Supplemental Material for "*Ab initio* electron-phonon interactions in correlated electron systems"

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Additional derivations on the projector derivatives

The generalized projector $\hat{P}$ on the space of the localized atomic orbitals φ^I_m is defined as

$$\hat{P}^I_{m_2m_1} = \hat{S}|\varphi^I_{m_2}\rangle\langle\varphi^I_{m_1}|\hat{S}, \tag{1}$$

where m_1 and m_2 are magnetic quantum numbers, I is the atomic index, and $\hat{S}$ is the overlap operator in the ultrasoft (US) or projector-augmented-wave (PAW) framework, which is defined as

$$\hat{S} = 1 + \sum_{J\mu\nu} q^J_{\mu\nu}|\beta^J_\mu\rangle\langle\beta^J_\nu|. \tag{2}$$

In Eq. (2), β^J_μ and β^J_ν are the localized atom-centered projector functions for the US or PAW schemes, labeled by an atomic (J) and a state (greek letter) index, and the coefficients $q^J_{\mu\nu}$ are integrals of the augmentation functions $Q^J_{\mu\nu}(\mathbf{r})$:

$$q^J_{\mu\nu} = \int Q^J_{\mu\nu}(\mathbf{r})d\mathbf{r}. \tag{3}$$

The bare derivative of the generalized projector $\partial_{I\alpha}\hat{P}^I_{m_2m_1}$ with respect to a unit displacement of atom I in the direction α becomes [1]:

$$\partial_{I\alpha}\hat{P}^I_{m_2m_1} = |\partial_{I\alpha}(\hat{S}\varphi^I_{m_2})\rangle\langle\varphi^I_{m_1}|\hat{S} + \hat{S}|\varphi^I_{m_2}\rangle\langle\partial_{I\alpha}(\hat{S}\varphi^I_{m_1})|. \tag{4}$$

In Eq. (4), the derivatives $\partial_{I\alpha}(\hat{S}\varphi^I_{m_2})$ can be further expanded as:

$$|\partial_{I\alpha}(\hat{S}\varphi^I_{m_2})\rangle = \partial_{I\alpha}(\hat{S})\,|\varphi^I_{m_2}\rangle + \hat{S}\,|\partial_{I\alpha}(\varphi^I_{m_2})\rangle, \tag{5}$$

where [see Eq. (2)]

$$\partial_{I\alpha}(\hat{S}) = \sum_{\mu\nu} q^J_{\mu\nu}\Big[|\partial_{I\alpha}(\beta^J_\mu)\rangle\langle\beta^J_\nu| + |\beta^J_\mu\rangle\langle\partial_{I\alpha}(\beta^J_\nu)|\Big]. \tag{6}$$

The derivatives $\partial_{I\alpha}(\varphi^I_{m_2})$ and $\partial_{I\alpha}(\beta^J_\mu)$ can be computed efficiently in reciprocal space, as discussed in Ref. [1].

In the case of norm-conserving pseudopotentials, $\hat{S} = 1$ and thus Eqs. (1) and (4) simplify to

$$\hat{P}^I_{m_2m_1} = |\varphi^I_{m_2}\rangle\langle\varphi^I_{m_1}|, \tag{7}$$

and

$$\partial_{I\alpha}\hat{P}^I_{m_2m_1} = |\partial_{I\alpha}(\varphi^I_{m_2})\rangle\langle\varphi^I_{m_1}| + |\varphi^I_{m_2}\rangle\langle\partial_{I\alpha}(\varphi^I_{m_1})|. \tag{8}$$

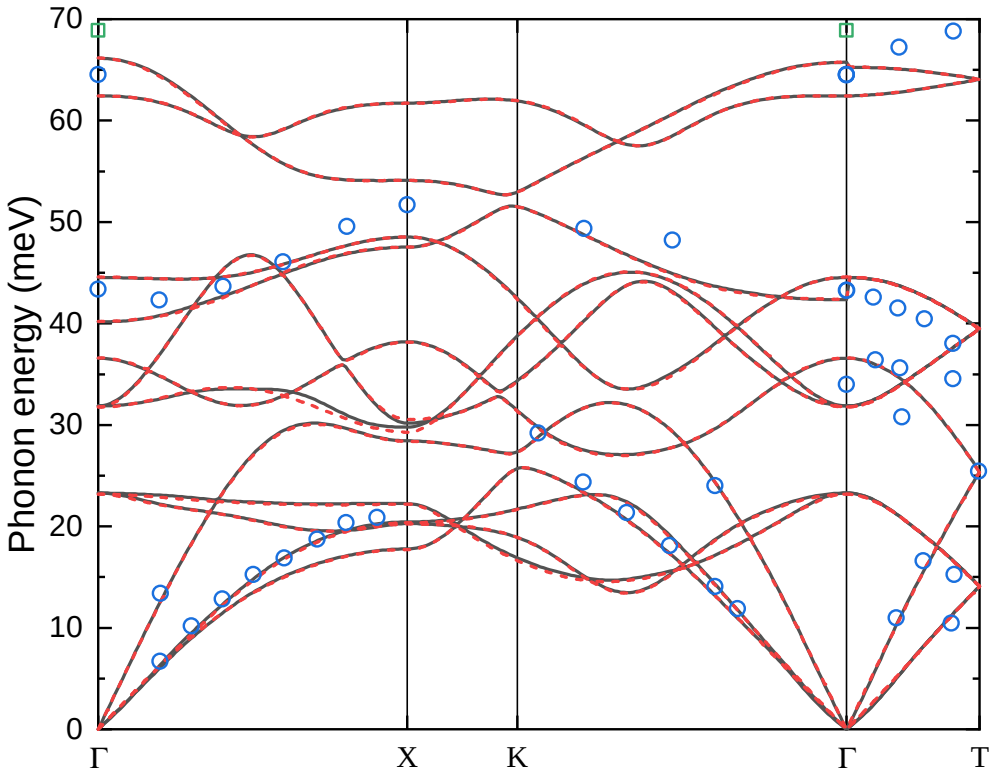

FIG. S1. CoO phonon dispersion in an equivalent (distorted) rock-salt cell. Shown are the DFPT+U results from our work (black solid line, $8 \times 8 \times 8$ coarse $\boldsymbol{q}$-point grid), DFPT+U results from Ref. [1] (red dashed line, $4 \times 4 \times 4$ coarse $\boldsymbol{q}$-point grid), and experimental results from Ref. [2] (blue circles) and Ref. [3] (green squares). Experimental data along the Γ-T direction were folded to account for the doubled periodicity of the four-atoms rhombohedral unit cell along the [111] direction [1].

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