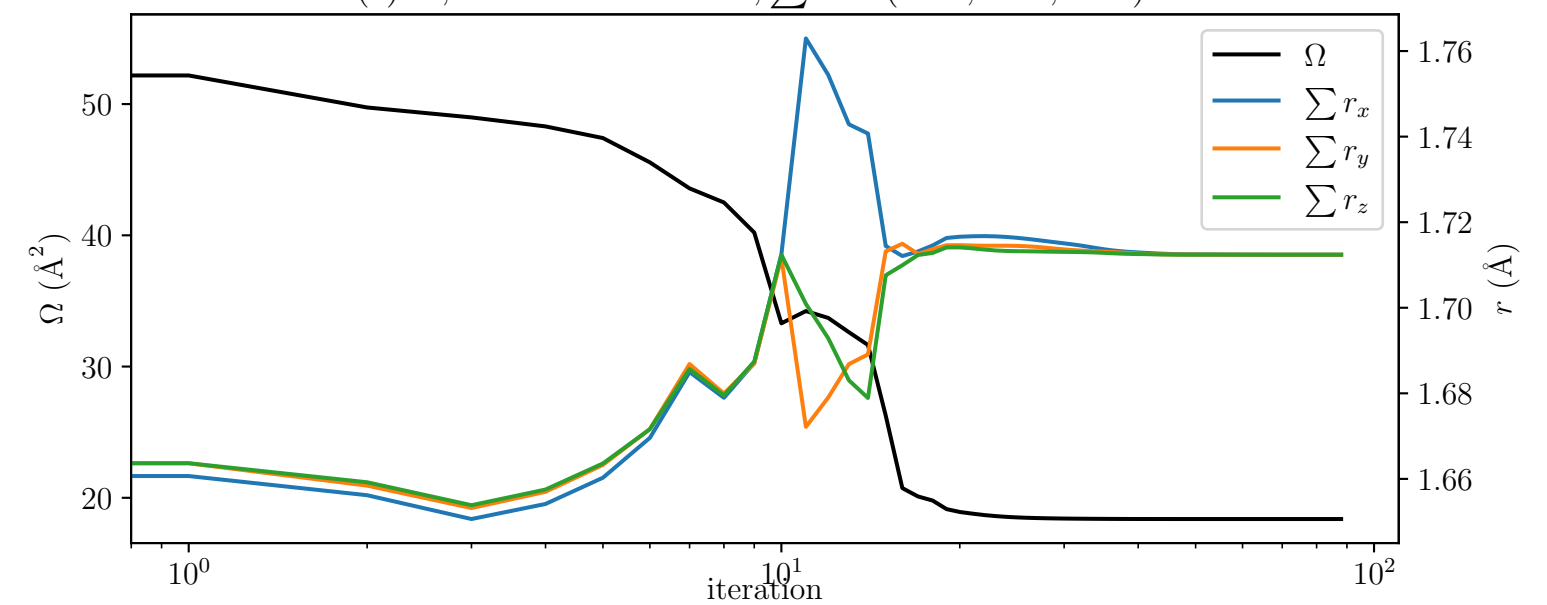
(a) VC; final $\Omega = 42.48 \text{ \AA}^2$, $\sum r = (3.59, 6.26, 9.04) \text{ \AA}$



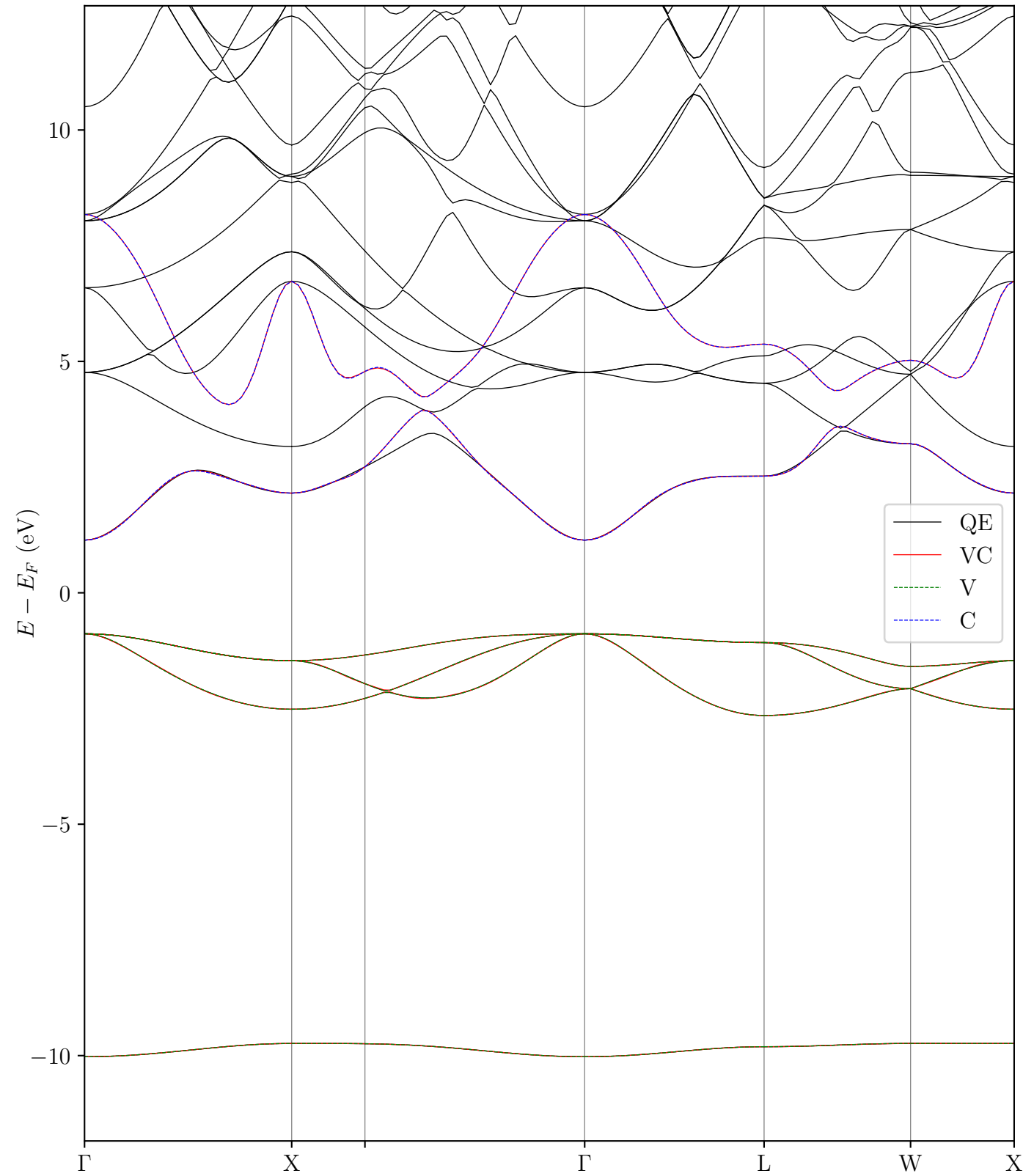
(b) V; final $\Omega = 7.46 \text{ \AA}^2$, $\sum r = (0.00, -0.00, -0.00) \text{ \AA}$



(c) C; final $\Omega = 18.38 \text{ \AA}^2$, $\sum r = (1.71, 1.71, 1.71) \text{ \AA}$

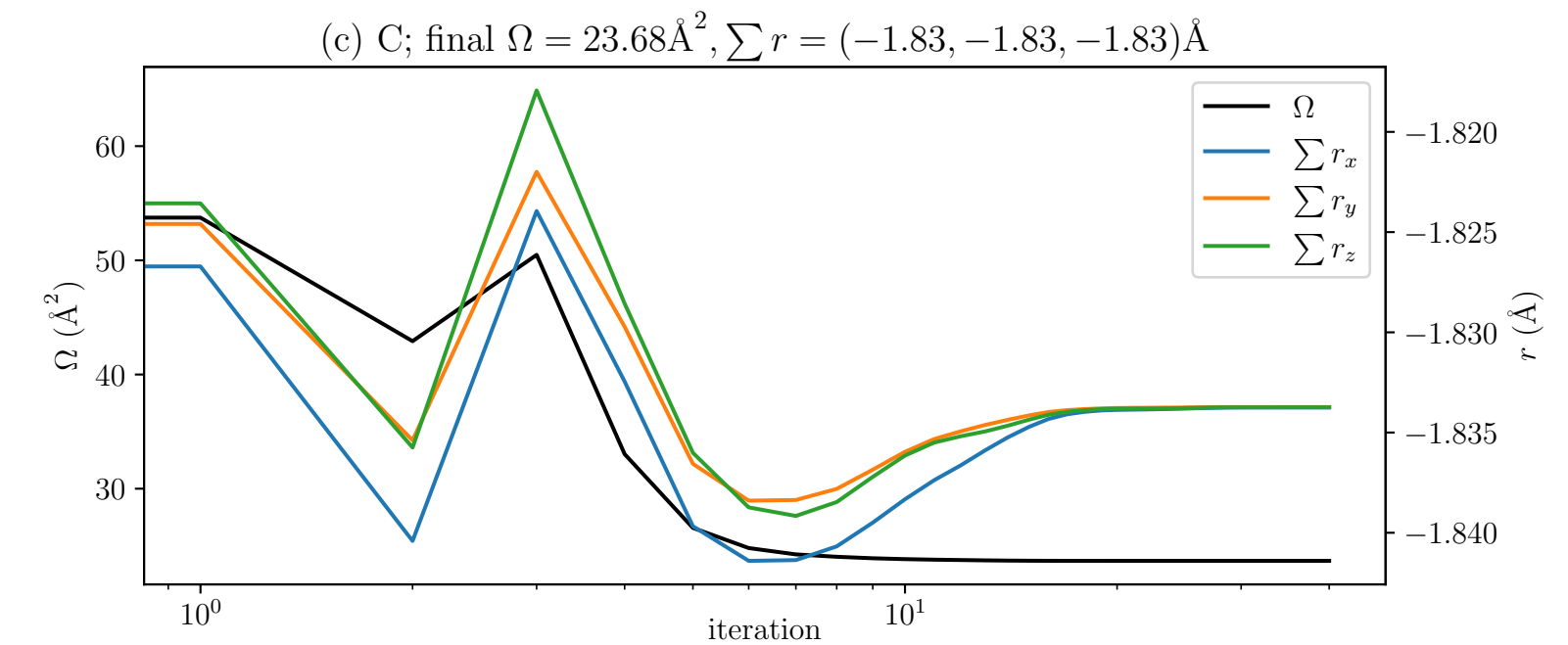
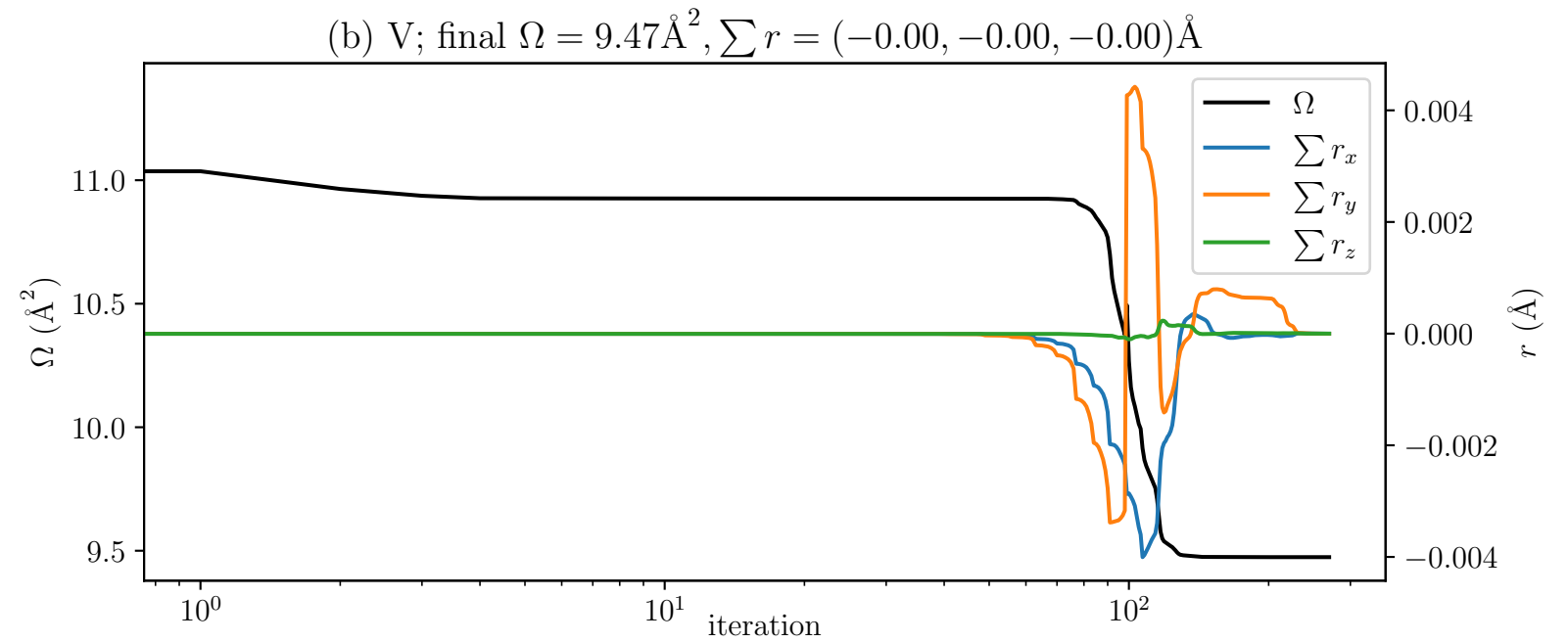
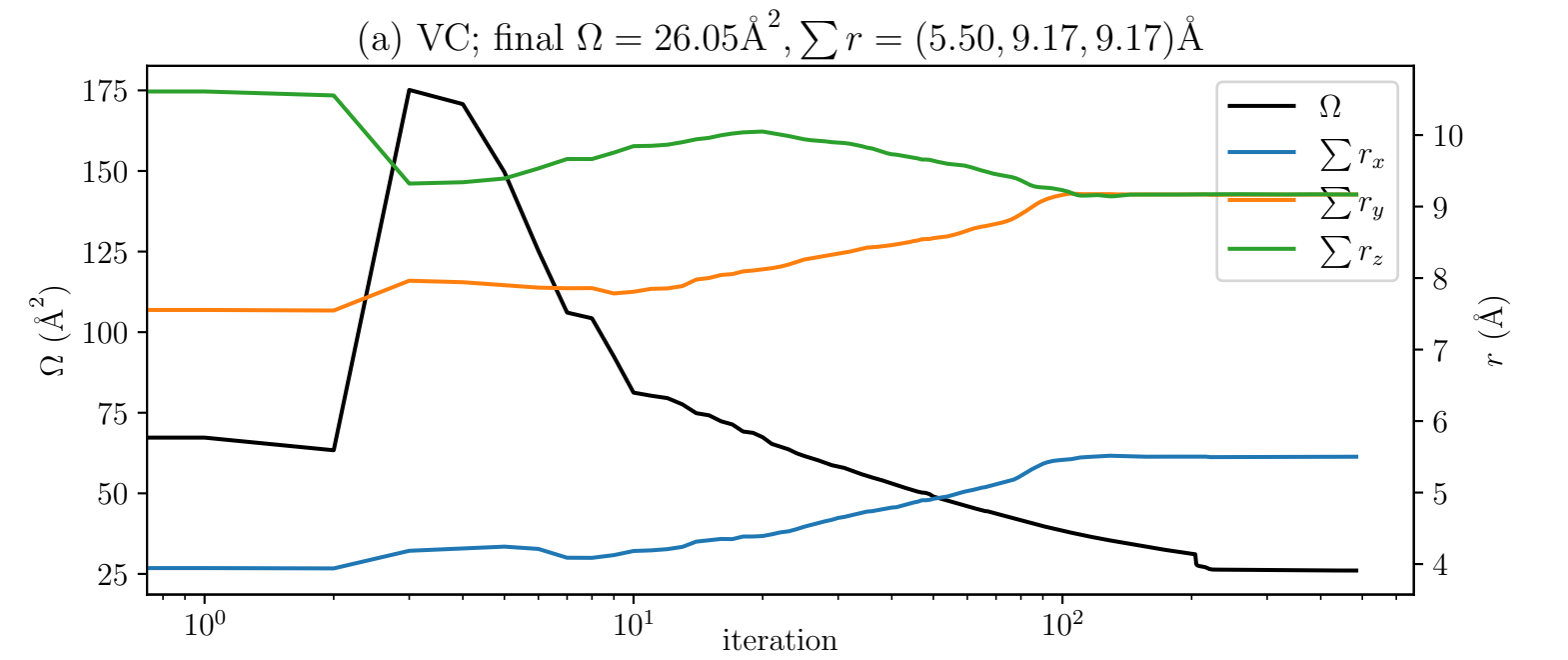


Na₂Te (exclude semicore)
PW AiiDA UUID: 5129d58a-6569-433c-b74e-4ffff50c6d26
W90 AiiDA UUID: 6c2b6057-27c1-489e-9af4-8dac7dc38ad0

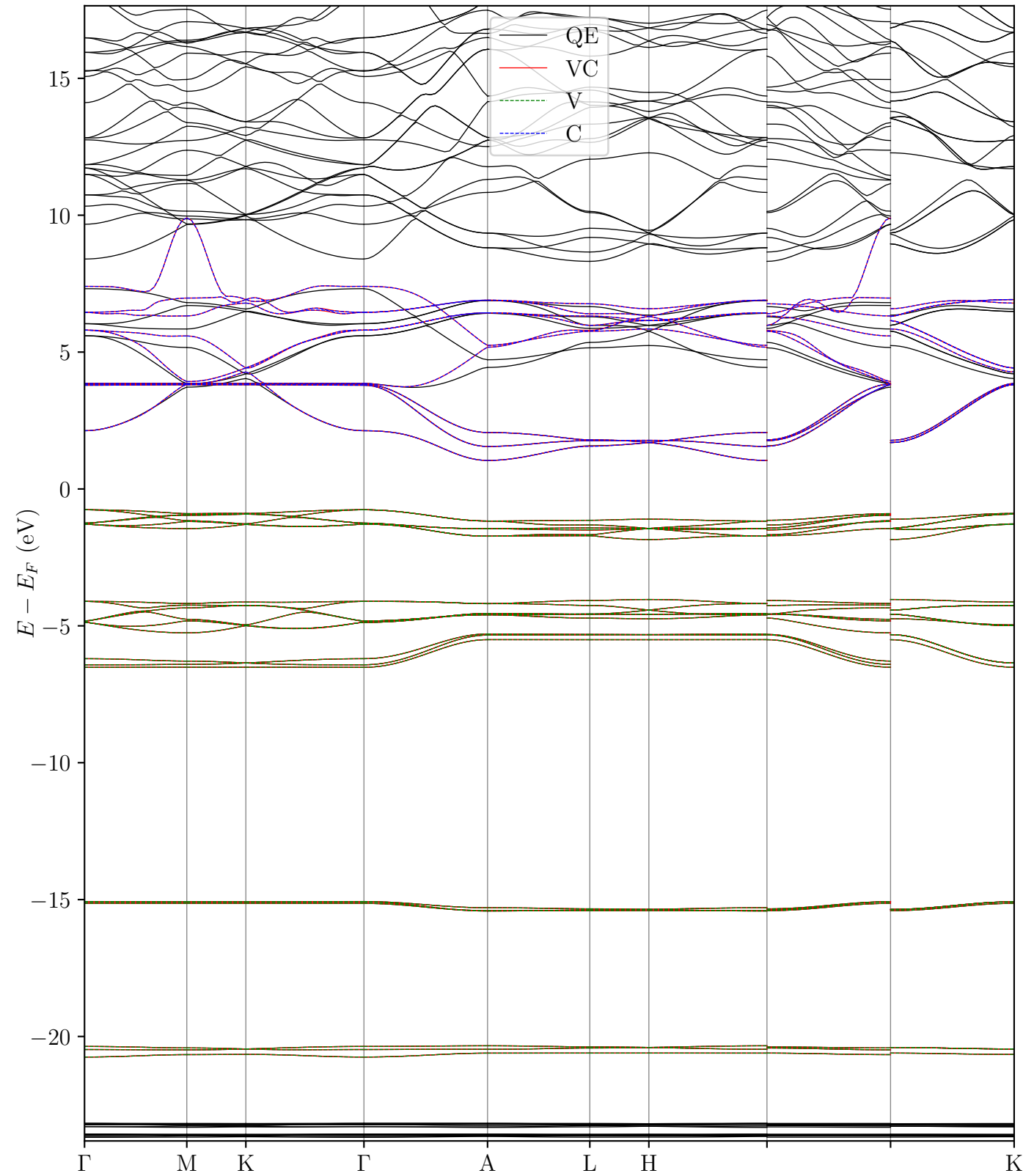


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	3.3	3.1	0.8	3.5	5.1	11.2	5.2
η_{max}	14.9	14.9	4.9	15.4	8.5	19.2	17.1

