Supplemental Material for “Ab initio electron-phonon interactions in correlated electron systems”

Jin-Jian Zhou,1,2,* Jinsoo Park,2,* Iurii Timrov,3 Andrea Floris,4 Matteo Cococcioni,5 Nicola Marzari,3 and Marco Bernardi2,†

1School of Physics, Beijing Institute of Technology, Beijing 100081, China.
2Department of Applied Physics and Materials Science, California Institute of Technology, Pasadena, CA 91125, USA.
3Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
4School of Chemistry, University of Lincoln, Brayford Pool, Lincoln LN6 7TS, United Kingdom
5Department of Physics, University of Pavia, Via A. Bassi 6, I-27100 Pavia, Italy
Additional derivations on the projector derivatives

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

\[
\hat{P}^I_{m2m1} = \hat{S}|\varphi^I_{m2}\rangle\langle\varphi^I_{m1}|\hat{S},
\]

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

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

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

\[
q^J_{\mu\nu} = \int Q^J_{\mu\nu}(r)dr.
\]

The bare derivative of the generalized projector \( \partial_I\alpha \hat{P}^I_{m2m1} \) with respect to a unit displacement of atom \( I \) in the direction \( \alpha \) becomes [1]:

\[
\partial_I\alpha \hat{P}^I_{m2m1} = |\partial_I\alpha (\hat{S}\varphi^I_{m2})\rangle\langle\varphi^I_{m1}| + |\varphi^I_{m2}\rangle\langle\partial_I\alpha (\hat{S}\varphi^I_{m1})|.
\]

In Eq. (4), the derivatives \( \partial_I\alpha (\hat{S}\varphi^I_{m2}) \) can be further expanded as:

\[
|\partial_I\alpha (\hat{S}\varphi^I_{m2})\rangle = \partial_I\alpha (\hat{S}) |\varphi^I_{m2}\rangle + \hat{S} |\partial_I\alpha (\varphi^I_{m2})|,
\]

where [see Eq. (2)]

\[
\partial_I\alpha (\hat{S}) = \sum_{\mu\nu} q^J_{\mu\nu} \left[ |\partial_I\alpha (\beta^J_{\mu})\rangle\langle\beta^J_{\nu}| + |\beta^J_{\mu}\rangle\langle\partial_I\alpha (\beta^J_{\nu})| \right].
\]

The derivatives \( \partial_I\alpha (\varphi^I_{m2}) \) 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

\[
\hat{P}^I_{m2m1} = |\varphi^I_{m2}\rangle\langle\varphi^I_{m1}|,
\]

and

\[
\partial_I\alpha \hat{P}^I_{m2m1} = |\partial_I\alpha (\varphi^I_{m2})\rangle\langle\varphi^I_{m1}| + |\varphi^I_{m2}\rangle\langle\partial_I\alpha (\varphi^I_{m1})|.
\]
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 $q$-point grid), DFPT+U results from Ref. [1] (red dashed line, $4 \times 4 \times 4$ coarse $q$-point grid), and experimental results from Ref. [2] (blue circles) and Ref. [3] (green squares). Experimental data along the $\Gamma$-T direction were folded to account for the doubled periodicity of the four-atoms rhombohedral unit cell along the $[111]$ direction [1].
* J.-J.Z. and J.P. contributed equally to this work
† Corresponding author: bmarco@caltech.edu

