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Master Thesis Defense

Entitled

"BAND GAP TUNING OF $MOSE_2$ AND WSE_2 MONOLAYERS THROUGH ALLOYING AND SUBSTITUTION: AN AB INITIO STUDY"

by

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Abstract

2D materials gained a huge interest among the research community after the first report of the preparation of graphene by a simple micromechanical exfoliation of highly oriented pyrolytic graphite in 2004.

For example, monolayer $MoSe_2$ and WSe_2 transistors have been demonstrated with on/off ratios of 10^8 and ultralow standby power dissipation. Graphene electrodes have been applied in developing fully transparent resistive memory to suppress undesired surface effects present in oxide memory devices. Photodetectors based on few-layered $MoSe_2$ have exhibited excellent photodetection properties.

Phototransistors based on monolayer WSe_2 have also been reported to exhibit a photoresponsivity as high as 2200 AW demonstrating the emerging applications of 2D materials for high-efficiency optoelectronic devices. In particular, the 2D monolayers of semiconducting transition-metal dichalcogenides (TMDs) have direct band gaps, possessing intriguing optical properties suitable for optoelectronic applications in light-emitting diodes and photovoltaics. To realize the highly efficient optoelectronic devices based on the TMD monolayers, it is also important to develop a strategy to tune the band gaps of the TMD monolayers.

One major disadvantage in graphene is that it lacks the existence of a band gap therefore it is not considered as an optimal material for light emission devices, and it minimized its application in the electronic industry where semiconductor materials maybe of much use. On the contrary, single layer TMDCs such as WSe_2 and WSe_2 are considered as direct band gap semiconductors and they exhibit good light emitting properties.

In this project, we will use theoretical and experimental methods to perform systematic studies of layered $MoSe_2$. Theoretically, we take transition metals and rare-earth metals to perform systematic studies of layered $MoSe_2$ and WSe_2 via substitutional doping, with the aim of identifying appropriate dopants which can effectively enhance or modify the electrical and optical properties of these materials.

Keywords: Transition Metal, Band gap, Monolayer,2D material, doping, point defects. DFT, VASP