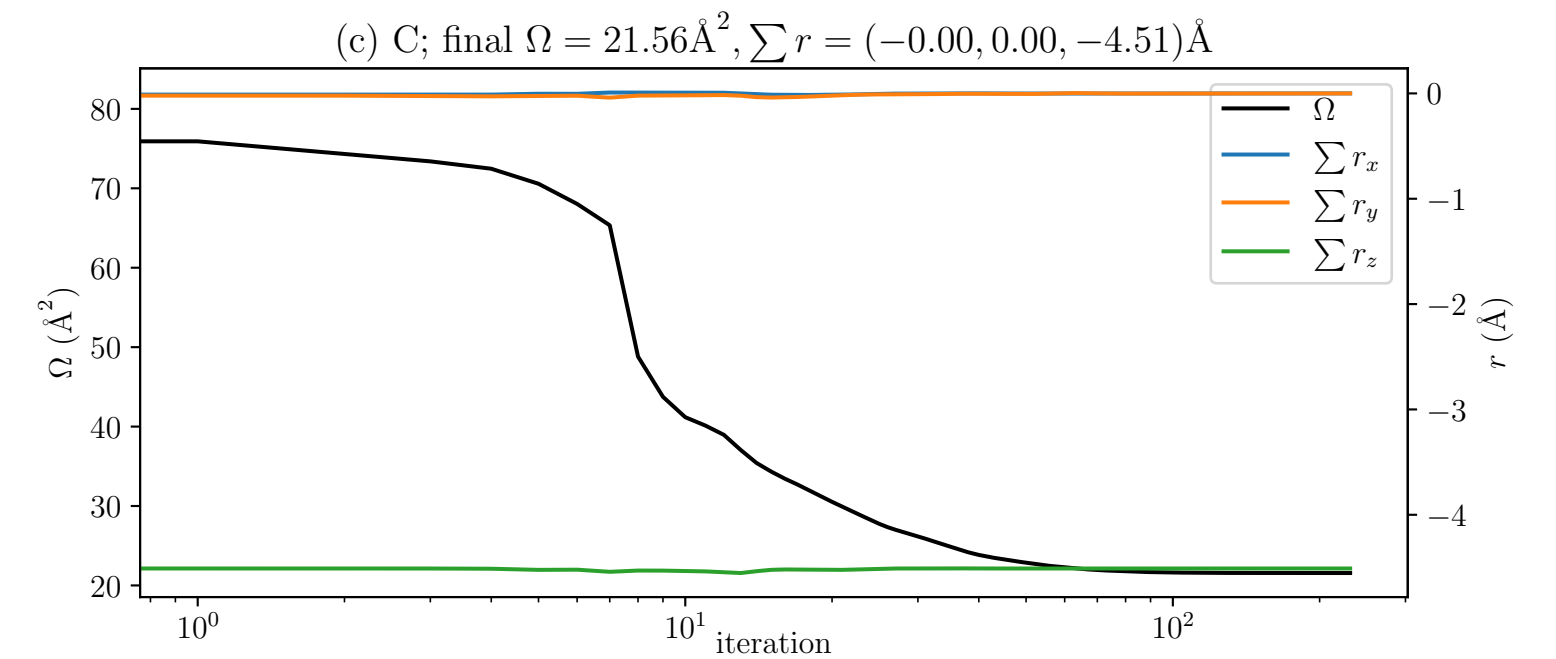
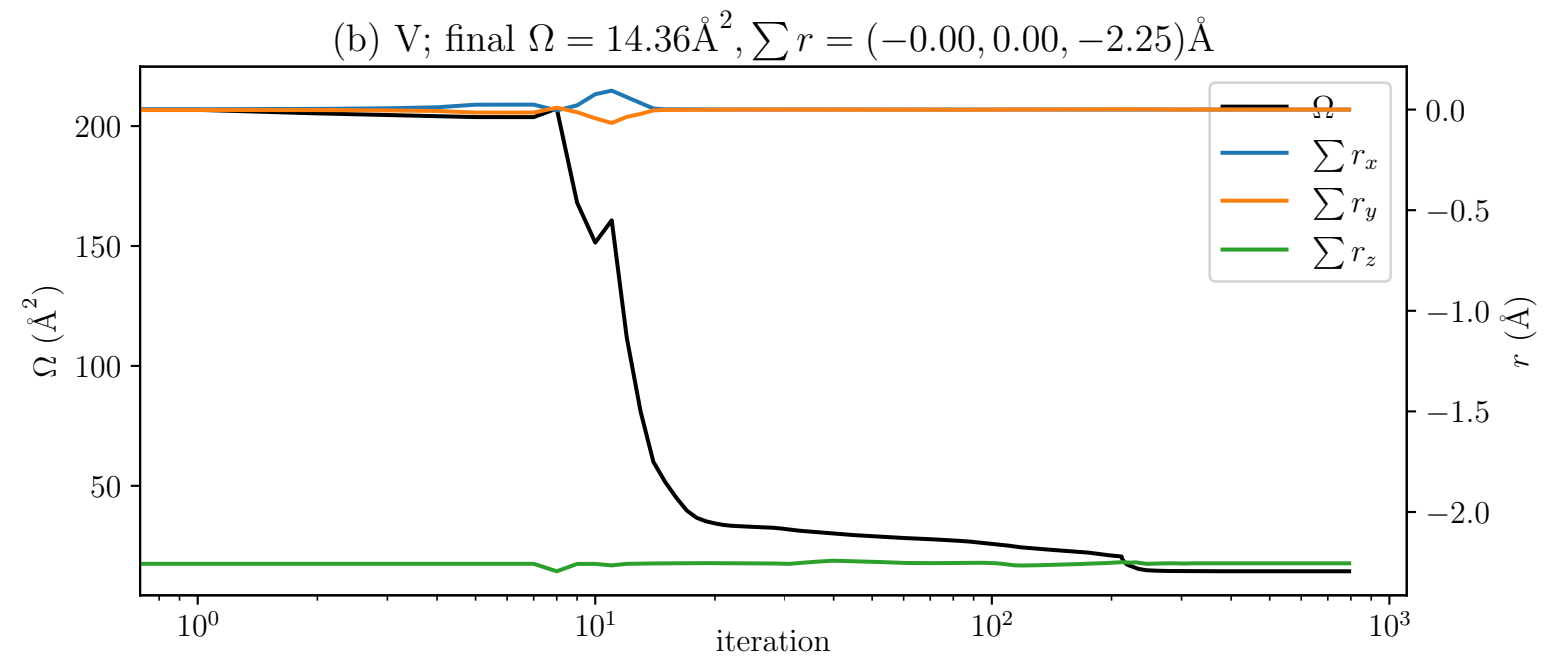
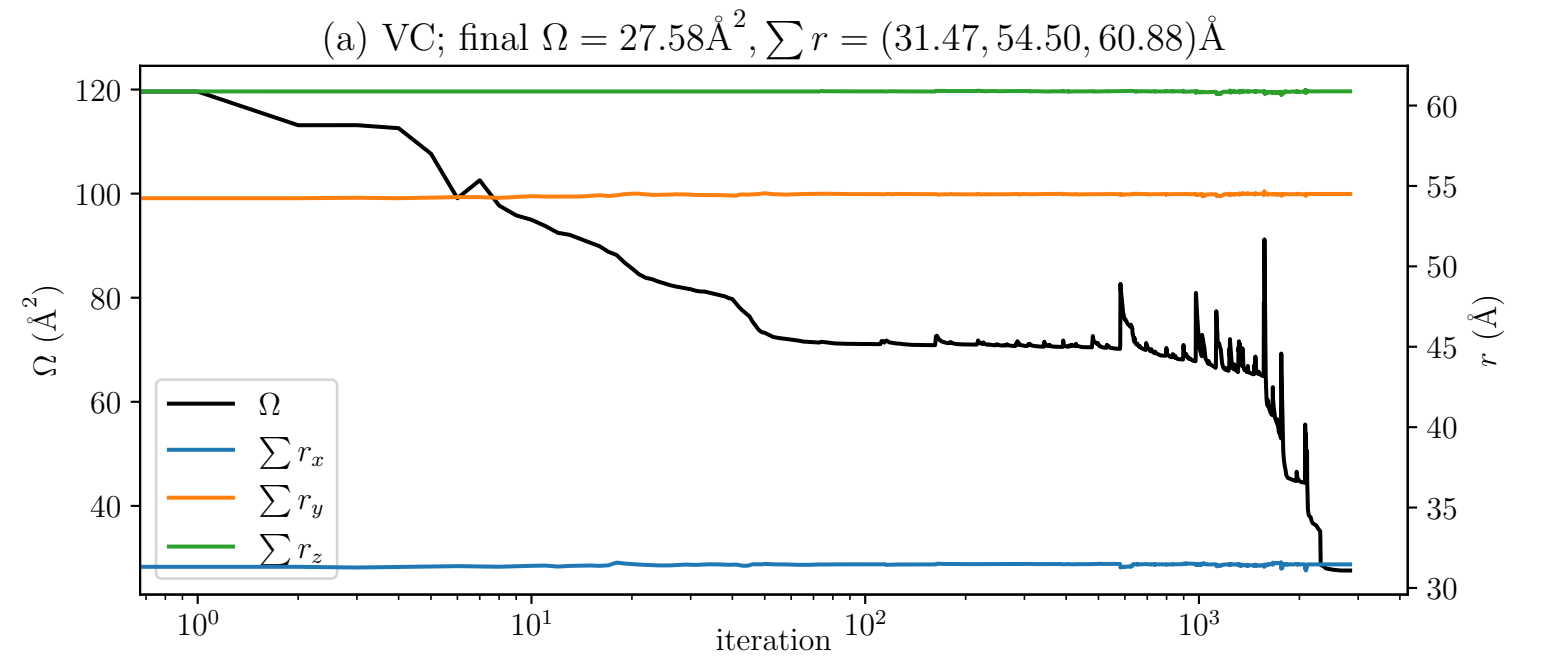


Na₆O₆ (exclude semicore)
PW AiiDA UUID: 1f157867-e615-4e16-82a0-f466b0f2f9f4
W90 AiiDA UUID: 325115e0-4948-468f-b369-721264ec72bf

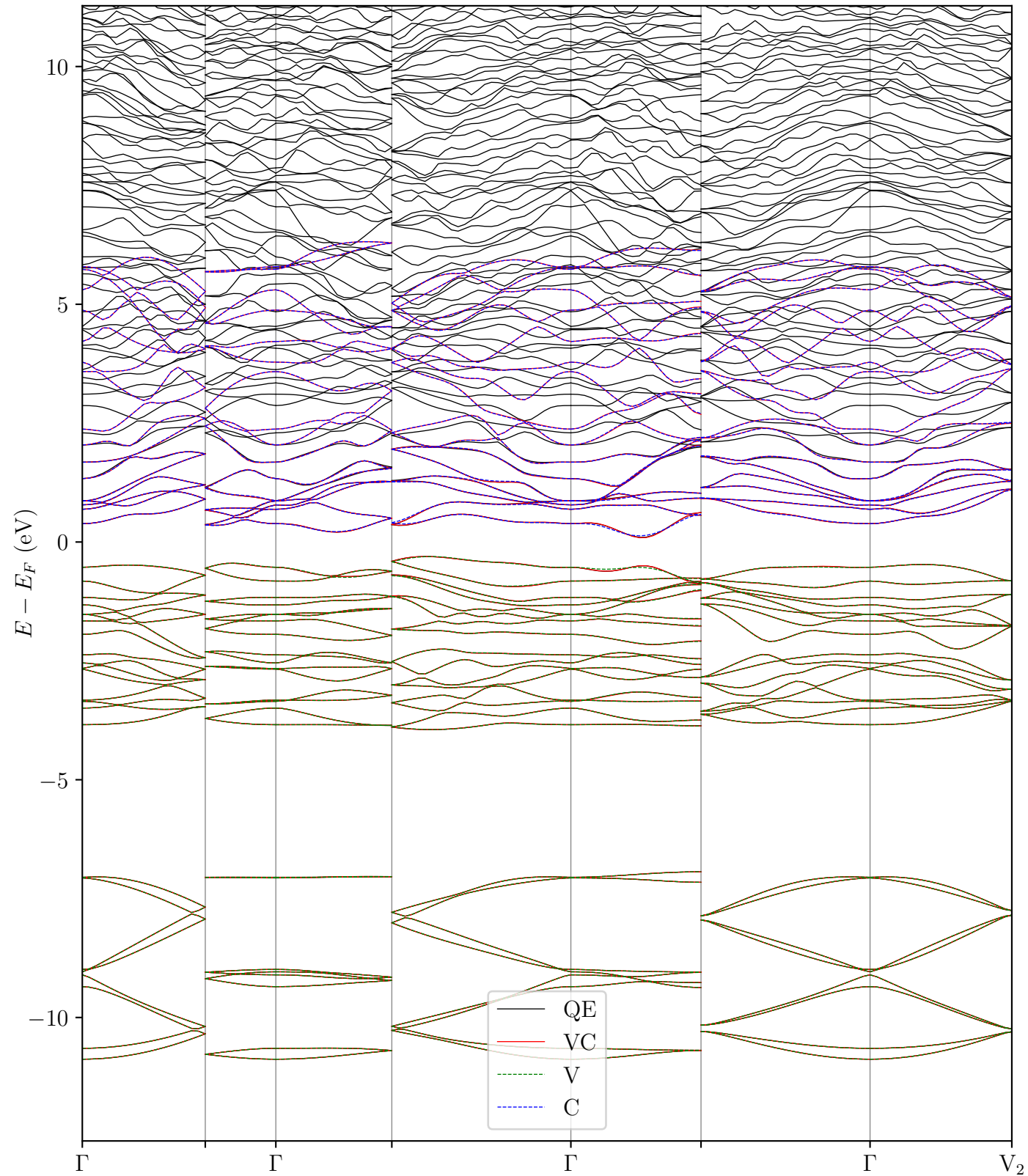


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.3	1.1	0.1	1.1	3.2	4.8	2.8
η_{max}	13.4	13.4	0.4	13.4	11.5	20.0	31.4

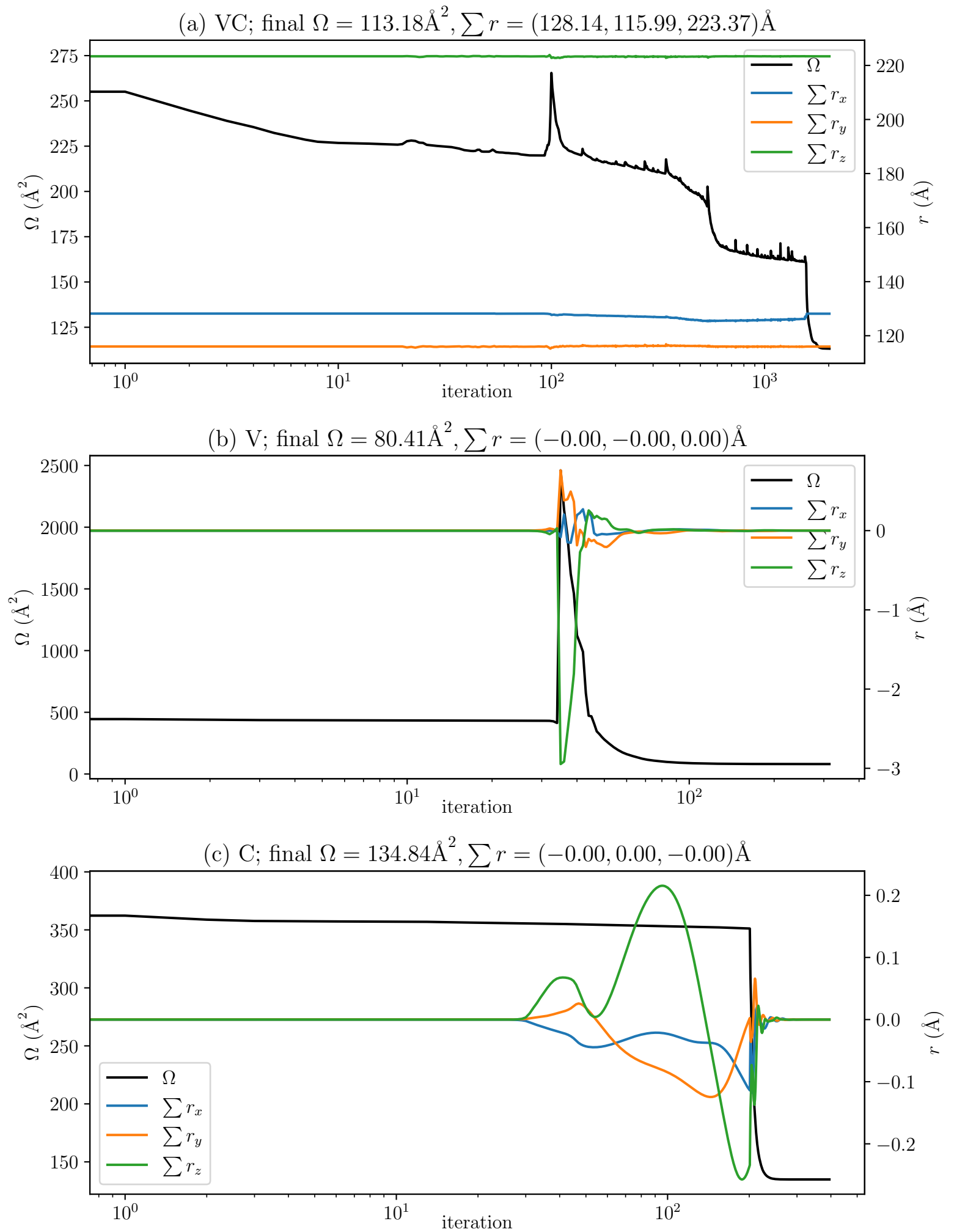


Na₈Sb₈ (exclude semicore)
PW AiiDA UUID: b9729c68-5954-4d9a-aeef-63853216c556
W90 AiiDA UUID: 18b5009c-4373-4ea5-96df-5604fd1a70d2

