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Disorder effect on the anisotropic resistivity of phosphorene determined by a tight-binding model CARLOS PAEZ, Universidade Estadual de Campinas, KURSTI DELELLO, DUY LE, University of Central Florida, ANA PEREIRA, Universidade Estadual de Campinas, EDUARDO MUCCIOLO, University of Central Florida — In this work we develop a compact multi-orbital tight-binding model for phosphorene that accurately describes states near the main band gap[1]. The model parameters are adjusted using as reference the band structure obtained by a density-functional theory calculation with the hybrid HSE06 functional. We use the optimized tight-binding model to study the effects of disorder on the anisotropic transport properties of phosphorene. In particular, we evaluate how the longitudinal resistivity depends on the lattice orientation for two typical disorder models: dilute scatterers with high potential fluctuation amplitudes, mimicking screened charges in the substrate, and dense scatterers with lower amplitudes, simulating weakly bounded adsorbates. We show that the intrinsic anisotropy associated to the band structure of this material, although sensitive to the type and intensity of the disorder, is robust. [1] Paez et al. Physical Review B, 94 (16) 165419 (2016)

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