Electronic Structure of MoSe₂/Graphene Van der Waals Heterostructures: an ab-initio Study

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1. Introduction

Two-dimensional layered Transition Metal Dichalcogenides (TDMs), especially MoS₂, are promising materials for developing a new class of optoelectronic devices due to their high photosensitivity, which is the result of its indirect to direct band gap transition when the bulk dimension is reduced to a single monolayer. using a commercial software package named Materials Studio, which is developed by Accelrys Inc. This software includes the modules DMol3 and CASTEP, that use DFT with a numerical radial function basis and with a plane wave basis set. We theoretically investigate the electronic structure of a van der Waals heterojunctions formed between single layers of MoSe₂ and graphene. The present study may shedding light on essential features such as doping, Fermi velocity, hybridization, and band-offset of the low energy electronic dynamics found at the interface.

2. Methodology

The DFT calculations presented here were carried out using a commercial software package named Materials Studio, which is developed by Accelrys Inc. This software includes the modules DMol3 and CASTEP, that use DFT with a numerical radial function basis and with a plane wave basis set, respectively, to calculate the electronic properties of molecules, clusters, surfaces and crystalline solid materials from first principles. Here we calculate the electronic and optical properties of MoSe₂/Graphene heterojunctions by using the methods LDA/PW91 and GGA/PBE on DFT, as implemented in the modules CASTEP and DMol3.

3. Results

Based on the DFT calculations, we investigate the electronic band structures of MoSe₂/Graphene heterojunctions. The results show that there is a non-uniform strain between two different orientation angles of MoSe₂ monolayer on top of epitaxial bilayer graphene. Hence, our results show that strain-induced bandgap engineering of single layered MoSe₂ is dependent on the orientation angle between stacked layers. This finding could be an interesting novel way to take advantage of the possibilities of

MoSe₂ and deeply exploit the capabilities of TMDs/graphene van der Waals heterostructures.

3. Conclusions

To conclude, we have reported that the orientation of MoSe₂ monolayer on bilayer graphene heterostructures affects the bandgap of MoSe₂. This suggests the dependency of the bandgap of layered TMD structures on the interfacial interactions within the heterostructures.

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5. References

- [1] M. M. Ugeda et. al. *Nature Materials*, **13**, 1091-1095, 2014.
- [2] Z. B. Aziz et. al. *Carbon*, **110**, 396-403, 2016.