Abstract Submitted
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Slater-Koster Tight-Binding parametrization of single and few-layer Black-Phosphorus from first-principles calculations[1] MARCOS MENEZES, RODRIGO CAPAZ, Instituto de Fsica, Universidade Federal do Rio de Janeiro — Black Phosphorus (BP) is a promising material for applications in electronics, especially due to the tuning of its band gap by increasing the number of layers. In single-layer BP, also called Phosphorene, the P atoms form two staggered chains bonded by sp^3 hybridization, while neighboring layers are bonded by Van-der-Waals interactions. In this work, we present a Tight-Binding (TB) parametrization of the electronic structure of single and few-layer BP, based on the Slater-Koster model within the two-center approximation. Our model includes all 3s and 3p orbitals, which makes this problem more complex than that of graphene, where only 2pz orbitals are needed for most purposes. The TB parameters are obtained from a least-squares fit of DFT calculations carried on the SIESTA code. We compare the results for different basis-sets used to expand the ab-initio wavefunctions and discuss their applicability. Our model can fit a larger number of bands than previously reported calculations based on Wannier functions. Moreover, our parameters have a clear physical interpretation based on chemical bonding. As such, we expect our results to be useful in a further understanding of multilayer BP and other 2D-materials characterized by strong sp^3 hybridization.

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Marcos Menezes
Universidade Federal do Rio de Janeiro

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