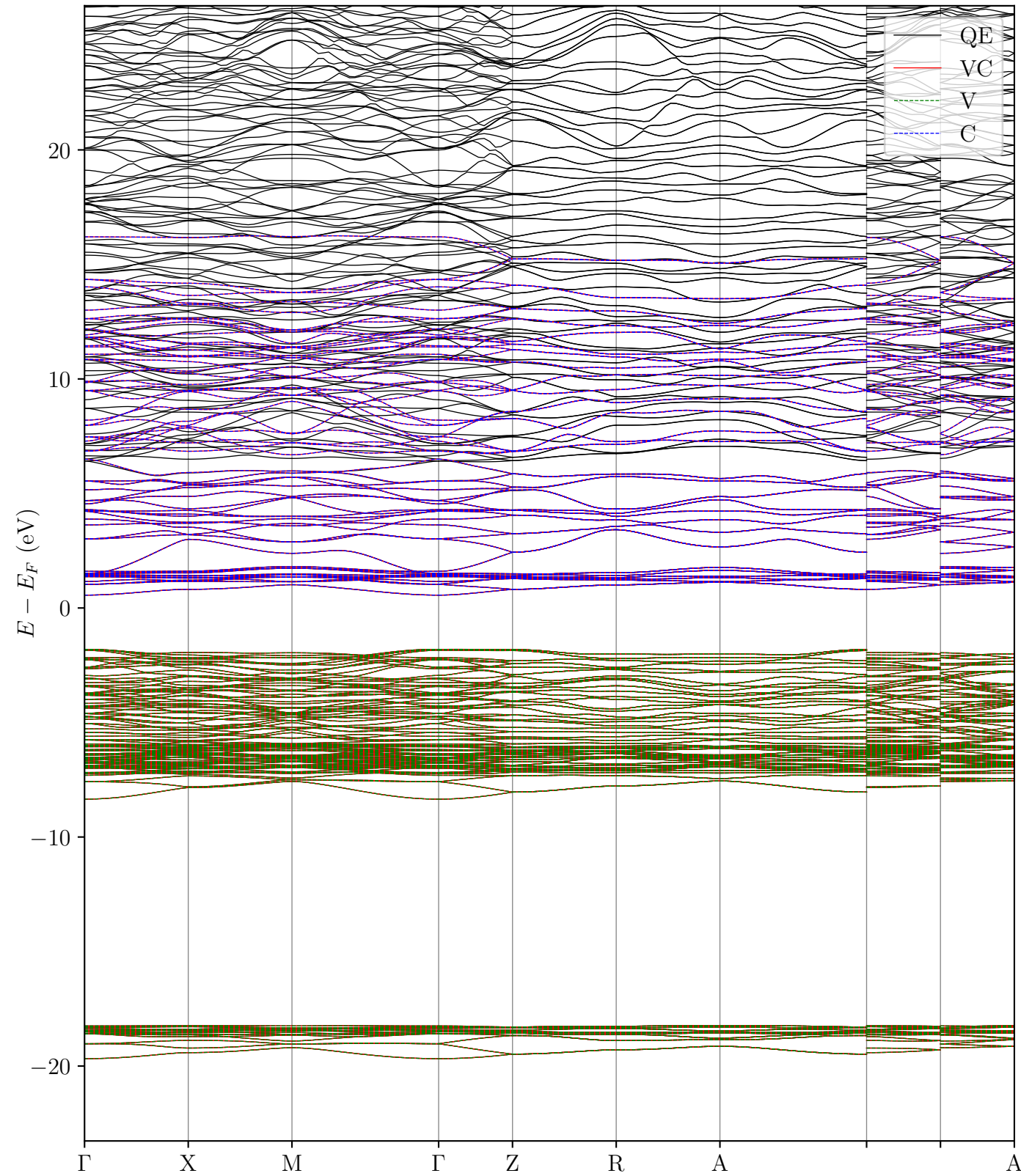


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	7.0	1.5	3.1	3.3	15.0	16.8	5.5
η_{max}	36.4	12.3	43.0	41.6	36.4	43.9	46.5



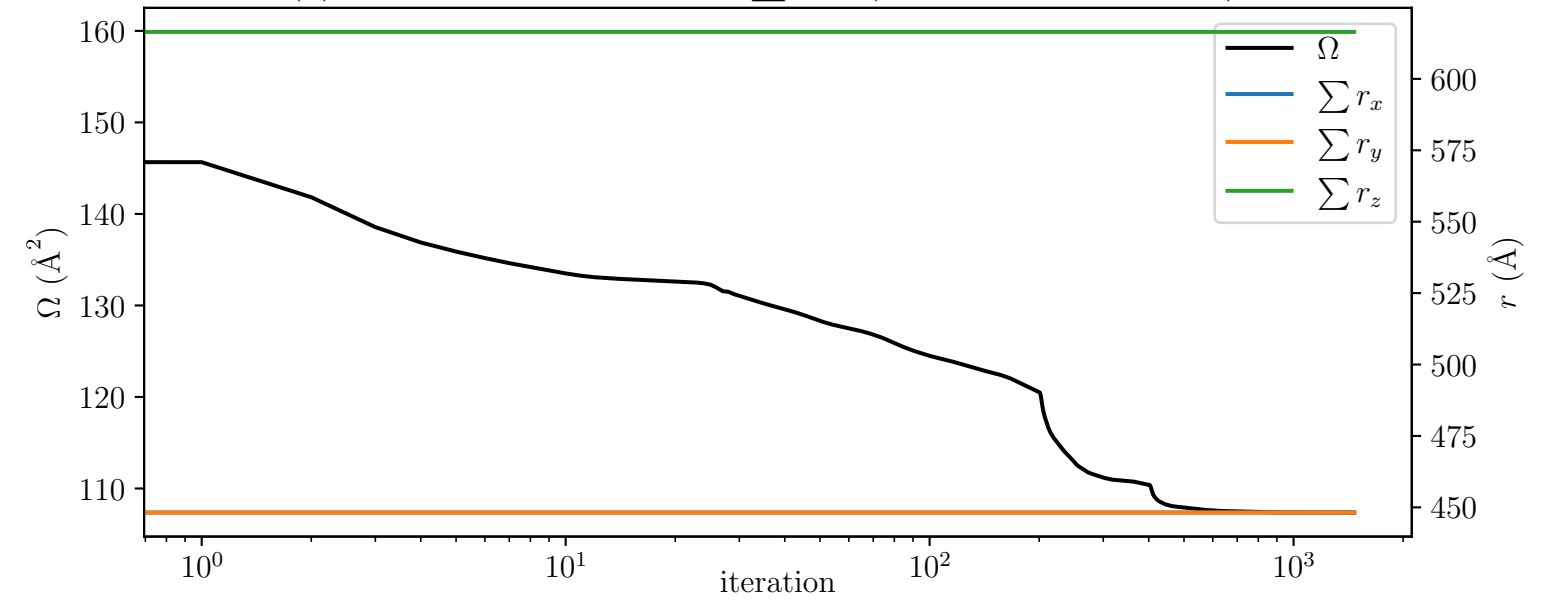
O₁₆Ti₄Zn₈ (exclude semicore)
PW AiiDA UUID: a8280fac-4c79-44c9-98bf-1d04574b918a
W90 AiiDA UUID: 08e9a02e-fd4d-4f3b-98fa-025ca39aea60



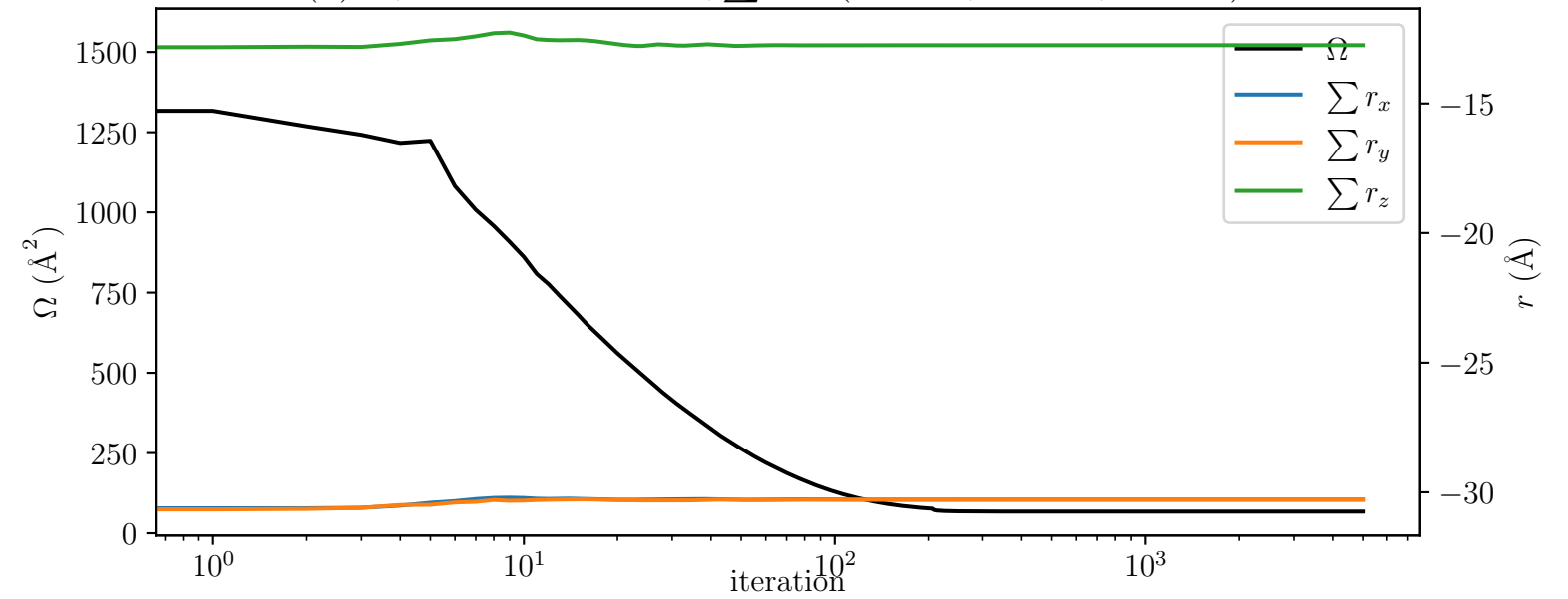
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.1	0.1	0.0	0.1	0.1	0.1	0.4
η_{max}	2.2	2.2	0.4	2.1	0.6	0.5	4.6

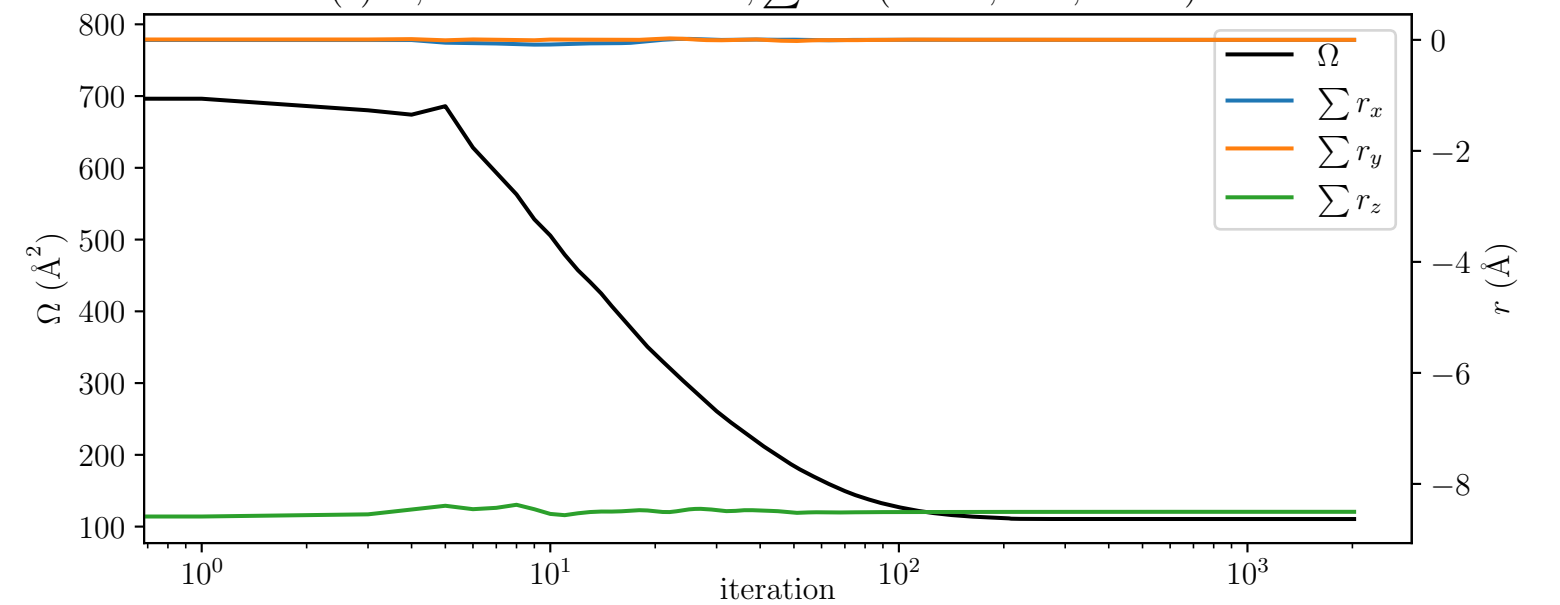
(a) VC; final $\Omega = 107.37 \text{ \AA}^2$, $\sum r = (448.19, 448.19, 616.44) \text{ \AA}$



(b) V; final $\Omega = 67.52 \text{ \AA}^2$, $\sum r = (-30.28, -30.28, -12.75) \text{ \AA}$



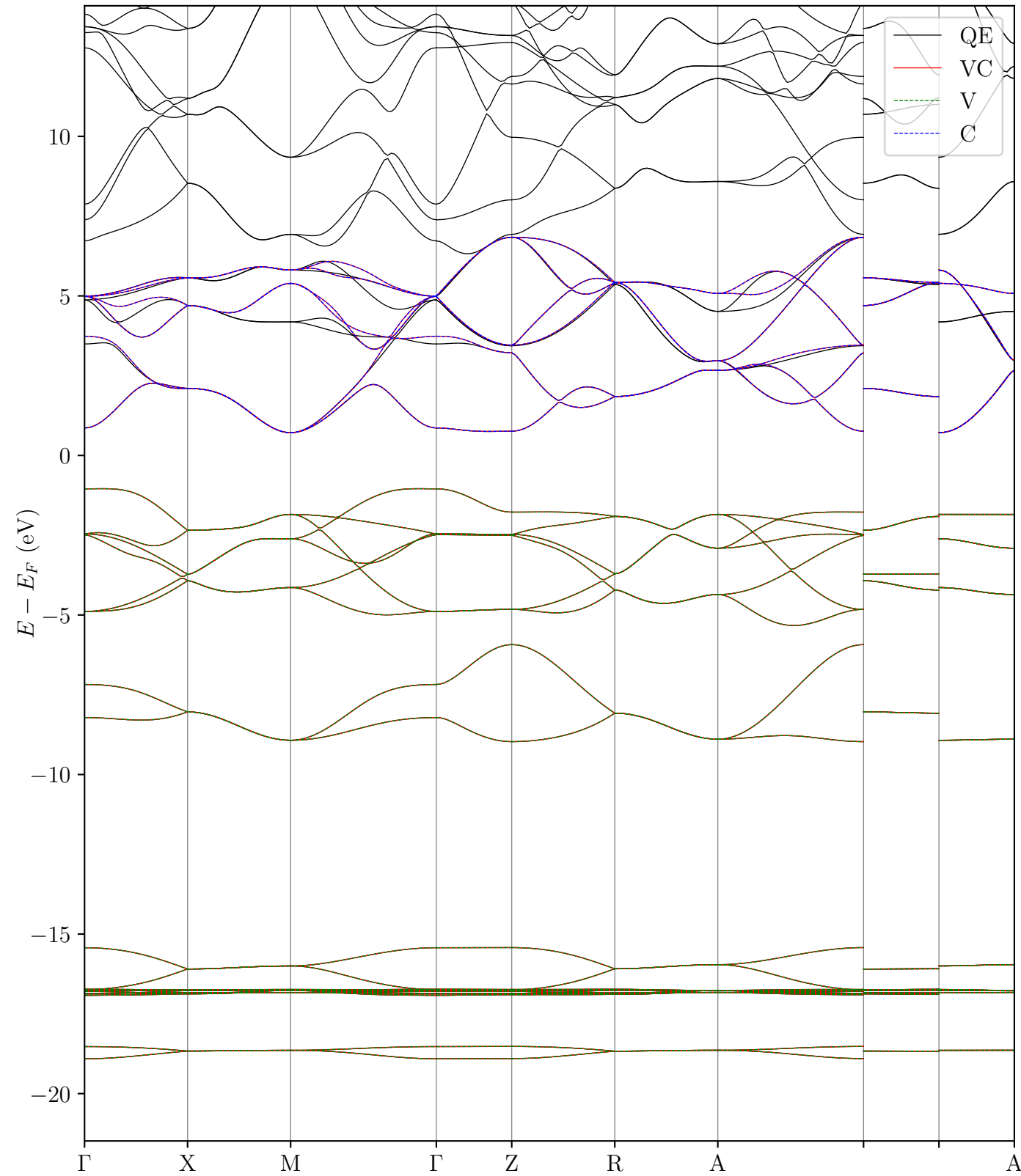
(c) C; final $\Omega = 110.55 \text{ \AA}^2$, $\sum r = (-0.00, 0.00, -8.50) \text{ \AA}$



O₂Pb₂ (**include** semicore)

PW AiiDA UUID: 94782b56-4c9d-42eb-bc63-5066fda64732

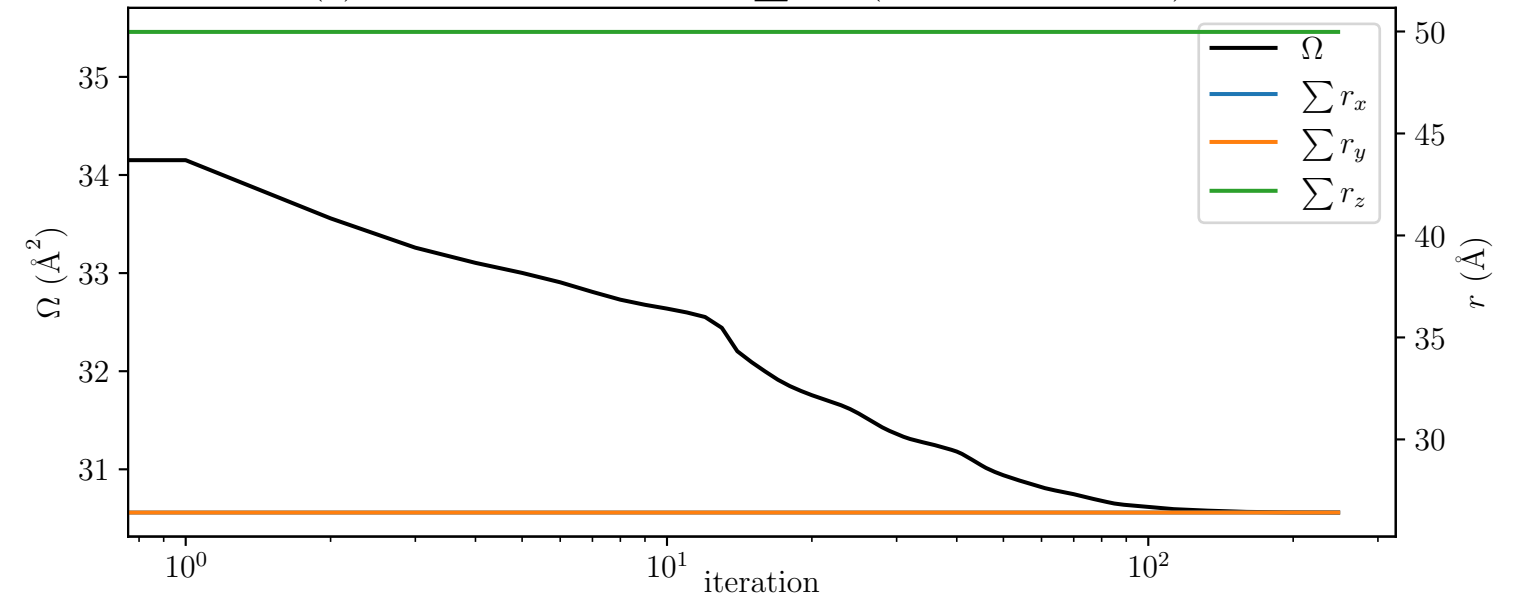
W90 AiiDA UUID: 595d95b4-1792-4d01-a37a-698d516f7212



