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An Accurate and Compact Tight-binding Model for Phosphorene

CARLOS PAEZ, ANA PEREIRA, University of Campinas, EDUARDO MUCCIOLO, University of Central Florida — In recent years, a variety of tight-binding models have been proposed for phosphorene. Although capturing key features such as the main band gap and the effective masses near the gamma point, they are not sufficiently accurate for the determination of electronic transport properties, particularly when probing states near the vicinity of extreme points of the valence and conductance bands. We propose a new tight-binding model parameterization based on the hybridization of s and p orbitals. For that purpose, we use theslater-koster method to construct a four-band model. We optimized the tight-binding parameters to fit the main features of ab-initio electronic band structure calculations and to reproduce the correct orbital composition at high-symmetry and low-symmetry points. Using this new tight-binding model, we compute some electronic transport properties of phosphorene ribbons in the presence of disorder.

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