Abstract Submitted
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A tight-binding model for MoS_2 monolayers[1] EMILIA RIDOLFI, Universidade Federal Fluminense, DUY LE, TALAT RAHMAN, EDUARDO MUCCIOLO, University of Central Florida, CAIO LEWENKOPF, Universidade Federal Fluminense — We propose an accurate tight-binding parametrization for the band structure of MoS_2 monolayers near the main energy gap. We introduce a generic and straightforward derivation for the band energies equations that could be employed for other monolayer dichalcogenides. A parametrization that includes spinorbit coupling is also provided. The proposed set of model parameters reproduce both the correct orbital compositions and location of valence and conductance band in comparison with ab initio calculations. The model gives a suitable starting point for realistic large-scale atomistic electronic transport calculations.

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