Wannier-Based Tight-Binding Modelling of Spin properties of pentagonal $PdSe_2$

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Two-dimensional materials have attracted significant attention due to their tunable electronic properties and potential applications in next-generation devices. Among them, $PdSe_2$ has emerged as a promising system due to its intrinsic anisotropy and unique electronic structure.

In this work, we investigate the electronic properties of monolayer $PdSe_2$ using *ab initio* calculations based on density functional theory. Particular attention is devoted to the analysis of the band structure and the orbital character of the states near the Fermi level, where strong hybridization between Se *p* and Pd *d* orbitals is observed.

To gain deeper insight and enable efficient modelling, we construct a Wannier-based tight-binding Hamiltonian by projecting the *ab initio* bands onto a minimal set of localized orbitals. This approach preserves the essential physics while significantly reducing computational cost. We show that a nearest-neighbor model with eight Wannier orbitals accurately reproduces the key features of the band dispersion.

Finally, we analyse the origin of the anisotropic electronic behaviour and discuss how the developed model can be used to study transport properties and other emergent phenomena in $PdSe_2$-based systems.

References

[1] J. F. Sierra, J. Světlík, W. Savero Torres, L. Camosi, F. Herling, T. Guillet, K. Xu, J. S. Reparaz, V. Marinova, D. Dimitrov, and S. O. Valenzuela, Nature Materials 24 (2025) 876–882
[2] X. Wang, G. Niu, J. Jiang, L. Sui, X. Zeng, X. Liu, Y. Zhang, G. Wu, K. Yuan, and X. Yang, Nano Letters 24 (2024) 9058–9064
[3] E. A. Moujaes and A. C. Dias, Journal of Physics and Chemistry of Solids 182 (2023) 111573
[4] F. Florio, M. Camanas-Gómez, G. Ohad, D. Naveh, L. Kronik, and A. Ramasubramaniam, Applied Physics Letters 126 (2025) 143101
[5] T. Olsen, E. Andersen, T. Okugawa, D. Torelli, T. Deilmann, and K. S. Thygesen, Physical Review Materials 3 (2019) 024005
[6] S. Bravo, M. Pacheco, J. D. Correa, and L. Chico, Physical Chemistry Chemical Physics 24 (2022) 15749–15755
[7] L. Elcoro, Z. Song, and B. A. Bernevig, Physical Review B 102 (2020) 035110
[8] J. Qiao, J. Zhou, Z. Yuan, and W. Zhao, Physical Review B 98 (2018) 214402
[9] P. Miró, M. Audiffred, and T. Heine, Chemical Society Reviews 43 (2014) 6537–6554
[10] D. Qin, P. Yan, G. Ding, X. Ge, H. Song, and G. Gao, Scientific Reports 8 (2018) 2764

Figures

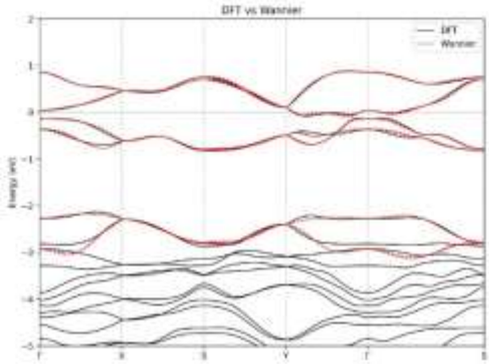

Figure 1: Comparison between *ab initio* DFT band structure (black solid lines) and the Wannier-interpolated tight-binding model for monolayer $PdSe_2$ along high-symmetry directions.