# Equivalence of charged and neutral density functional formulations for correcting the many-body self-interaction of polarons

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## I. RESULTS OBTAINED WITH UNIT-CELL METHOD FOR POLARONS

We illustrate the results obtained with the unit-cell method for the various polarons considered in this work. Specifically, in Fig. S1 we show the generalized Fourier amplitudes $A_{n\mathbf{k}}$ and $B_{\mathbf{q}\eta}$, which describe the polaron wave function and the polaron lattice distortions, respectively. The strongly localized nature of small polarons is emphasized by the fact that the coefficients $A_{n\mathbf{k}}$ are spread across the entire Brillouin zone. Similarly, the localized nature of polaronic lattice distortions is related to the fact that the coefficients $B_{\mathbf{q}\eta}$ are spread across the phonon dispersion. In addition, we show in Fig. S1 the extrapolations of polaron formation energies for increasing $\mathbf{k}$ meshes, which are used to determine the polaron formation energies in the dilute limit.

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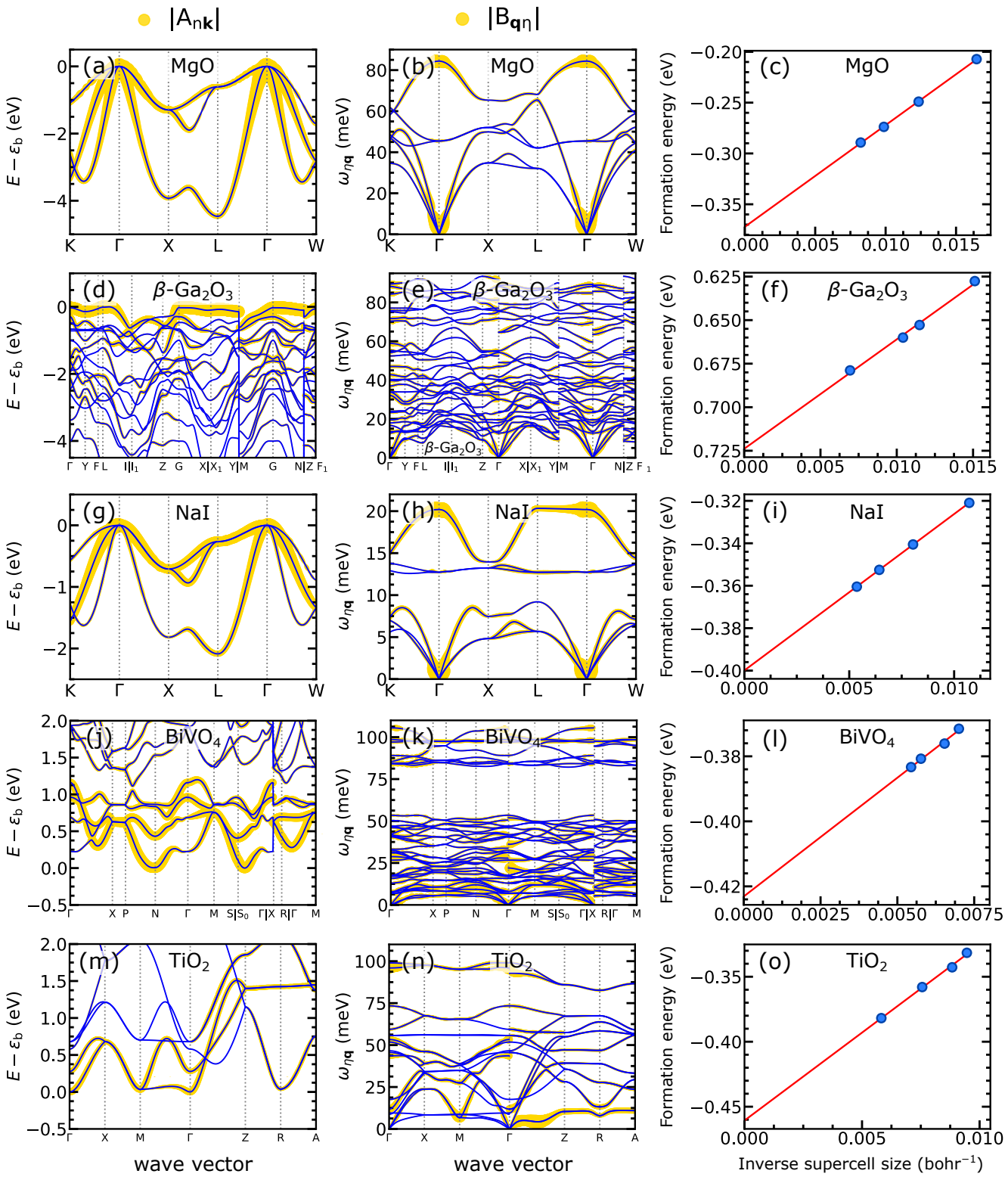


FIG. S1. Spectral decomposition of small polarons in MgO, $\beta$-$Ga_2O_3$, NaI, $BiVO_4$, and $TiO_2$ as obtained with the unit-cell method. (a,d,g,j,m) Generalized Fourier amplitudes $A_{n\mathbf{k}}$ plotted as circles on top of the band structure, with a radius proportional to $|A_{n\mathbf{k}}|^2$. Energies are referred to the top of the valence band for hole polarons, and to the top of the conduction band for electron polarons. (b,e,h,k,n) Generalized Fourier amplitudes $B_{\mathbf{q}\eta}$ plotted as circles on top of the phonon dispersion, with a radius proportional to $|B_{\mathbf{q}\eta}|^2$. (c,f,i,l,o) Scaling with inverse supercell size $L^{-1}$ of the polaron formation energy obtained by using increasingly dense $\mathbf{k}$-point meshes. The formation energies in the dilute limit are found by linear extrapolation.