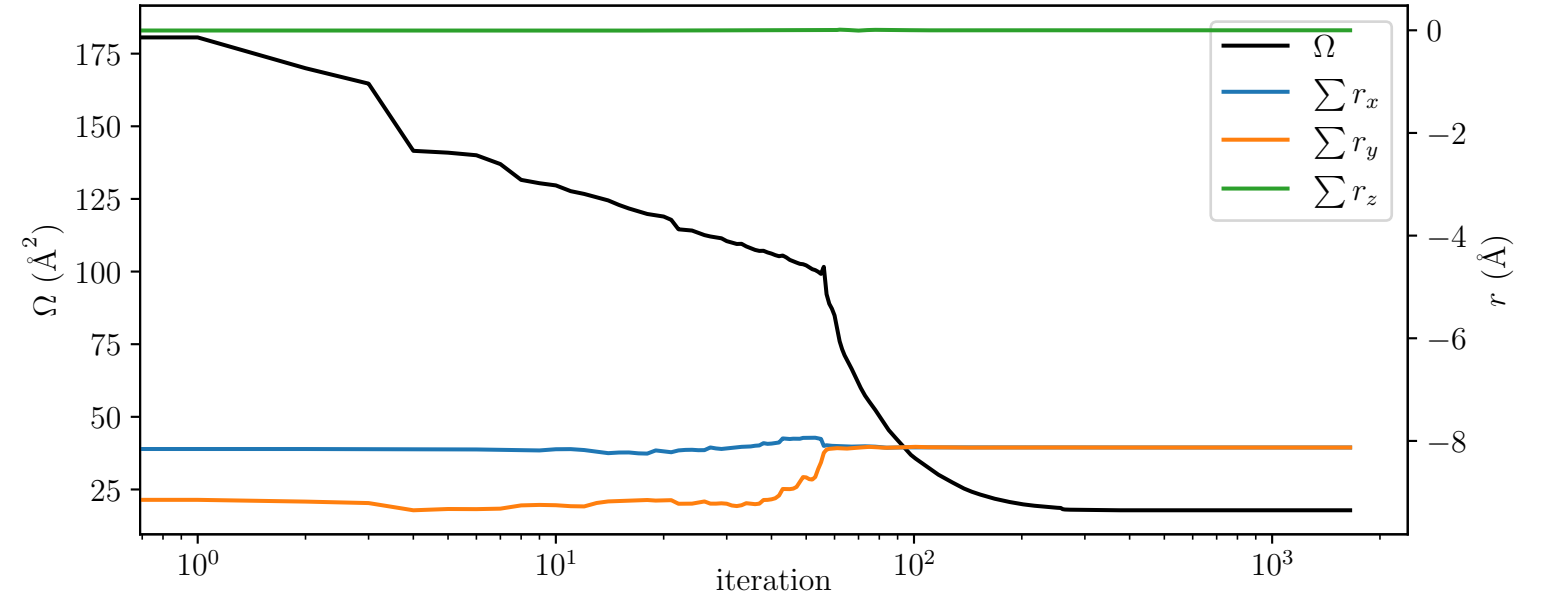
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.7	0.2	0.1	0.2	3.0	2.9	0.7
η_{max}	10.8	2.4	1.7	2.6	10.8	9.9	5.9

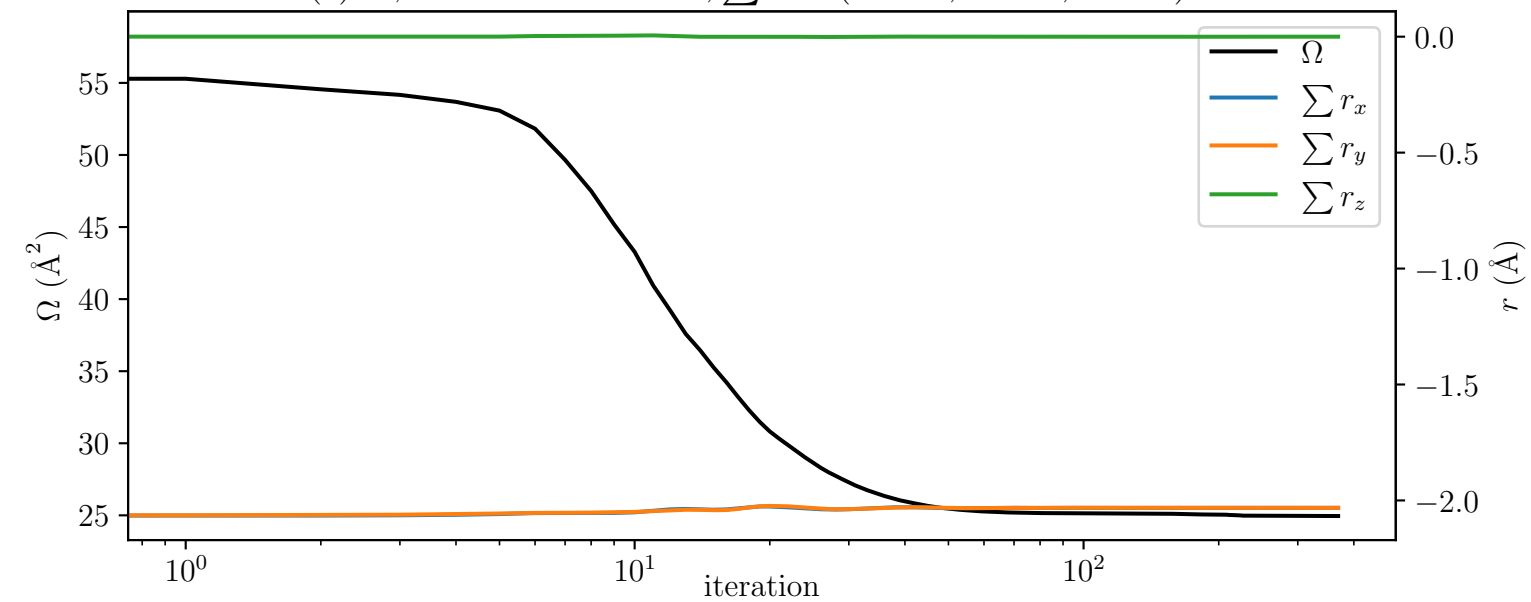
(a) VC; final $\Omega = 30.56 \text{\AA}^2$, $\sum r = (26.41, 26.41, 49.98) \text{\AA}$



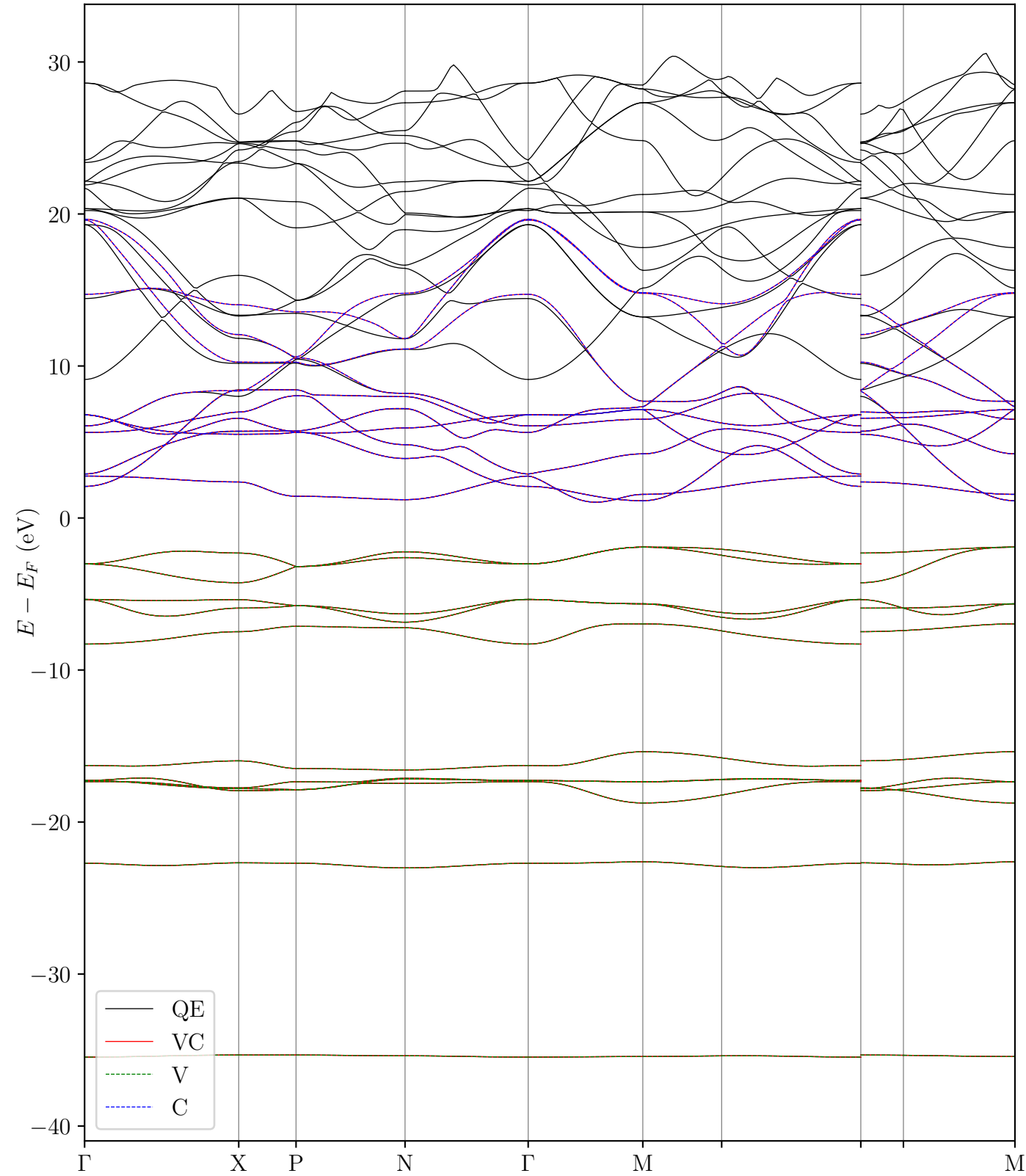
(b) V; final $\Omega = 17.84 \text{\AA}^2$, $\sum r = (-8.13, -8.13, 0.00) \text{\AA}$



(c) C; final $\Omega = 24.95 \text{\AA}^2$, $\sum r = (-2.03, -2.03, -0.00) \text{\AA}$



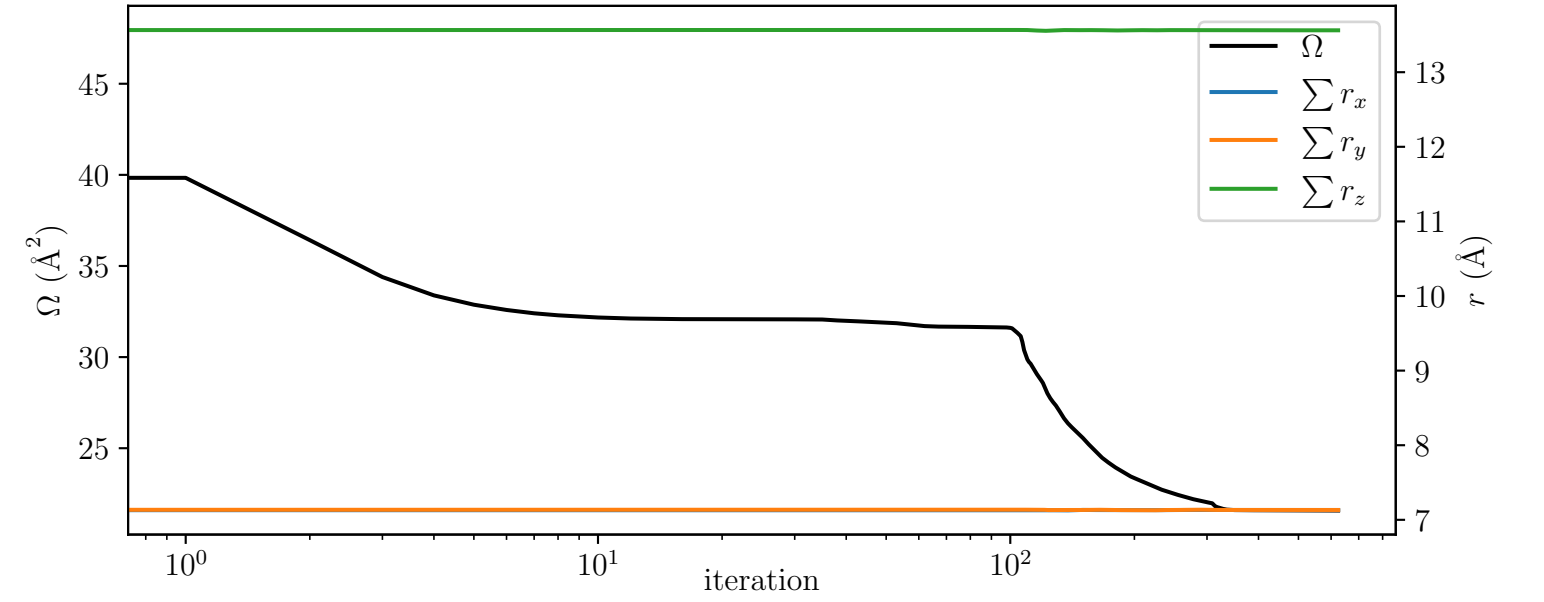
O₂Sr (**include** semicore)
PW AiiDA UUID: 9c175f49-1adc-408f-9963-bfce4d709f87
W90 AiiDA UUID: a1b1d6b7-7076-4575-8164-75d5056e112a



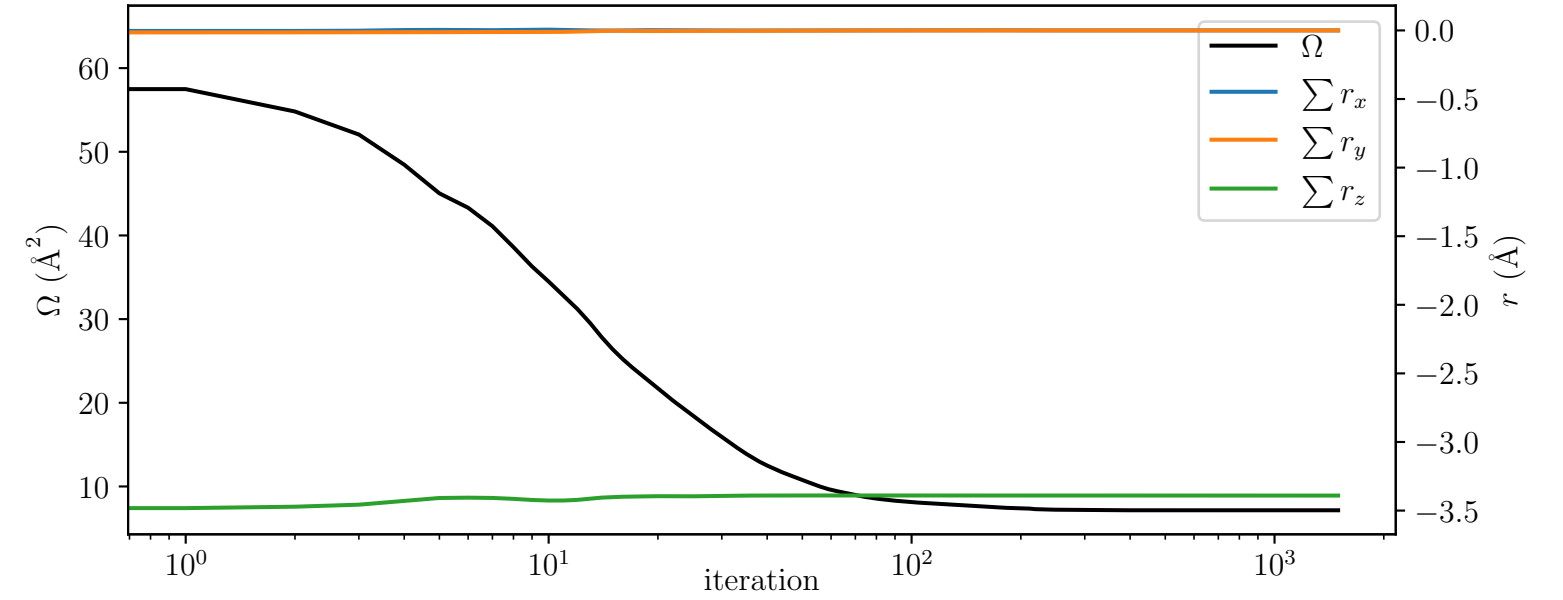
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.6	0.4	0.0	0.4	1.8	1.6	2.1
η_{max}	7.6	2.1	0.0	2.1	7.6	5.4	18.2

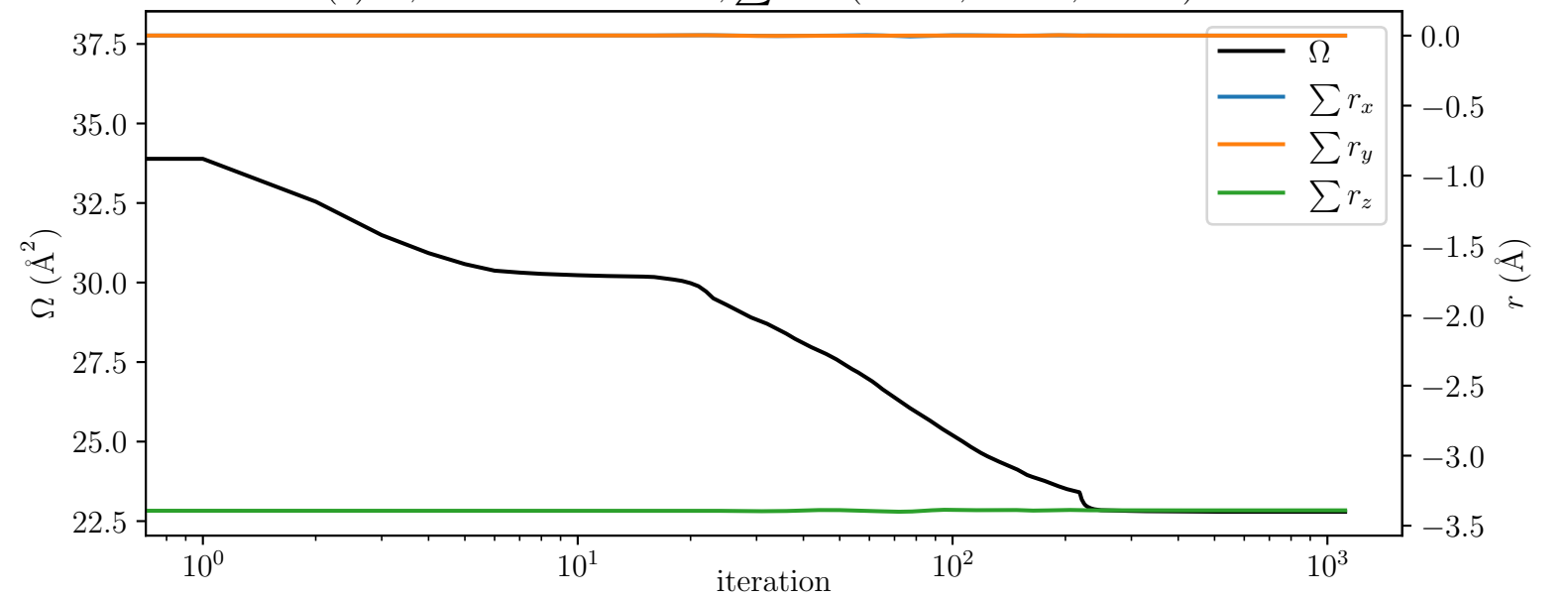
(a) VC; final $\Omega = 21.58 \text{ \AA}^2$, $\sum r = (7.13, 7.13, 13.56) \text{ \AA}$



