

Structural and electronic properties in the graphene/MoS₂ heterostructure

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Abstract

Graphene is one of the most promising materials for future electronics. Due to its specific bandstructure, its charge carrier mobility is very important, in addition to its thermal conductivity and its high mechanical resistance. Therefore, these properties open the way to the elaboration of graphene based electronic devices like field-effect transistors (FET).

The design of graphene-based FET goes through the elaboration of heterostructures where graphene is associated to other materials in order to create interface Schottky barrier. For example, MoS₂ represents an interesting candidate for the creation of such new heterostructure. However, this heterostructure equilibrium is ruled by van der Waals interactions, as there exist in supramolecular chemistry, graphitic materials (graphene, carbon nanotubes, ...) or biological membranes for example. The modeling of such interactions is of high fundamental interest to determine the interface electronic properties.

From the last numerical developments to describe van der Waals interactions in the frame of Density Functional Theory (DFT), we aim at studying different possible configurations of graphene/MoS₂ heterostructures, by considering different rotation angles between the graphene and the MoS₂ monolayers. To characterize these properties, we proceed to electronic density (DOS) and charge transfer calculations as well as current determination perpendicular to the interface from a Keldysh-Green formalism implemented in DFT.

Moreover, this system could be refined or modulated by considering graphene/MoS₂ multilayers (sandwich-like systems) or atom or molecules intercalation to modulate the graphene electronic properties.

References

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