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Low-Dimensional Semiconductors beyond Graphene: An Insight from Theory*

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Abstract

If graphene had a band gap, it would probably be the optimum 2D system for electronics applications. Layered transition metal dichalcogenides (TMDs) with a robust intrinsic band gap appear as the next-best alternative. Only after a long search, however, optimum strategies have been devised to make low-resistance, ohmic contacts to TMDs [1]. In the meantime, a new class of 2D semiconductors has been rapidly gaining attention, namely layered black phosphorus and related phosphorene monolayers [2]. These 2D systems display a tunable, direct fundamental band gap and thus are ideal candidates for optoelectronics applications. Recent Quantum Monte Carlo (QMC) calculations show that the inter-layer bonding, while weak, is not well described by dispersive van der Waals (vdW) interactions [3]. As seen in Fig. 1, QMC results differ qualitatively from vdW-enhanced DFT functionals and the common designation of similar systems as "van der Waals solids" is strictly incorrect. Also other group V systems including monolayers of As_xP_{1-x} [4], IV-VI compounds such as SiS [5] with the same average valence, and related 2D phosphorus carbide [6] share the same nonplanarity of their structure with phosphorene. Same as in phosphorene, the fundamental band gap in these systems depends sensitively on the number of layers and in-layer strain. Predictive *ab initio* calculations provide here a useful guidance to experimental studies.

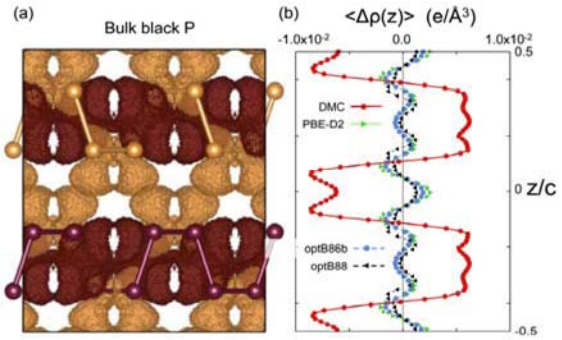

FIG.1. Calculated electron density difference $\Delta\rho=\rho_{tot}(bulk)-\Sigma\rho_{tot}(monolayers)$ representing the charge redistribution caused by assembling the bulk structure from isolated monolayers. (a) Diffusion Monte Carlo (DMC) isosurfaces bounding regions of excess electron density (dark brown) and electron deficiency (light brown), with respective values $\pm 6.5\times10^{-3}$ e/Å^3. (b) $<\Delta\rho(z)>$ for DMC and selected DFT functionals averaged across the *x*−*y* plane of the layers, with *z/c* indicating the relative position of the plane in the unit cell. (From Ref. [2]).

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References:

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