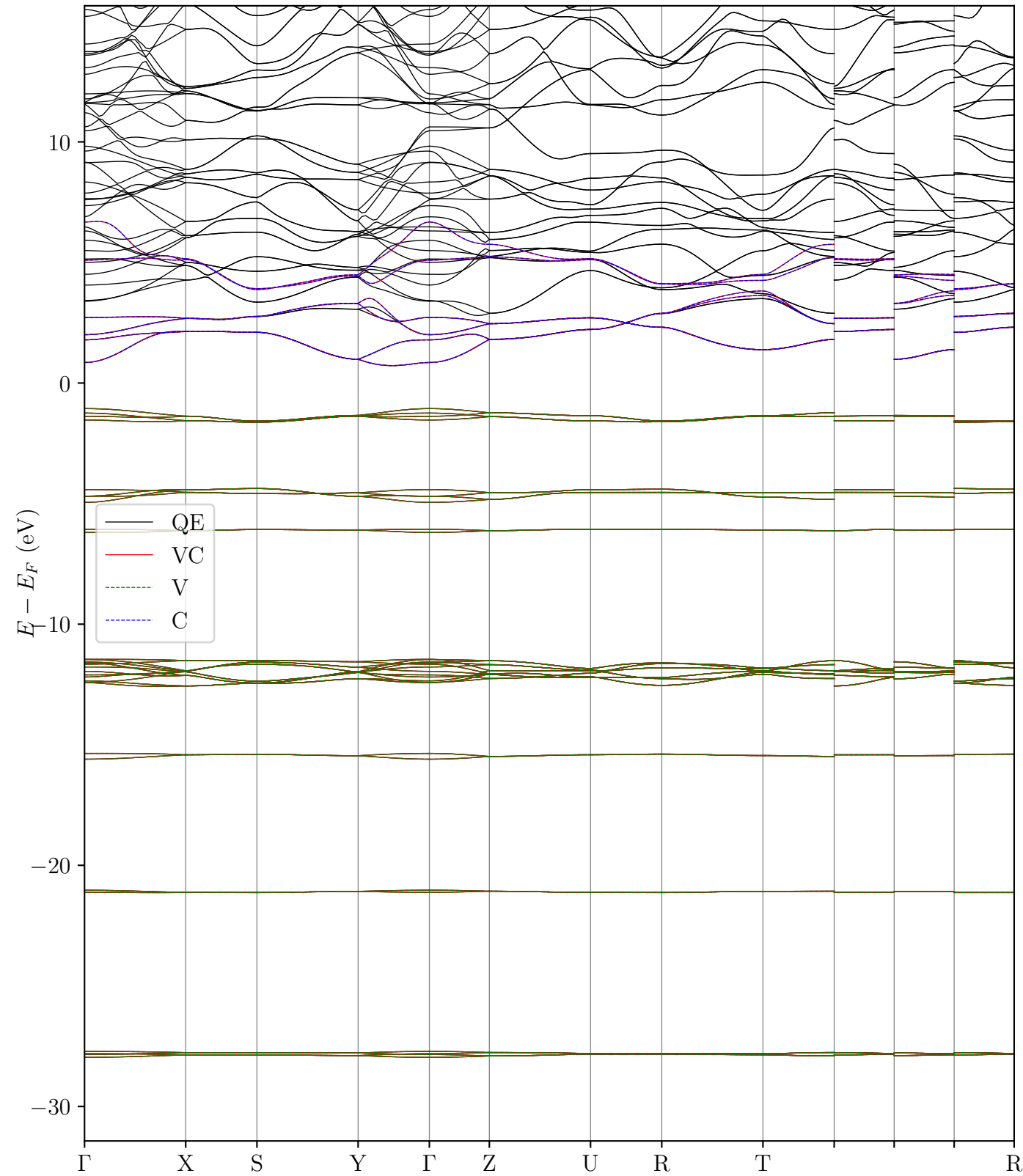
(b) V; final $\Omega = 7.15 \text{ \AA}^2$, $\sum r = (0.00, 0.00, -3.39) \text{ \AA}$



(c) C; final $\Omega = 22.79 \text{ \AA}^2$, $\sum r = (-0.00, -0.00, -3.39) \text{ \AA}$

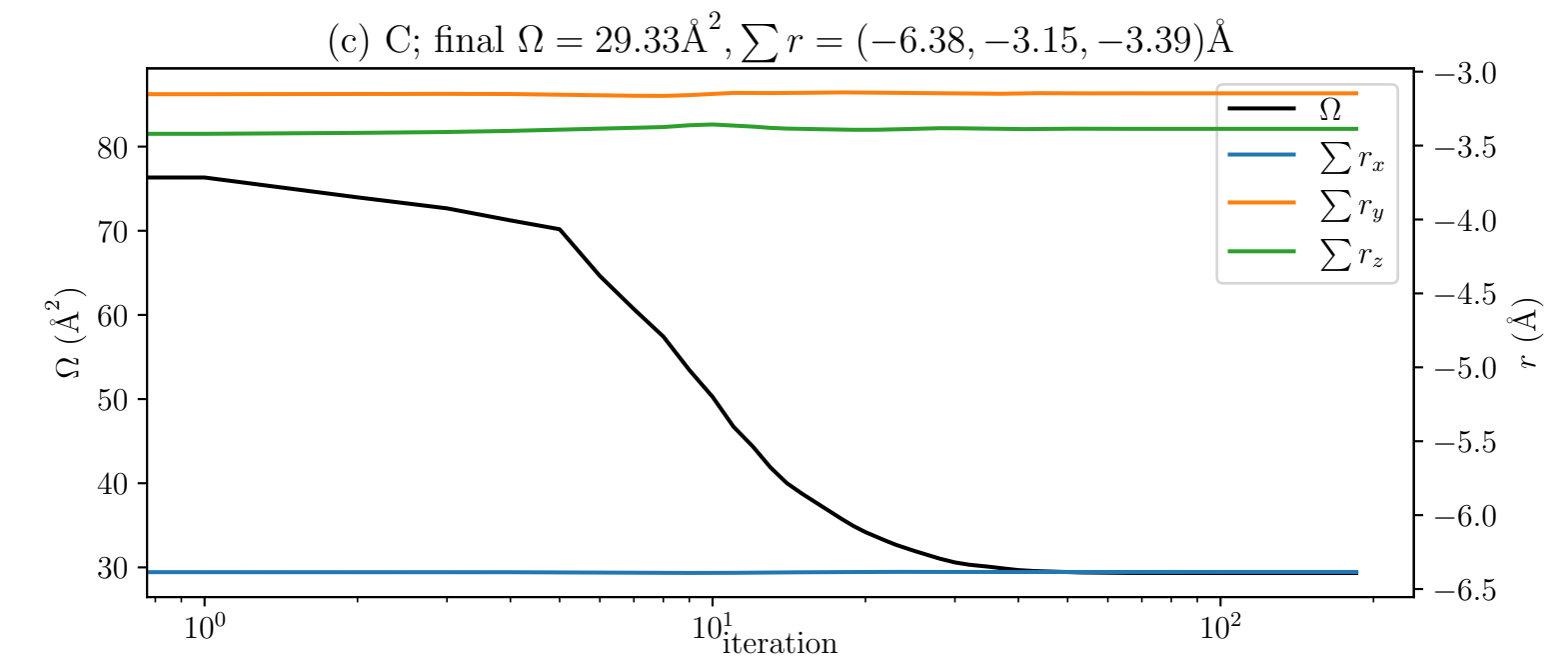
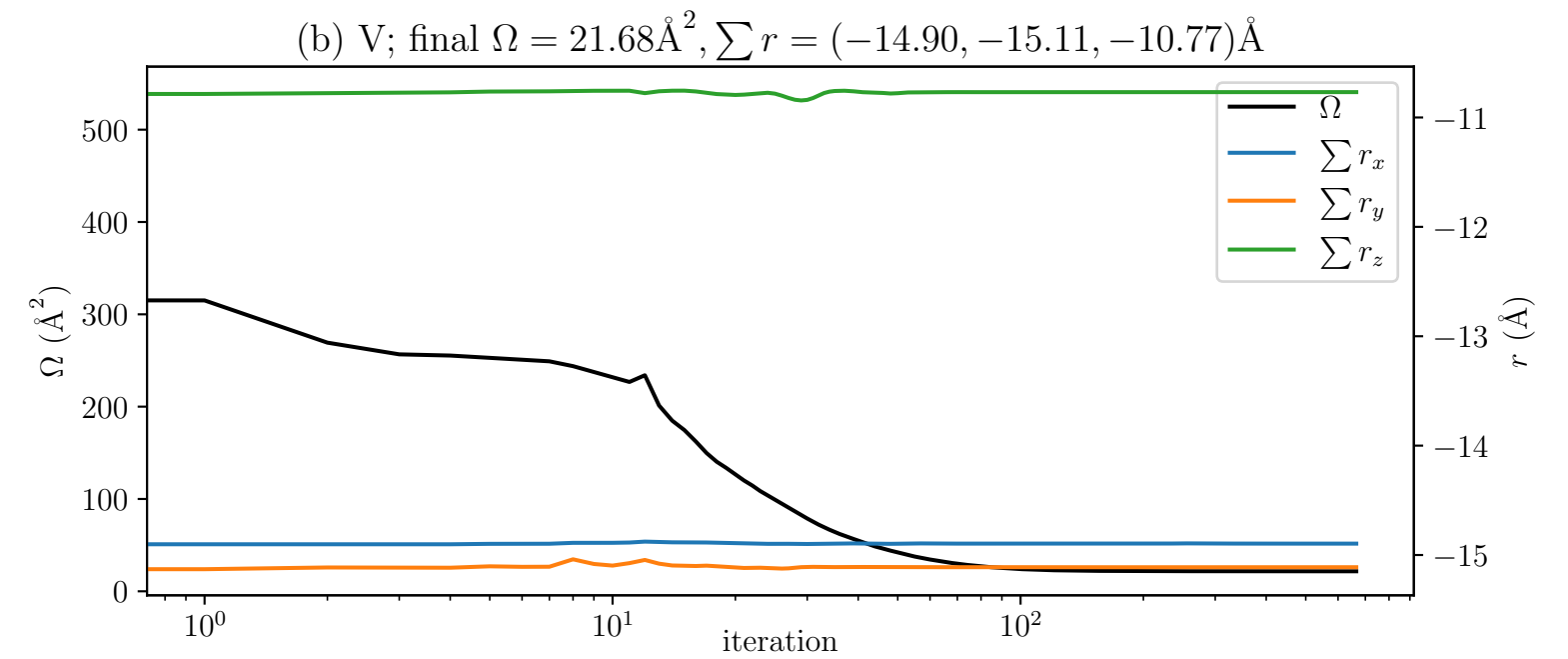
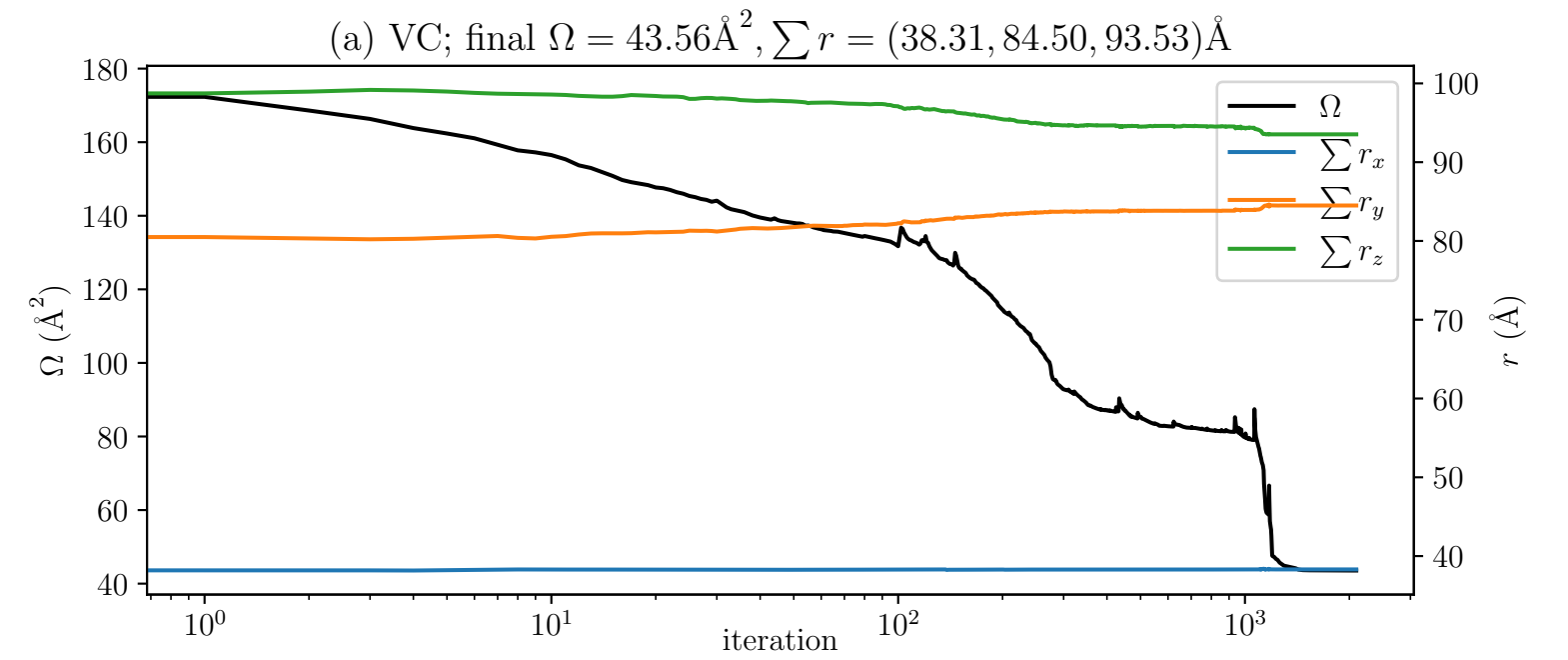


O₄Rb₄ (**include** semicore)
PW AiiDA UUID: 15e4547d-d9f4-4623-8839-e3a5392b0b12
W90 AiiDA UUID: b4f1a398-ab4c-4280-9935-cdbe58c91d01

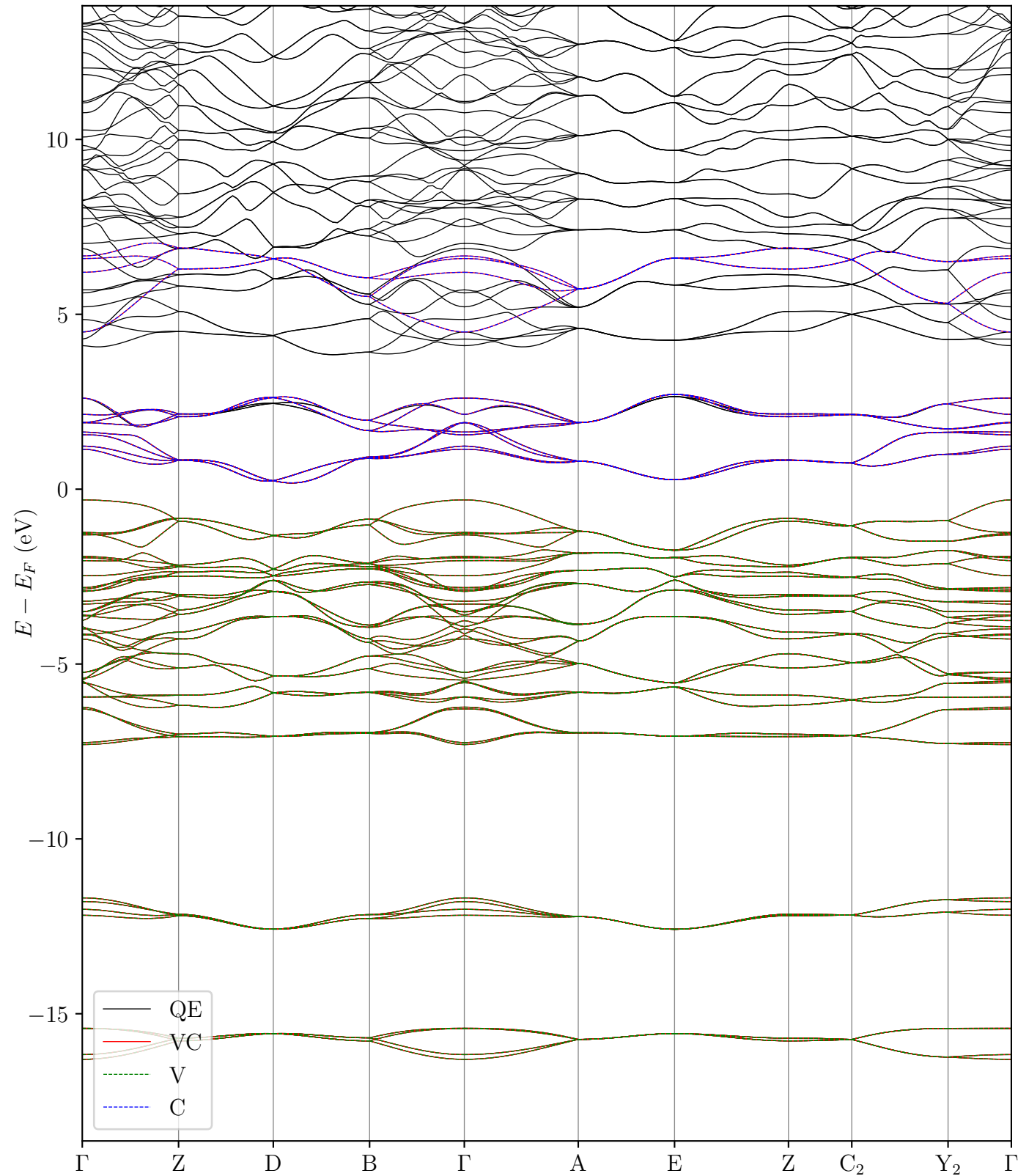


band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.6	0.3	0.0	0.3	2.4	2.6	0.9
η_{max}	8.5	5.6	0.0	5.6	8.5	8.2	6.7



