Tight-Binding Model of $TaSe_2$

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2H-$TaSe_2$ is a metallic layered transition metal dichalcogenide which, similarly to $NbSe_2$, hosts charge-density waves (CDW). In this material, these states are well-separated in the phase diagram from superconductivity providing a platform to study the physics intrinsic to CDW. We construct a Slater-Koster orbital basis tight-binding model for bulk 2H-$TaSe_2$ which reveals that around the Fermi energy contribution of the Ta $d_{3z^2-r^2}$ states dominates over those of other orbitals. Based on this, we develop an effective two-band model which we use to calculate the electron-phonon coupling following the approach in Ref. [1]. This, in turn, allows us to study the generalized static electronic susceptibility which peaks at the CDW wave vector in agreement with experiment [2].

References

[1] Varma, C. M., Blount, E. I., Vashishta, P. & Weber, W. Electron-phonon interactions in transition metals, *Phys. Rev. B* **19**, 6130–6141 (1979).
[2] Li, Y. W. *et al.* Folded superstructure and degeneracy-enhanced band gap in the weak-coupling charge density wave system 2H-TaSe2. *Phys. Rev. B* **97**, 115118 (2018).

Figures

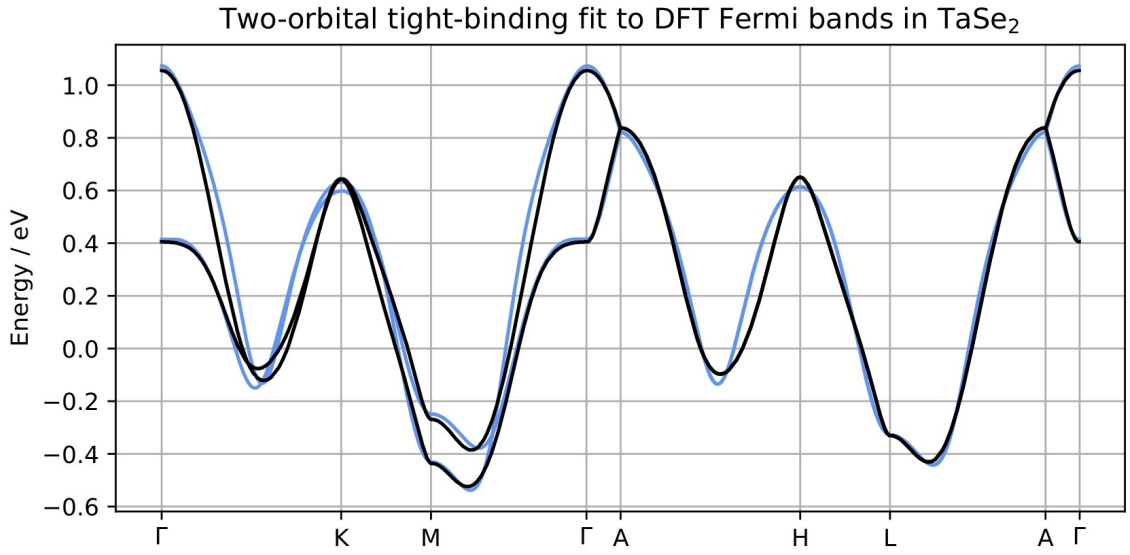

Figure 1: Two-orbital Slater-Koster tight-binding model, in blue, fitted to non-relativistic ab initio bandstructure for bulk $TaSe_2$, shown in black, optimized using a Monte Carlo method.