

Abstract Submitted
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Electronic Structures of Single-Layer Boron Pnictides HOULONG

L. ZHUANG, RICHARD G. HENNIG, Department of Materials Science and Engineering, Cornell University — Single layered materials such as graphene and boron nitride promise alternative routes to electronic devices. We use density-functional calculations to identify potential novel 2D materials in the boron pnictide family and determine their stability and electronic properties.¹Hybrid density functional calculations show that BN, BP, BAs and BSb in this family exhibit a direct bandgap of 6.1, 1.4, 1.2 and 0.6 eV, respectively, that originates from the energy difference of the p_z orbitals of the species and is tunable by strain. The bandgap linearly decreases with strain for BN, while it increases non-linearly for BP, BAs, and BSb. The calculated natural band offsets between the various boron pnictides are all of type I. We expect that these results will provide valuable guidance in designing electronic devices based on single-layer boron pnictides.

¹H. L. Zhuang and R. G. Hennig. Appl. Phys. Lett., **101**, 153109 (2012)

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