UNUSUAL 2D SEMICONDUCTORS BEYOND GRAPHENE: AN INSIGHT FROM THEORY

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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]. 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. These systems share another similarity with phosphorene, namely the dependence of the fundamental band gap on the number of layers and in-layer strain. Predictive *ab initio* calculations provide here a useful guidance to experimental studies.

Partly supported by the NSF/AFOSR EFRI 2-DARE grant number #EFMA-1433459.

Keywords: phosphorene, ab initio calculations, band gap

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