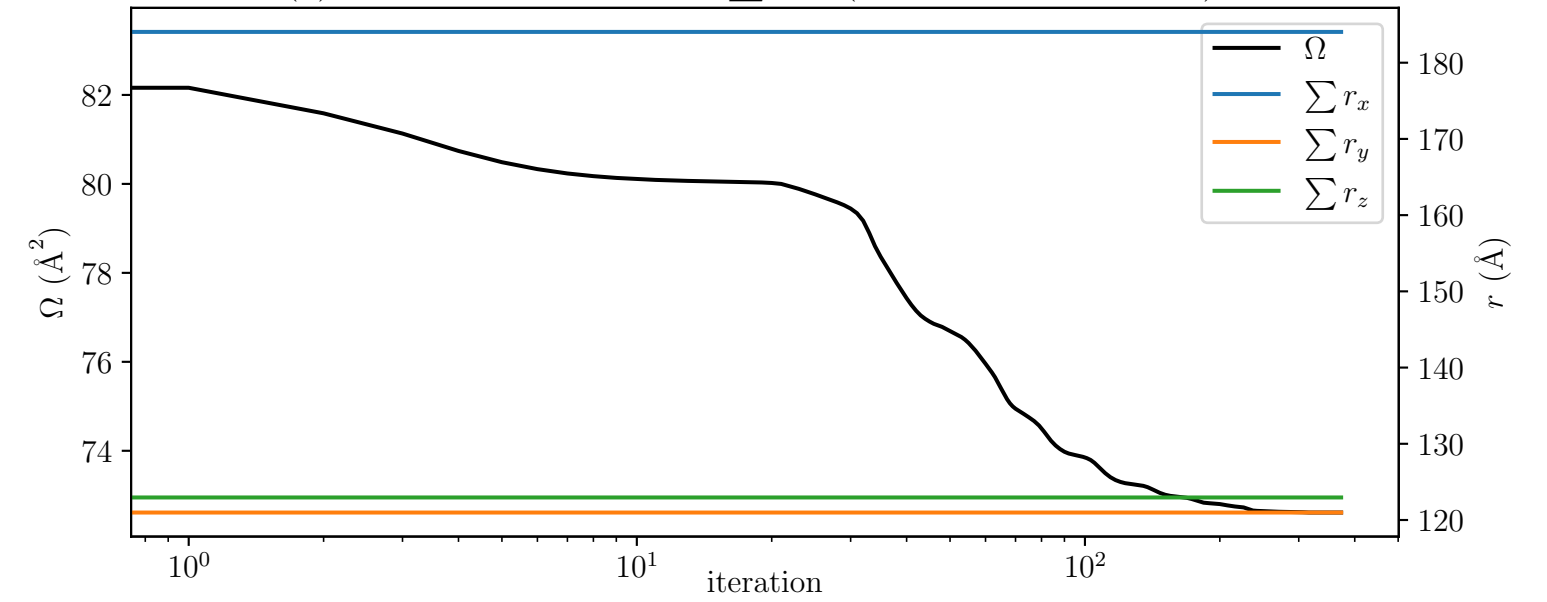
Pd₄S₈ (exclude semicore)
PW AiiDA UUID: c87b7e08-8db6-40e9-bca1-66aa0c637465
W90 AiiDA UUID: cc2afb5b-66bd-4203-b0c0-11b491775822



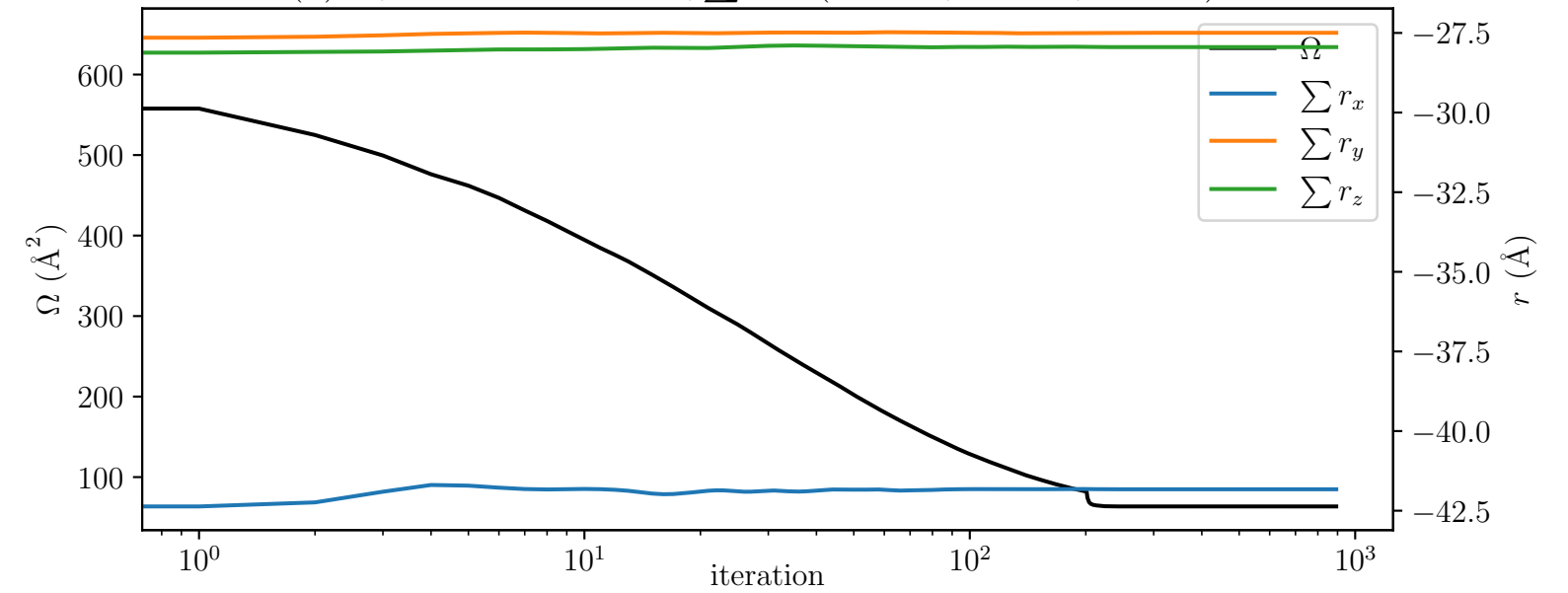
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.5	0.3	0.3	0.4	4.6	4.7	0.7
η_{max}	20.7	2.8	3.3	3.0	20.7	20.9	3.2

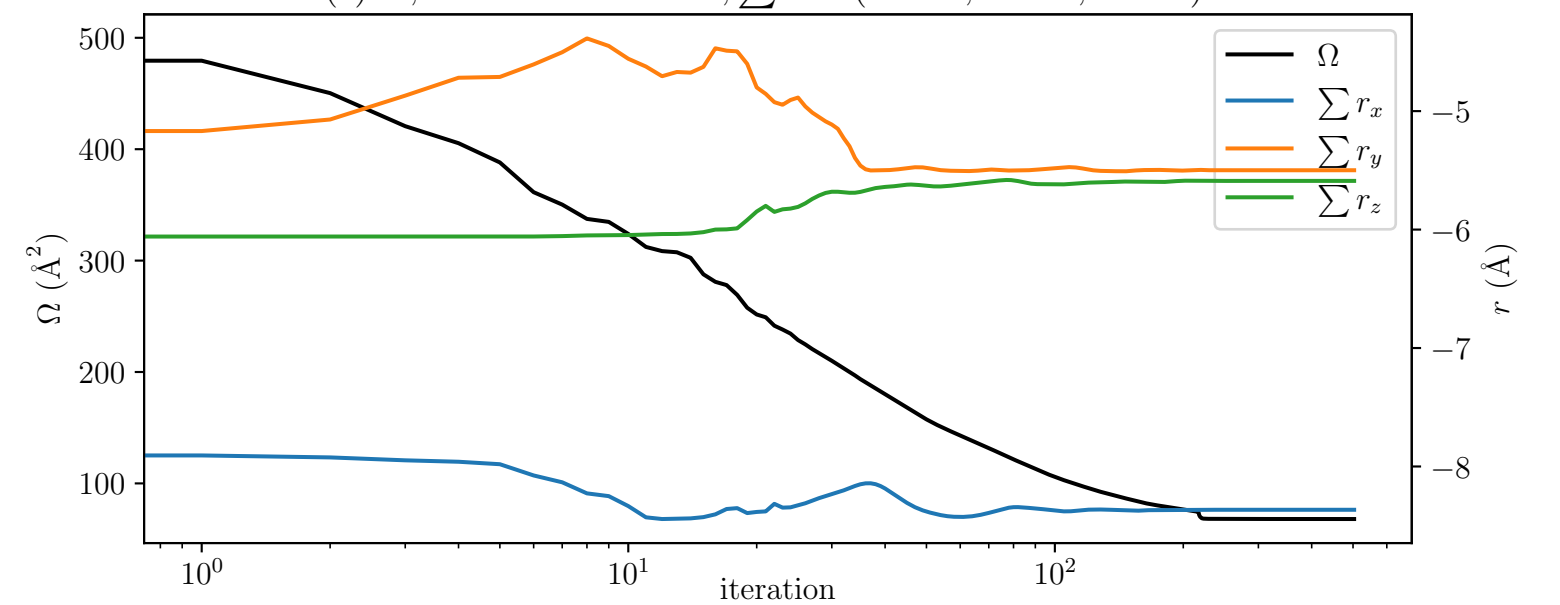
(a) VC; final $\Omega = 72.61 \text{ \AA}^2$, $\sum r = (184.04, 120.98, 122.96) \text{ \AA}$



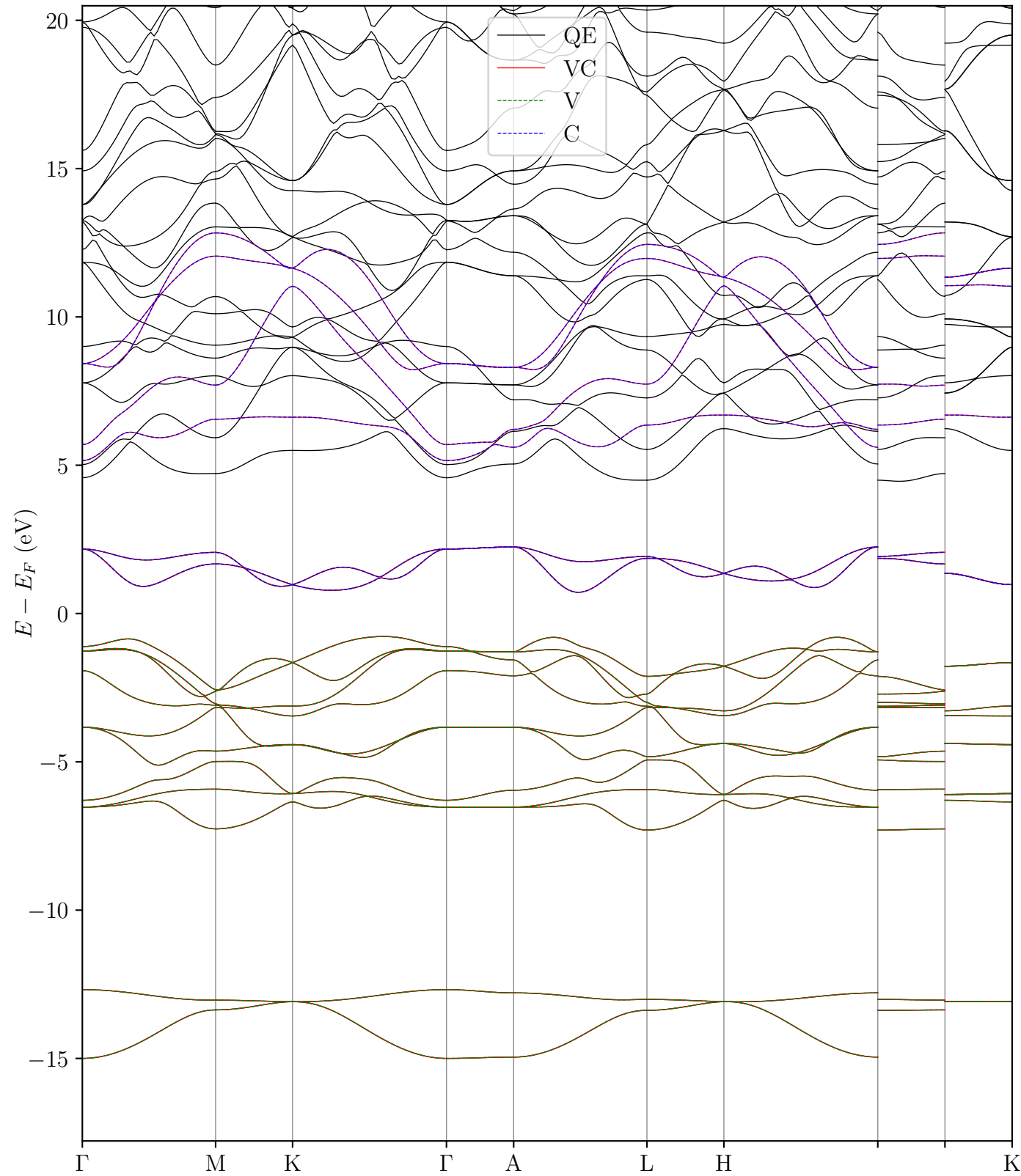
(b) V; final $\Omega = 63.55 \text{ \AA}^2$, $\sum r = (-41.83, -27.50, -27.94) \text{ \AA}$



(c) C; final $\Omega = 68.02 \text{ \AA}^2$, $\sum r = (-8.37, -5.50, -5.59) \text{ \AA}$

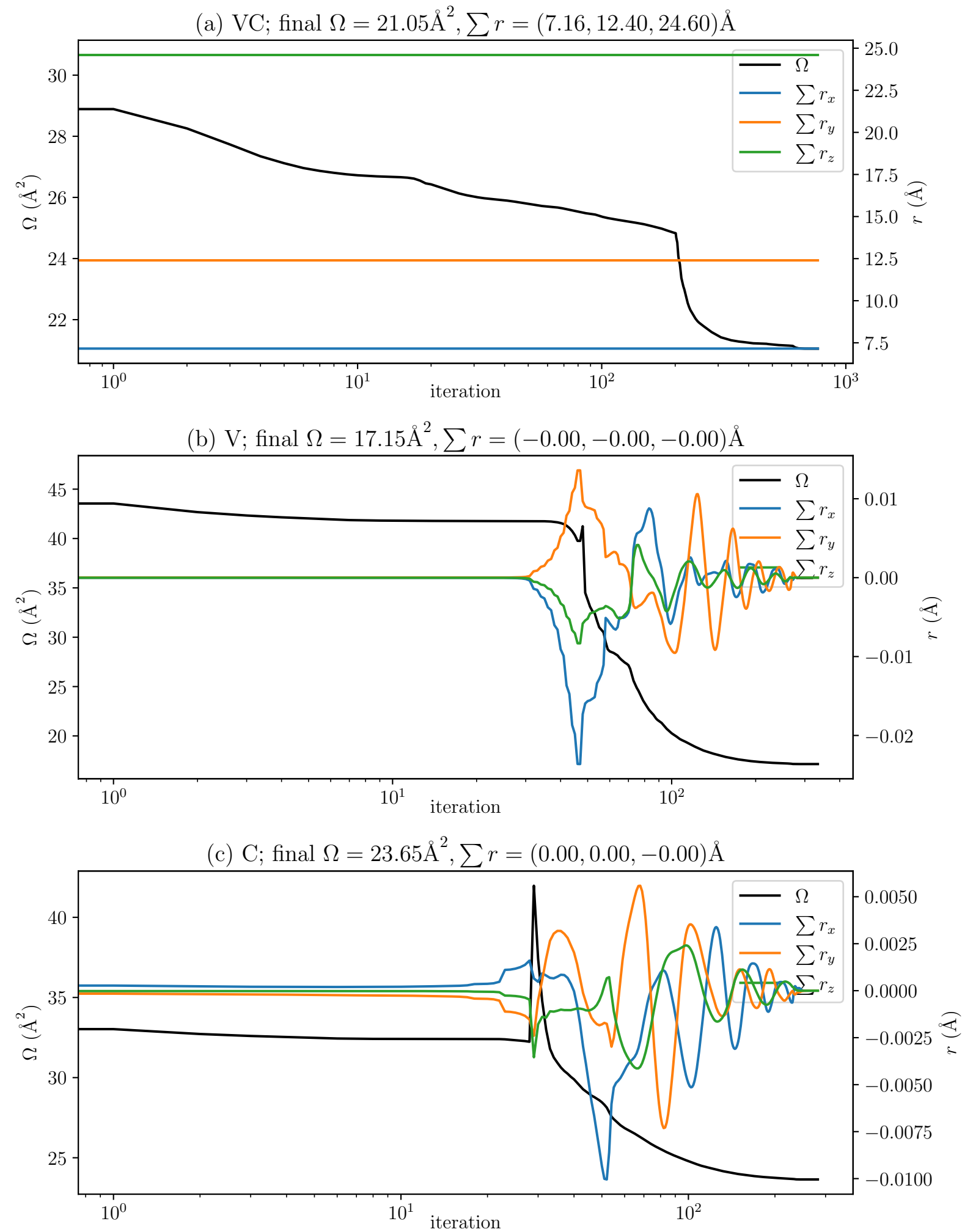


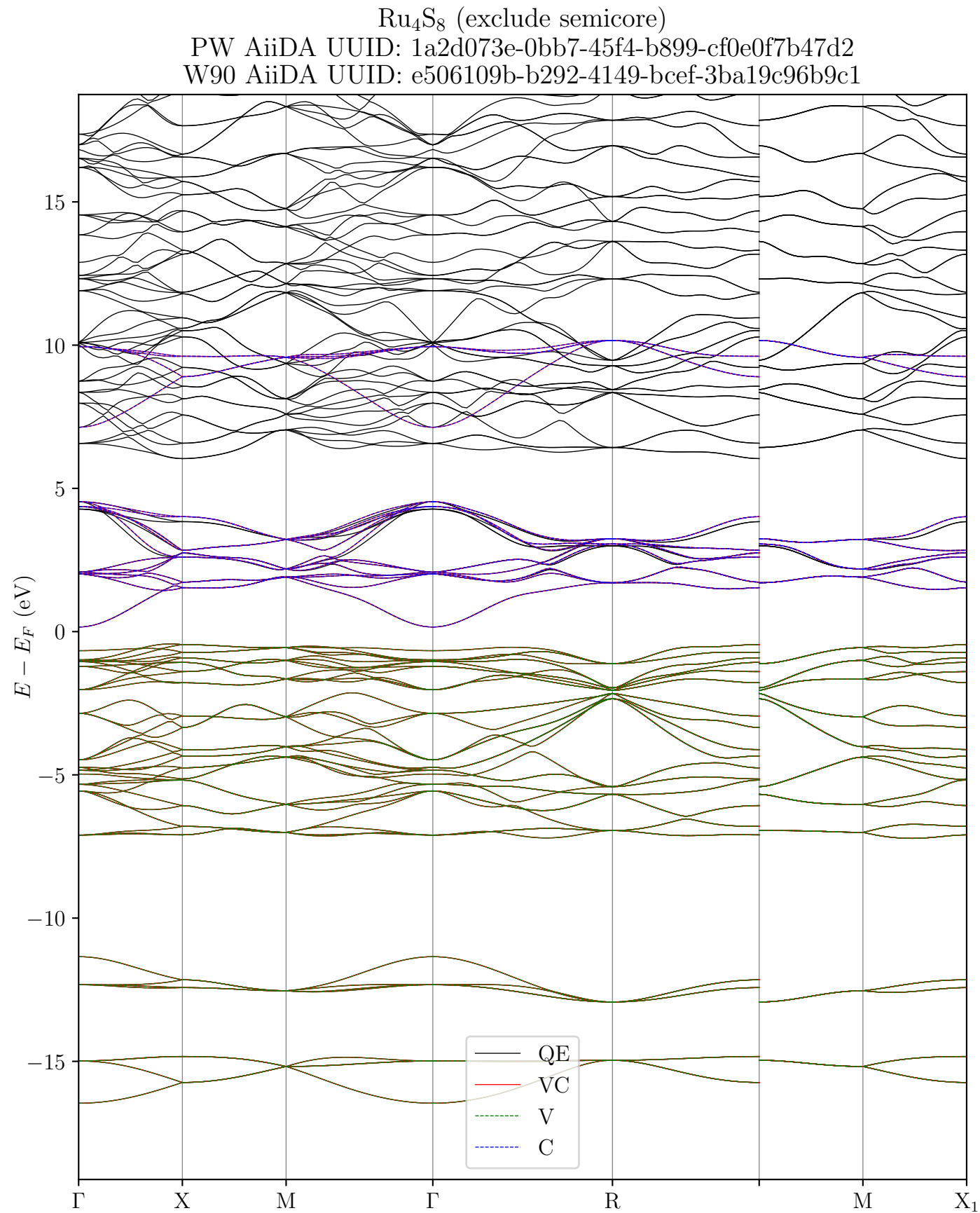
PtS₂ (exclude semicore)
PW AiiDA UUID: c3e724f4-cd9c-46bc-bfab-6e4930592618
W90 AiiDA UUID: b43d6848-5d50-4d6a-be75-b2a000f83397



