

# Appendix to *First-principles calculation of electron-phonon coupling in doped $\text{KTaO}_3$*

Tobias Esswein\* and Nicola A. Spaldin†  
 Materials Theory, Department of Materials, ETH Zurich, Switzerland  
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This document contains data and information on the 2D to 3D charge carrier conversion, electronic band structures and numerical convergence of the calculations presented in the main text.

## A. Conversion between 2D and 3D carrier densities

The interpolation used for conversion between  $n_{2D}$  and  $n_{3D}$  carrier densities is shown in figure A1. It is based on data from figure S6 of the supplementary information of Ref. 1.

The corresponding interpolation formula is

$$n_{3D} [\text{cm}^{-3}] = 6.108 \times 10^{-3} \text{ cm}^{-1} * n_{2D}^{1.596} [\text{cm}^{-2}] .$$

According to this conversion, a 3D carrier concentration of  $1.4 \times 10^{20} \text{ cm}^{-3}$  corresponds to  $1.0 \times 10^{14} \text{ cm}^{-2}$ , and  $2 \times 10^{21} \text{ cm}^{-3}$  to  $5.4 \times 10^{14} \text{ cm}^{-2}$ .

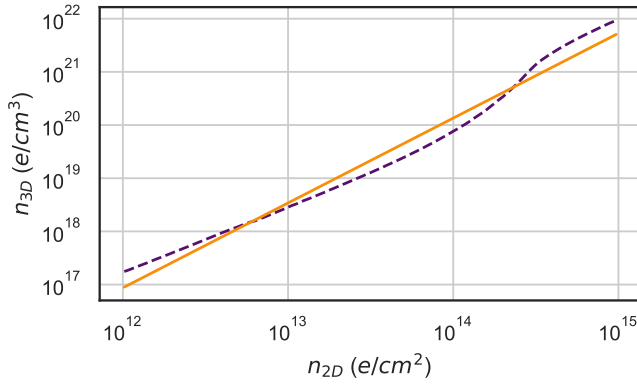


FIG. A1. Interpolation used for conversion between  $n_{2D}$  and  $n_{3D}$  carrier densities (solid lighter line), based on data for KTO from figure S6 of the supplementary information of Ref. 1 (dashed dark line). The corresponding interpolation formula is  $n_{3D} = 6.1078 \times 10^{-3} * n_{2D}^{1.5960}$ .

## B. Convergence with coarse q mesh

To test the convergence of our results, we calculate the phonons and the electron-phonon coupling strength  $\lambda$  along the same high-symmetry path using three different q meshes (q4 ( $4 \times 4 \times 4$ ), q6, and q8). Our results are shown in figure A2. The phonon frequencies at the high-symmetry points are well converged at q4, with only minor variations between q4 and q6 or q8. The colorscale is the same as that in Figure 2 of the main text. The

actual  $\lambda$  values are about twice as large in the q6 and q8 cases compared to the q4 case.

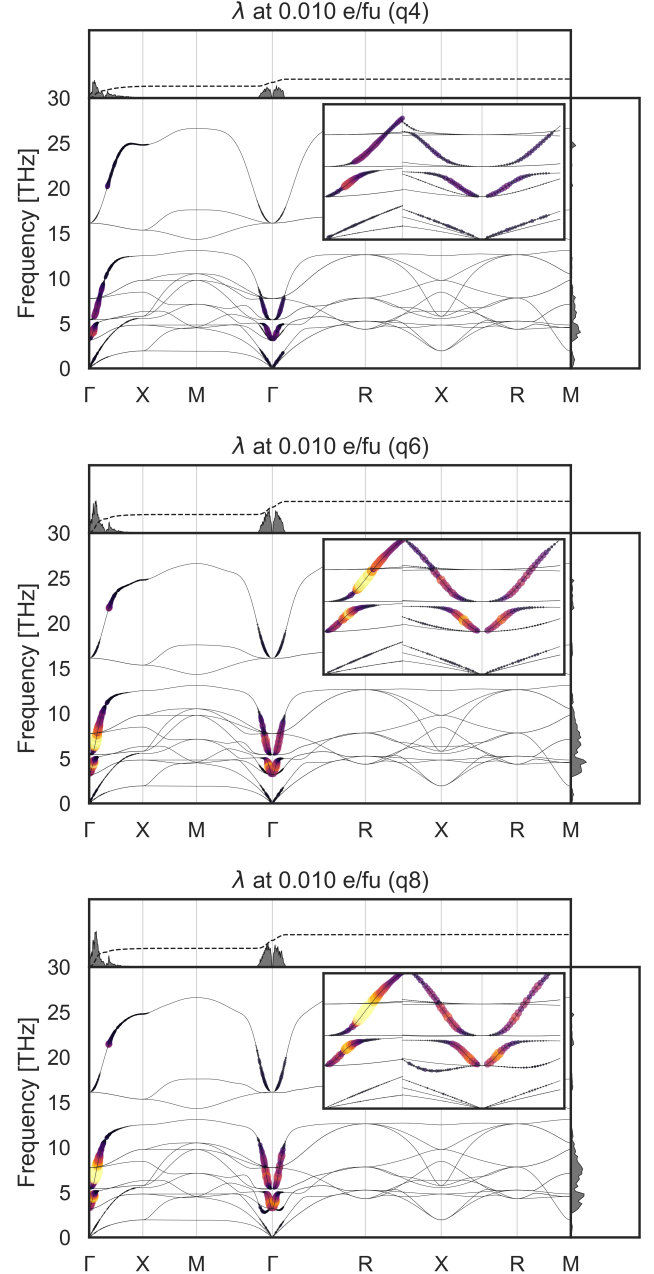


FIG. A2. Calculated phonon dispersion and mode-resolved electron-phonon coupling strength  $\lambda$  at a doping level of 0.01 e/fu for q4, q6 and q8 meshes (top to bottom).

