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T715: Modeling and simulation of nanoscale materials, structures and devices

Topological bands in the $PdSe_2$ pentagonal monolayer

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In this presentation a theoretical study of the topological features of pentagonal Palladium diselenide ($PdSe_2$) in its monolayer form will be developed. As a recently synthesized transition metal dichalcogenide, pentagonal $PdSe_2$ is an appealing platform to explore the interplay of reduced dimensionality, low crystalline symmetry, electronic correlations, and topological effects.

By means of first-principles calculations, using density functional theory along with topological quantum chemistry theory, we present a panorama of the symmetry-indicated electronic band topology of the material. A group of bands with strong topology is identified in the set of the low-lying conduction bands and an associated possible physical response is discussed, as presented in [1]. Also, the valence band manifold of the system is analyzed and an obstructed atomic phase is spotted. This novel phase is linked to a higher-order type of nontrivial topology and the presence of corner states and charges realizing a bulk-boundary correspondence is addressed.

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References

[1] Bravo S. et al. (2022), doi.org/10.1039/D2CP01822E