

Abstract Submitted
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Boundary conditions for transition-metal dichalcogenide monolayers in the continuum model CSABA G. PÉTERFALVI, ANDOR KORMÁNYOS, GUIDO BURKARD, Department of Physics, University of Konstanz, D-78464 Konstanz, Germany — We derive the boundary conditions for MoS₂ and similar transition-metal dichalcogenide honeycomb (2H polytype) monolayers with the same type of $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian within the continuum model around the K points. [1] In an effective 2-band description, the electron-hole symmetry breaking quadratic terms are also taken into account. We model the effect of the edges with a linear edge constraint method that has been applied previously to graphene. Focusing mainly on zigzag edges, we find that different reconstruction geometries with different edge-atoms can generally be described with one scalar parameter varying between 0 and 2π . We analyze the edge states and their dispersion relation in MoS₂ in particular, and we find good agreement with the results of previous density functional theory calculations for various edge types.

[1] Cs. G. Péterfalvi, A. Kormányos, G. Burkard, arXiv:1509.00184 (2015).

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