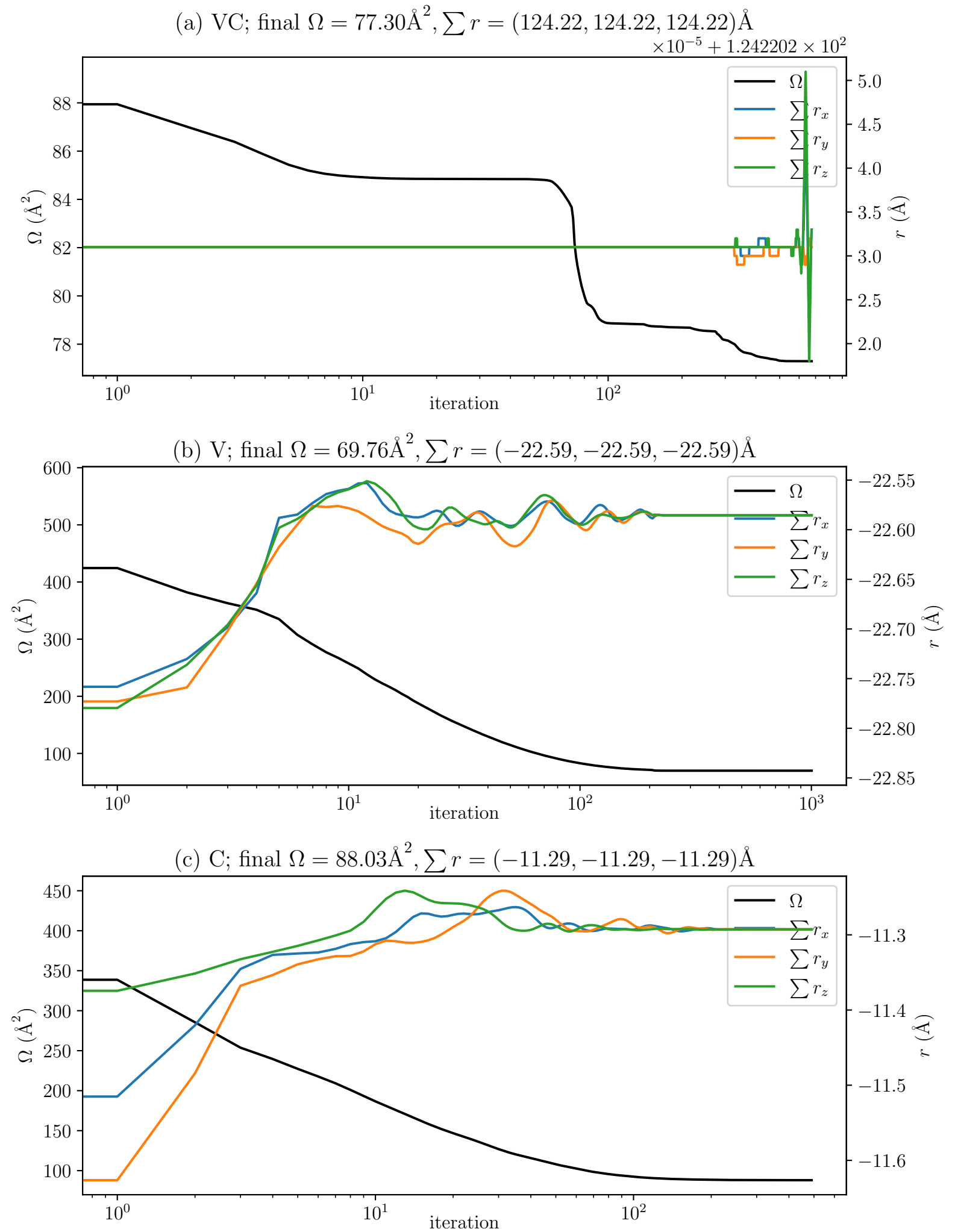
band distance (meV)

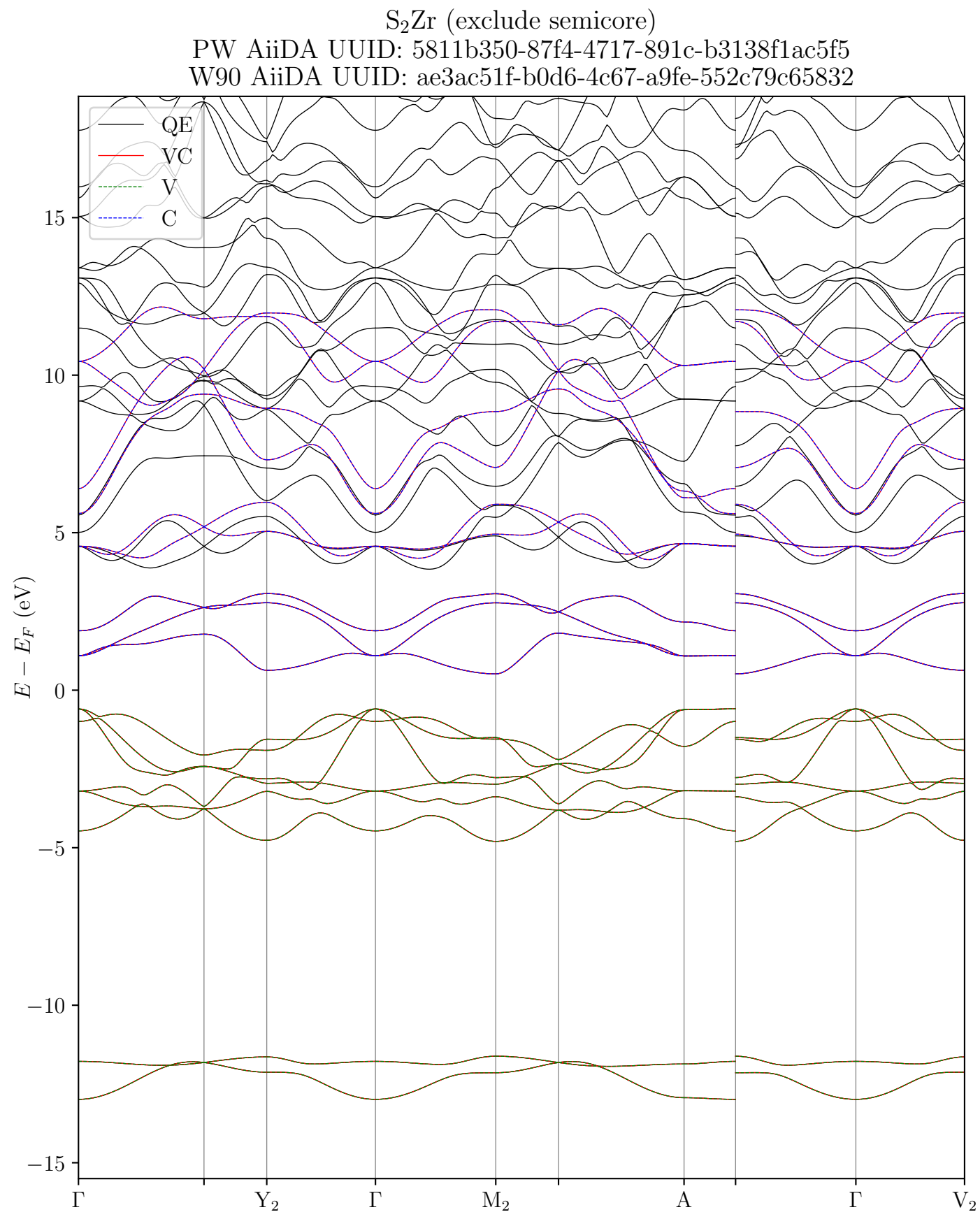
	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	0.6	0.6	0.4	0.7	0.6	2.3	2.1
η_{max}	4.6	4.6	3.5	4.7	2.3	6.9	12.5



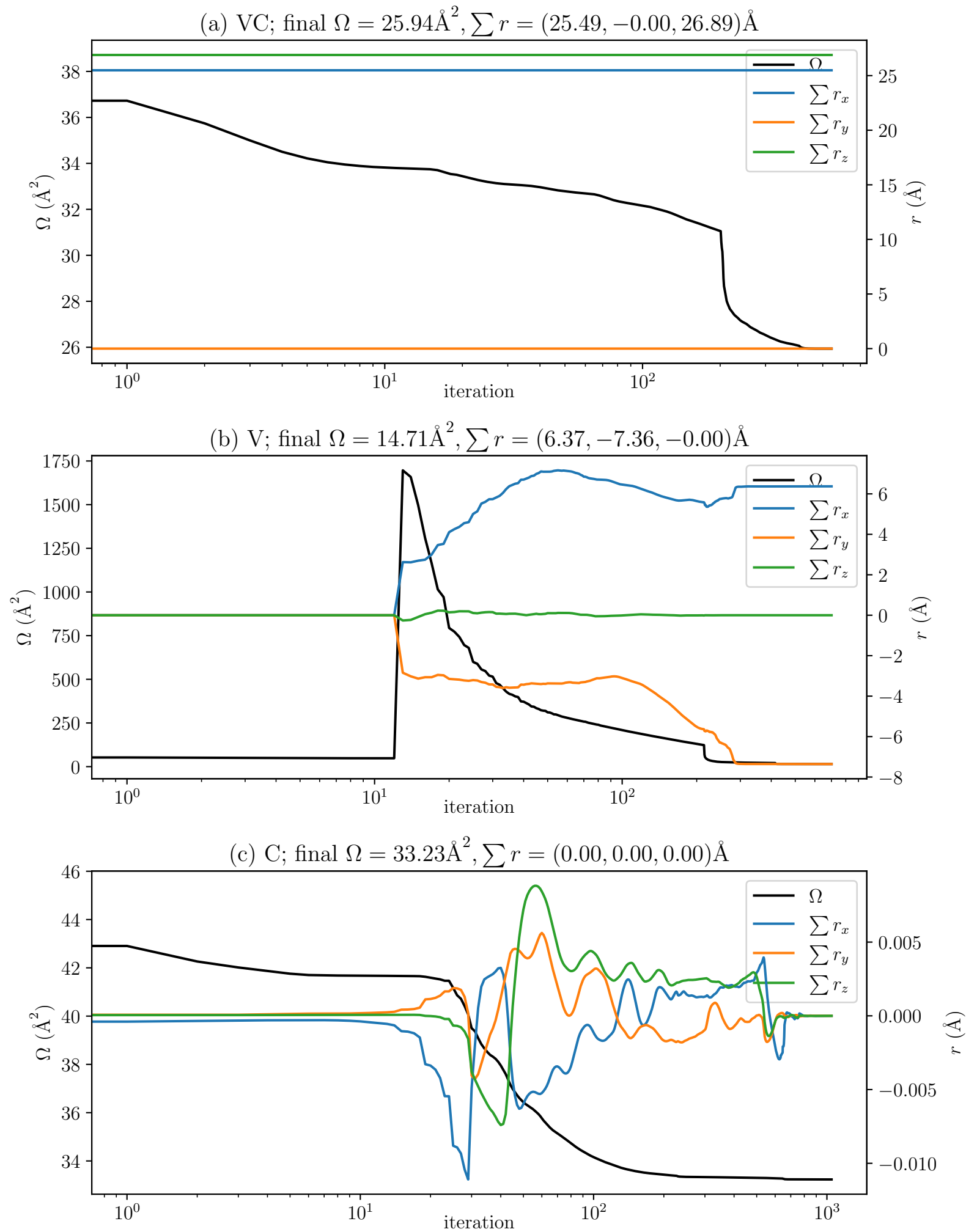


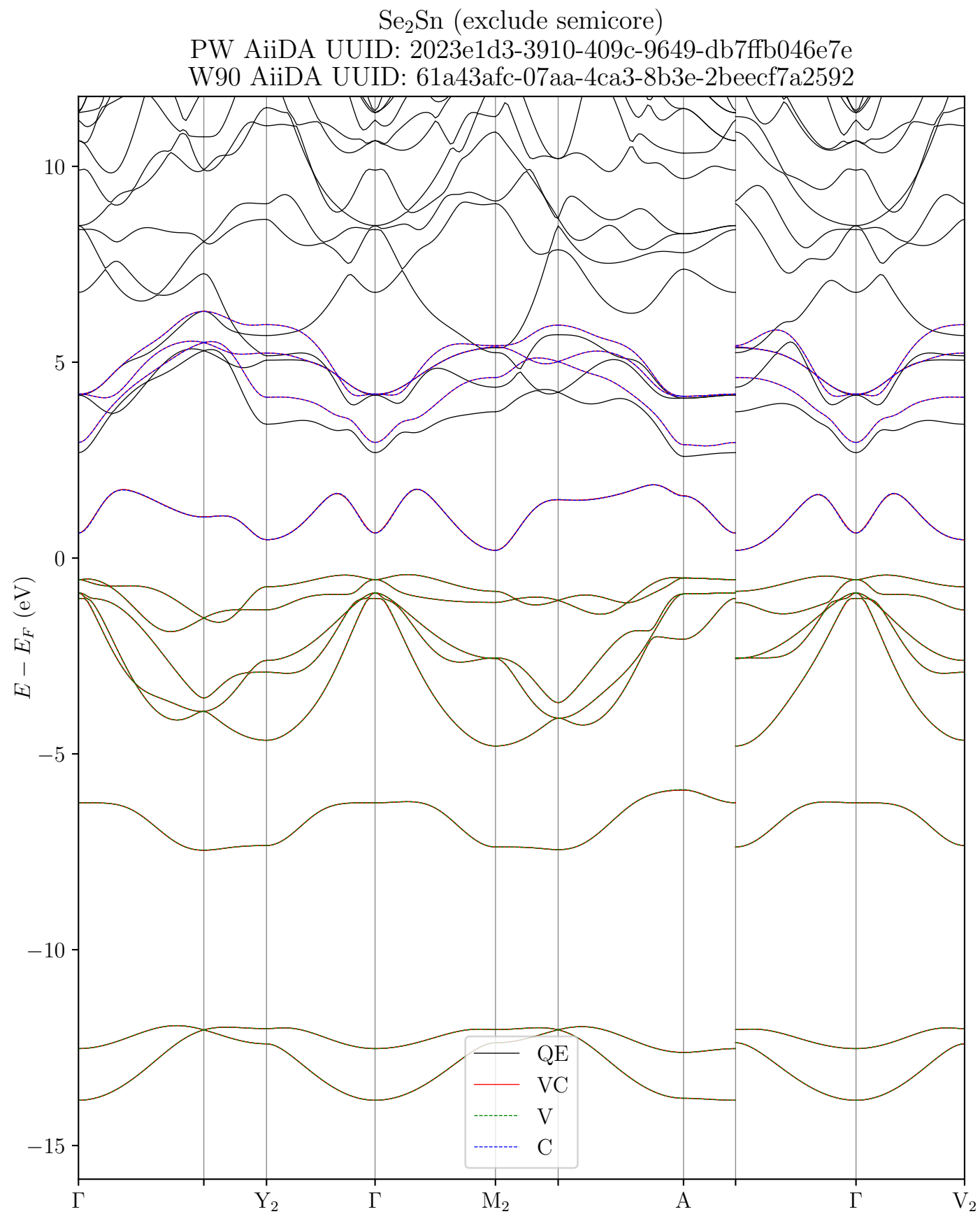
	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.1	0.4	0.2	0.5	3.7	3.8	0.6
η_{max}	12.6	3.4	2.2	3.8	12.6	12.8	2.8



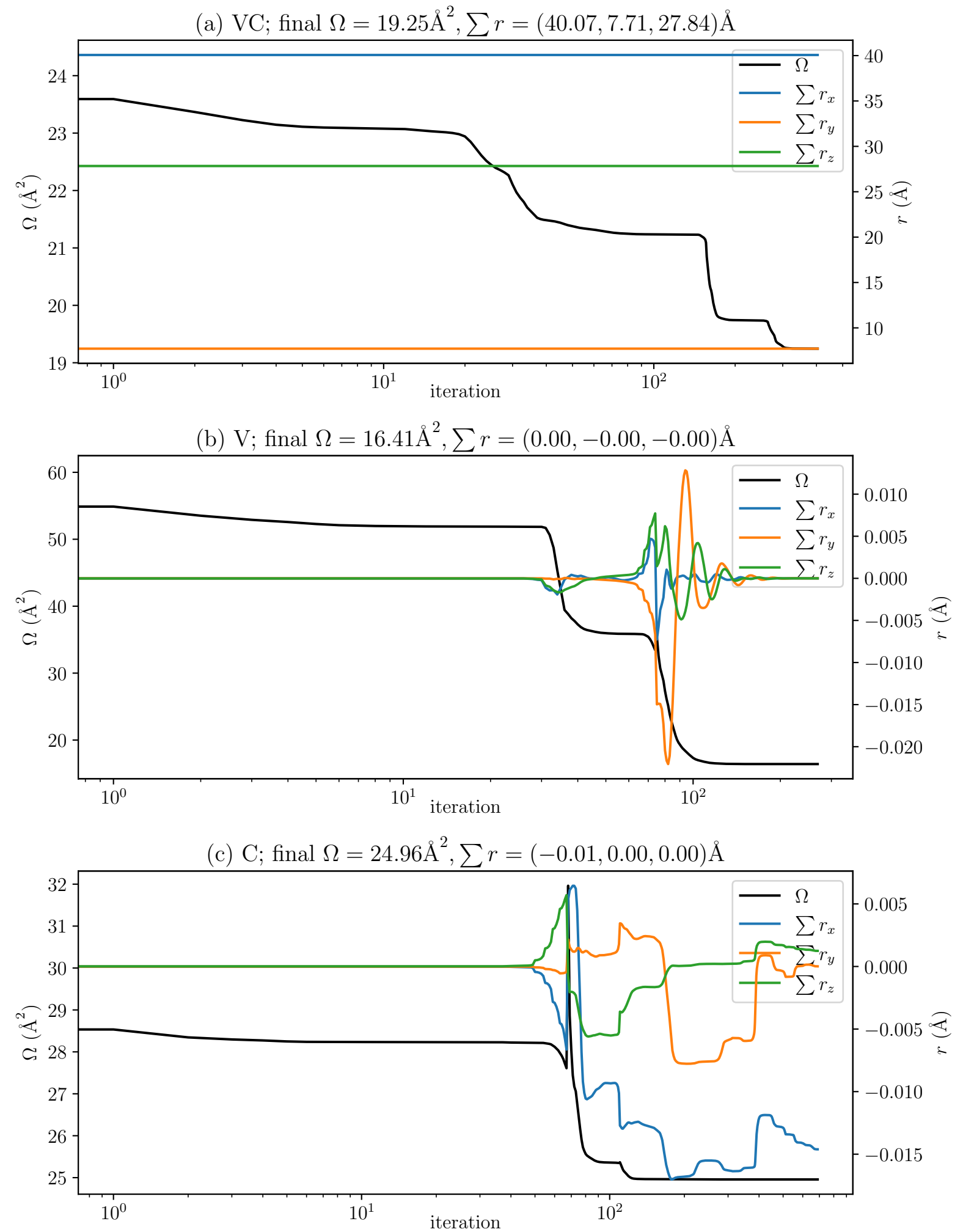


	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.1	1.2	1.3	1.9	0.8	2.0	2.1
η_{max}	7.9	7.9	7.6	10.5	2.2	10.6	12.3

