

Black Phosphorus and Phosphorene Properties From DFT and TD-DFT

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ABSTRACT

The successful exfoliation of bulk black phosphorus into monolayer and few-layer black phosphorus, also known as ‘ α -phosphorene’, has triggered intense interests in the nanoscience community. This is mainly related to the rather unusual in-plane anisotropy and thickness-dependent direct band gap of phosphorene, resulting in novel and intriguing properties with potential applications in optoelectronics, photovoltaic, and thermoelectrics. [1, 2, 3] In this contribution, we present a detailed investigation of the structural, vibrational, electronic and optical properties of bulk and few-layer black phosphorus, using a computational protocol combining periodic hybrid DFT with TD-DFT applied to non-periodic models embedded in an array of point charges devised to reproduce the periodic electrostatic environment. Our work not only provides a better understanding of the fundamental properties of bulk phosphorus and phosphorene, but also paves the way to the investigation of triphosphides-based van der Waals heterostructures with strong interlayer coupling.

References

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