Contribution ID: **72** Type: **Poster Presentation**

First-principles studies of Te line-ordered alloys in a molybdenum disulfide monolayer

Tuesday, 4 July 2017 17:10 (1h 50m)

The electronic and optical properties of a two dimensional (2D) semiconductor materials (MoS₂, MoSe₂, MoTe₂, etc.) are usually controllable by tuning their band gaps to meet the requirements of various electronic applications. The band gap of a molybdenum disulfide (MoS₂) monolayer can be tuned by creating alloys either at the molybdenum (Mo) sites or sulfur (S) sites. Different alloy isomers such as random, line and cluster configurations can be formed at each concentration. Computing all the possible alloy configurations using first-principles methods is practically impossible. In this work, the thermodynamic stability, structural and electronic properties of the Te line-ordered alloys at the S sites are investigated using the density functional theory (DFT) methods. Thirty four possible Te line-ordered alloy configurations are found in a 5×5 supercell of a MoS₂ monolayer. The calculated formation energies show that the Te line-ordered alloy configurations are thermodynamically stable at 0K. The lowest energy configuration at each concentration corresponds to the configuration where the Te atom rows are far away from each other (avoiding clustering). The variation in the lattice constants at different concentrations obeys Vegard's law. The Te line-ordered alloys fine tune the band gap of a MoS₂ monolayer although deviating from the linearity behavior. Our results suggest that the Te line-ordered alloys can be an effective way to modulate the band gap of a MoS₂ monolayer to fullfill the requirement of nanoelectronic, optoelectronic and nanophotonic applications.

Summary

A systematic study of the Te line-ordered alloys in a MoS₂ has been considered. The lowest energy configuration at each concentration of the Te line-ordered alloys in a MoS₂ monolayer has been identified. The incorporation of the Te line-ordered alloys affects the lattice constant as well as the electronic properties of the MoS₂ monolayer. The lattice constant variation obeys Vegard's law and the band gap of the 2D MoS₂ is tuned from 1.65 eV to 1.04 eV. This range of band gap is related to the solar spectrum, indicating the importance of this study in optoelectronic and photonic devices.

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Session Classification: Poster Session 1

Track Classification: Track G - Theoretical and Computational Physics