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Tunable and Sizable Band Gap of Single Layer Graphene Sandwiched between Hexagonal Boron Nitride JIAXIN ZHENG, HERUGE QU, QIHANG LIU, RUI QIN, JING ZHOU, DAPENG YU, ZHENGXIANG GAO, JING LU, State Key Laboratory of Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, GUANGFU LUO, SHIGERU NAGASE, Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Okazaki 444-8585, Japan, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266, USA —
It is a big challenge to open a tunable and sizable band gap of single layer graphene without big loss in structural integrity and carrier mobility. By using density functional theory calculations, we show that the band gap of single layer graphene can be opened to 0.16 (without electrical field) and 0.34 eV (with a strong electrical field) when sandwiched between two hexagonal boron nitride single layers in a proper way. The zero-field band gaps are increased by about 50% when many-body effects are included. Ab initio quantum transport simulation of a dual-gated FET out of such a sandwich structure further confirms an electrical field-enhanced transport gap. The tunable and sizeable band gap and structural integrity render this sandwich structure a promising candidate for high-performance single layer graphene field effect transistors.

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