First-principles study of Graphene/Transition metal dichalcogenide/Graphene Field-Effect Transistors

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Tunneling field-effect transistor (TFET) formed from atomic precision three-dimensional stacks of graphene and two-dimensional insulating crystals of a few atomic layers in thickness can have extraordinary properties. Good candidates for barrier layer materials in such a vertical TFET are transition metal dichalcogenides (TMDCs) such as WS_2 and MoS_2 due to their sizable bandgaps. We report first-principles study of the electronic properties of the Graphene/WS_2/Graphene and Graphene/MoS_2/Graphene sandwich structures revealing a high ON/OFF ratio with an appropriate number of atomic layers of the barrier material and a suitable range of the gate voltage. For both WS_2 and MoS_2 barrier layers, when the stack is in contact with the graphene electrodes the effective barrier height varies with layer thickness and can be reduced by a gate voltage. Layer thickness also affects the band splitting due to spin-orbit coupling and the dielectric constant of the WS_2 layer, making the latter slightly lower than that of bulk WS_2. These properties can be valuable in future nanoelectronic device designs.

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