

First-principles simulations of Graphene/Transition-metal-Dichalcogenides/Graphene Field-Effect Transistor

Xiang-Guo Li, Yun-Peng Wang, X.-G. Zhang and Hai-Ping Cheng

Department of Physics and Quantum Theory Project, University of Florida, Gainesville,
Florida 32611, USA

A prototype field-effect transistor (FET) with fascinating properties can be made by assembling graphene and two-dimensional insulating crystals into three-dimensional stacks with atomic layer precision. Transition metal dichalcogenides (TMDCs) such as WS₂, MoS₂ are good candidates for the atomically thin barrier between two layers of graphene in the vertical FET due to their sizable bandgaps. We investigate the electronic properties of the Graphene/TMDCs/Graphene sandwich structure using first-principles method. We find that the effective tunnel barrier height of the TMDC layers in contact with the graphene electrodes has a layer dependence and can be modulated by a gate voltage. Consequently a very high ON/OFF ratio can be achieved with appropriate number of TMDC layers and a suitable range of the gate voltage. The spin-orbit coupling in TMDC layers is also layer dependent but unaffected by the gate voltage. These properties can be important in future nanoelectronic device designs.

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