Multi-scale approach for strain-engineering of phosphorene

Dr. Alexander Croy

Abstract

A multi-scale approach for the theoretical description of deformed phosphorene is presented. This approach combines a recently developed valence-force model [1] to relate macroscopic strain to microscopic displacements of atoms and a tight-binding model [2] with distance-dependent hopping parameters to obtain electronic properties. The resulting self-consistent electromechanical model is suitable for large- scale modeling of phosphorene devices. We demonstrate this for the case of an inhomogeneously deformed phosphorene drum, which may be used as an exciton funnel [3]

[1] D. Midtvedt and A. Croy, Phys. Chem. Chem. Phys. 18, 23312 (2016).
[2] A. N. Rudenko, S. Yuan, and M. I. Katsnelson, Phys. Rev. B 92, 085419 (2015).
[3] P. San-Jose et al, Phys. Rev. X 6, 031046 (2016).