First principle study on the electronic properties and Schottky contact of graphene adsorbed on MoS_2 monolayer under applied out-plane strain

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Highlights

- Effects of interlayer distance on structural and electronic properties of Graphene/MoS2 heterointerface is studied using DFT calculations.
- A narrow band gap of 3.6 meV has opened in G/MoS2 heterointerface, and it can be modulated by the interlayer distance.
- The Schottky barrier and Schottky contact types in the G/MoS2 heterointerface can be controlled by the interlayer distance.
- The transition from n-type to p-type Schottky contact is occurred at d= 2.74 Å.
- Our studies may prove to promote the application of ultrathin G/MoS2 heterointerface in the next-generation nanoelectronic and photonic devices.