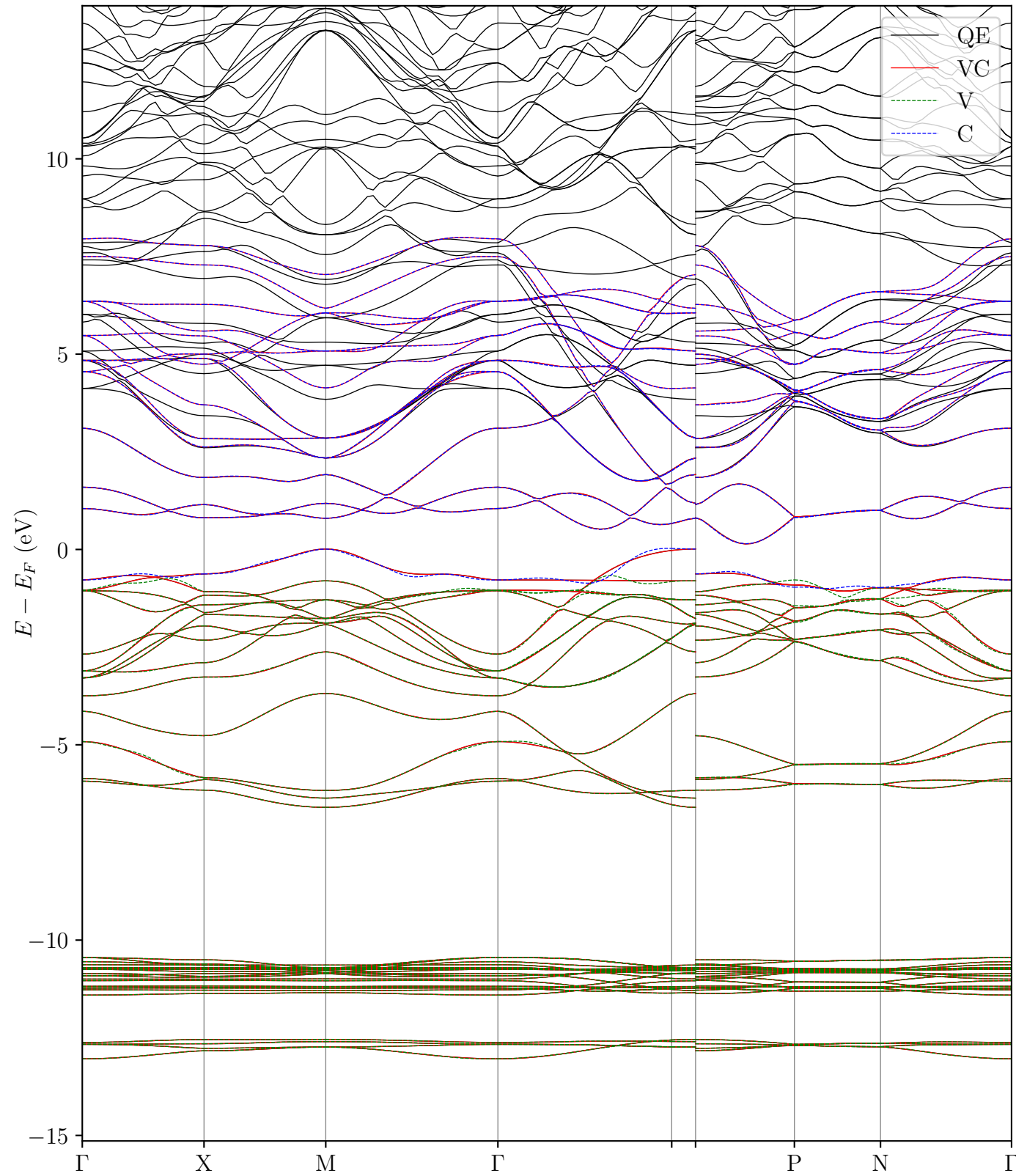




	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.1	0.6	2.7	2.7	2.9	7.3	3.9
η_{max}	6.4	3.3	23.6	22.9	6.4	23.0	22.3



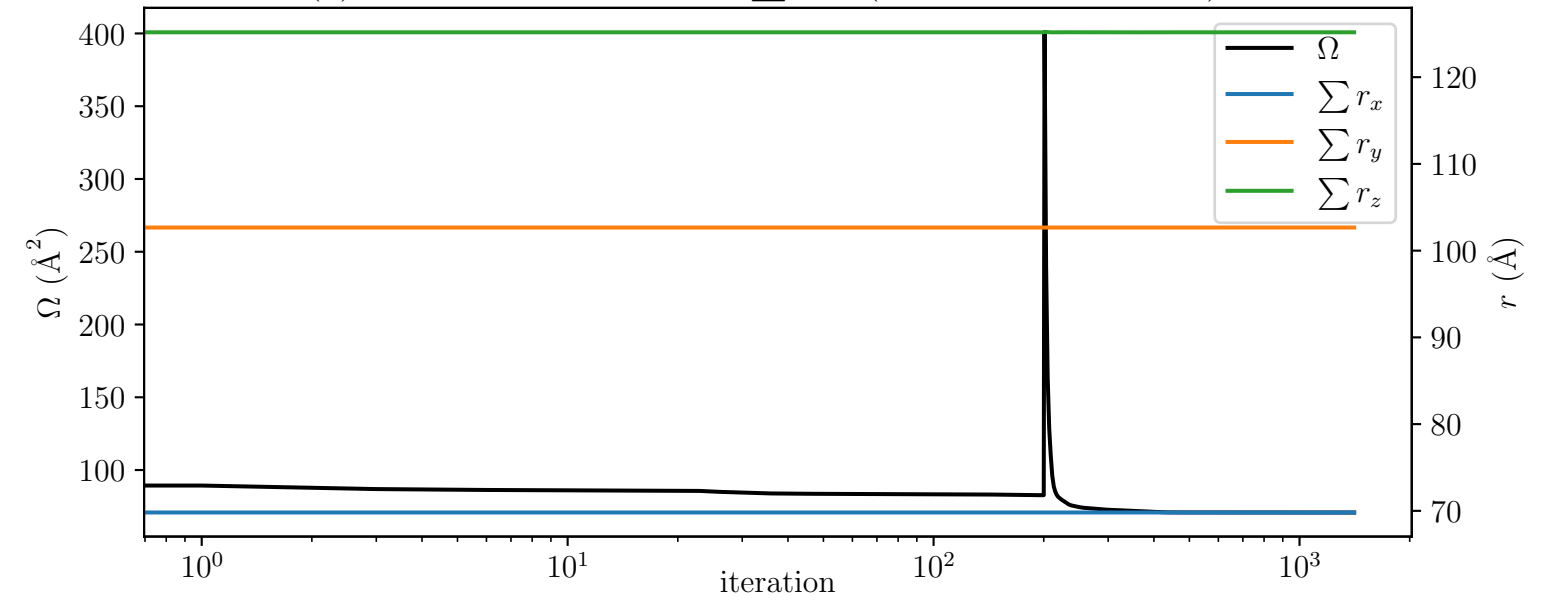
Se₄Tl₄ (**include** semicore)
PW AiiDA UUID: 9a1af3cc-017a-4e82-a65b-f8546931f7bb
W90 AiiDA UUID: 59b9dd26-b31c-4409-9391-4c9ac276f260



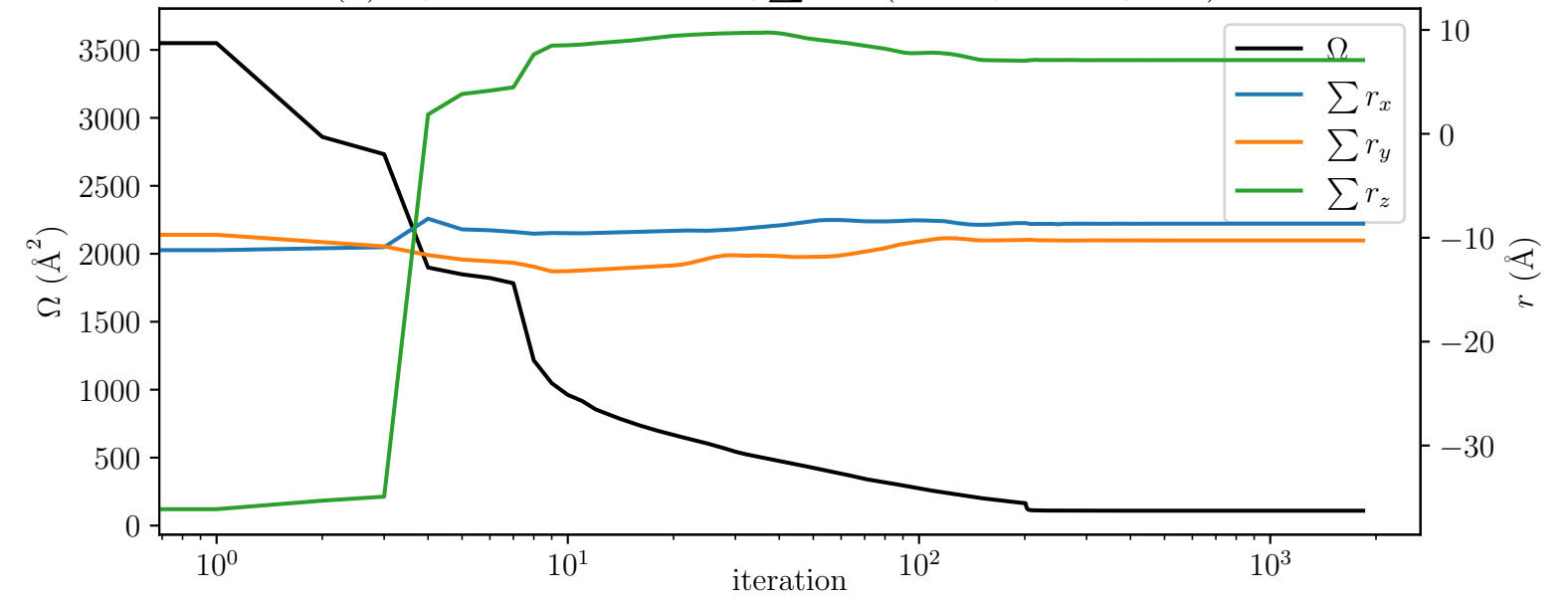
band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.2	1.0	10.9	11.0	2.4	24.6	12.9
η_{max}	10.1	7.2	204.3	203.9	10.1	145.7	152.1

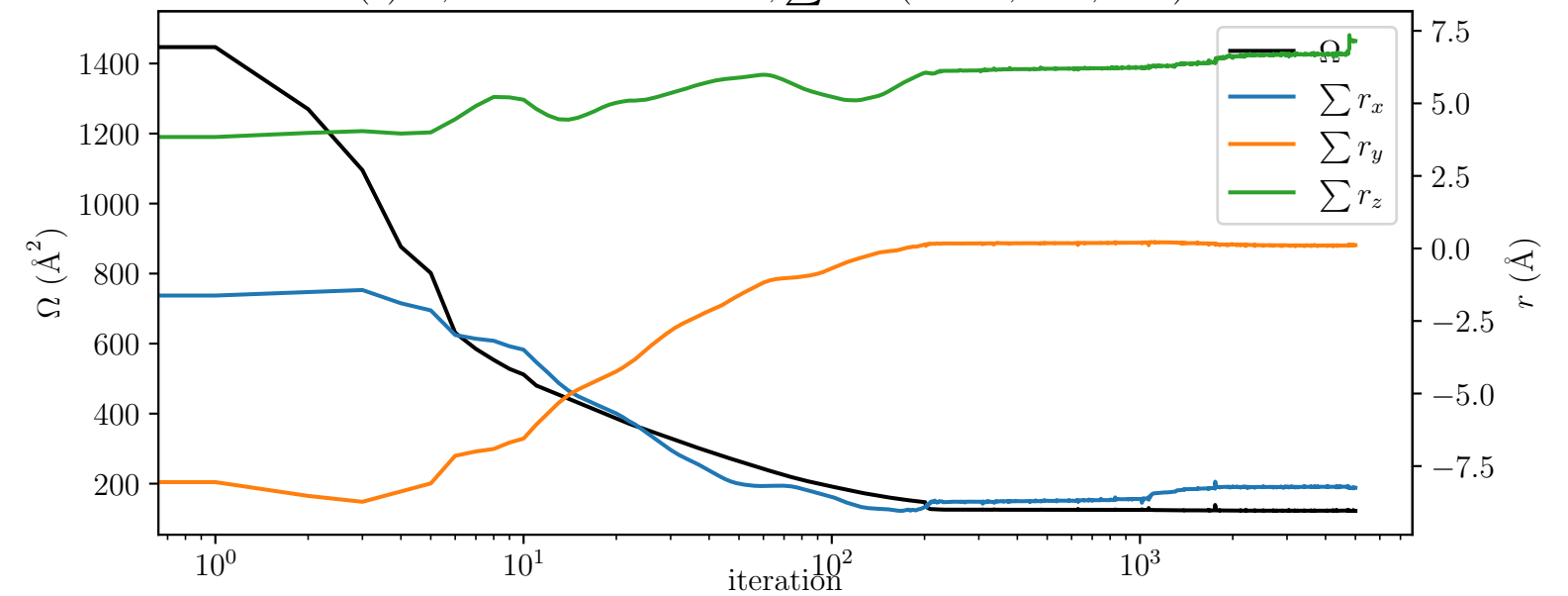
(a) VC; final $\Omega = 70.79 \text{\AA}^2$, $\sum r = (69.81, 102.67, 125.17) \text{\AA}$



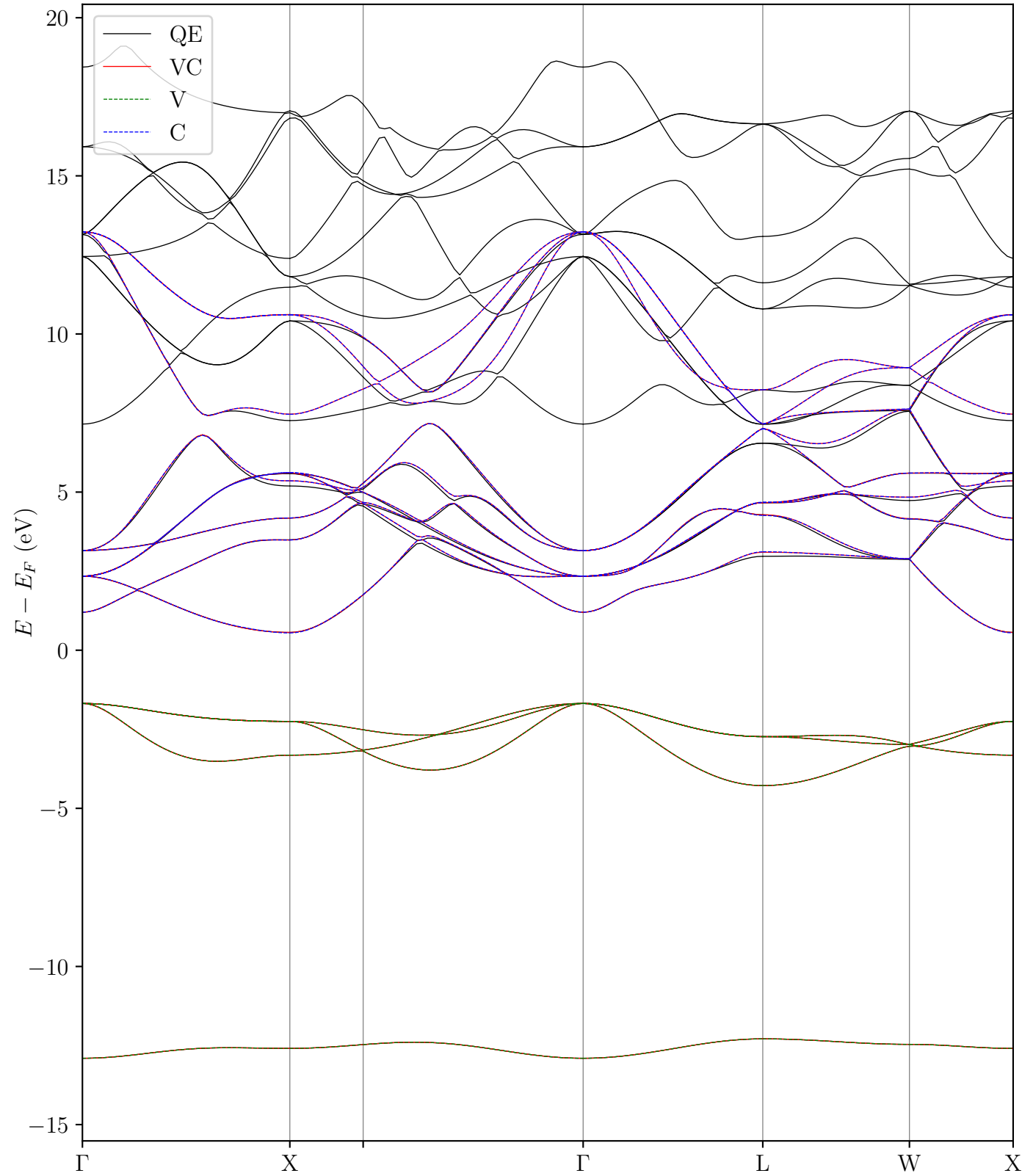
(b) V; final $\Omega = 109.43 \text{\AA}^2$, $\sum r = (-8.65, -10.26, 7.10) \text{\AA}$



(c) C; final $\Omega = 122.27 \text{\AA}^2$, $\sum r = (-8.25, 0.11, 7.15) \text{\AA}$



SeSr (exclude semicore)
PW AiiDA UUID: b5ac4414-c04f-4a9b-a1ae-745b5f35a655
W90 AiiDA UUID: 2ab87ed2-a8d5-4a83-91a3-28a93be1deb4



band distance (meV)

	VC-QE	V(VC)-QE	V-QE	V-VC	C(VC)-QE	C-QE	C-VC
	η_2	η_{isolated}	η_{isolated}	η_{isolated}	η_2	η_2	η_{isolated}
η	1.7	1.2	0.9	1.8	3.7	6.9	4.6
η_{max}	11.0	5.2	5.3	9.8	11.0	15.6	20.8