\* tobias.esswein@mat.ethz.ch

† nicola.spaldin@mat.ethz.ch

### C. Decay properties in real space

The spatial decay of the electron-phonon matrix elements in real space for the same three  $q$  meshes is shown in figure A3 (see Refs. 2 and 3 for more details). We observe a decay of the phonon perturbation of almost three orders of magnitude using all three meshes. The  $q6$  and  $q8$  meshes flatten after the decay, without further lowering the lowest value reached using the  $q4$  mesh, indicating that the  $q4$  mesh is accurate enough for the qualitative comparison we make. The decay of the electronic Wannier functions is well converged using the  $24 \times 24 \times 24$  coarse  $k$ -point mesh, as can be seen from the bottom right panel of figure A3.

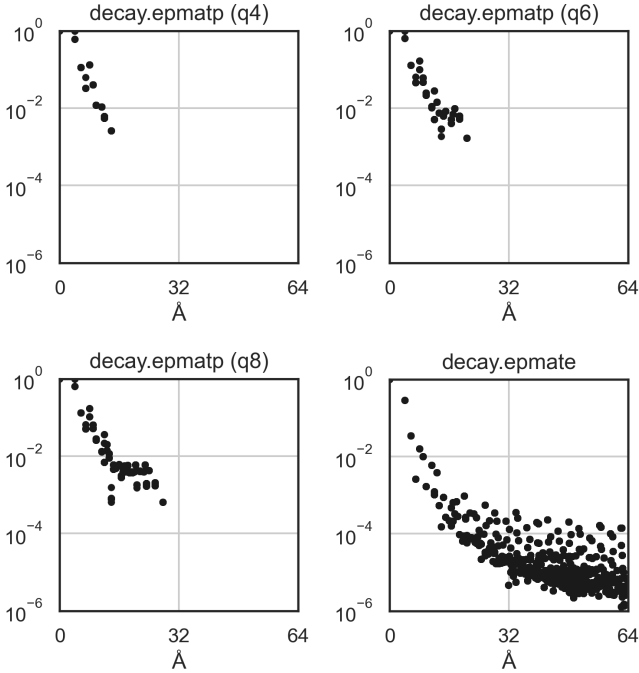


FIG. A3. Decay of the phonon perturbation part of the electron-phonon matrix elements in real space for  $4 \times 4 \times 4$  ( $q4$ ),  $6 \times 6 \times 6$  ( $q6$ ) and  $8 \times 8 \times 8$  ( $q8$ )  $q$  meshes (top left, top right and bottom left) and the electronic Wannier functions (bottom right), using a  $24 \times 24 \times 24$   $k$  mesh.

### D. Electronic band structure with and without spin-orbit coupling

Figure A4 shows our calculated electronic band structure of non-polar (upper panel) and polar (lower panel)

KTO without and with spin-orbit coupling, corresponding to Figure 4 in the main text.

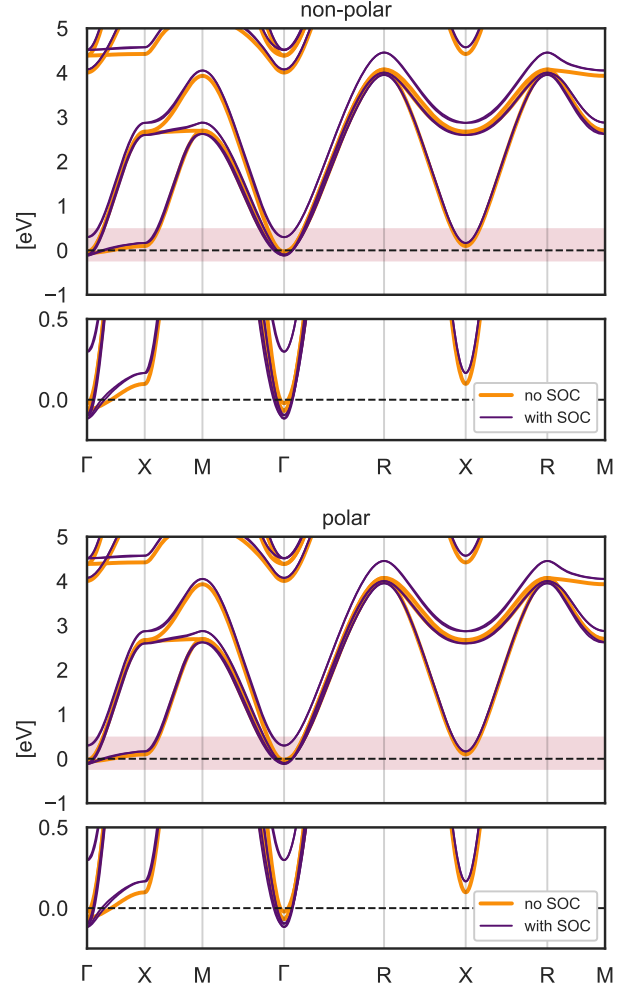


FIG. A4. Electronic bands of non-polar (upper plots) and polar (lower plots) KTaO<sub>3</sub> without and with spin-orbit coupling (SOC), aligned at their respective Fermi energies (dashed lines) as calculated from the fine  $k$  mesh. A band splitting of 400 meV from SOC is observed in both cases. The polar band width is smaller due to the increases lattice constant necessary to stabilize the [111]-polar structure. The narrower bottom panel in each subplot is a zoom on the shaded region of each main panel

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