SAIP2016



Contribution ID: 171

Type: Poster Presentation

First-principles studies of transition metal defects in a molybdenum disulfide (MoS₂) monolayer

Wednesday, 6 July 2016 16:10 (1h 50m)

Abstract content
 (Max 300 words)
Formatting &
Special chars

Over the past few years, two dimensional (2D) transition metal dichalcogenides (TMDs) MX₂ (M=Mo,Cr,Nb,W; X=S,Se,Te) have attracted tremendous attention due to their remarkable electronic, magnetic and optical properties. It is evident that TMDs are suitable for future nanoscale device applications. Using density functional theory (DFT) implemented within the

Vienna <i>ab-initio</i> simulation package (VASP), the effects of transition metal defects (Rhenium (Re) and Tantalum(Ta)) on the thermodynamic stability and electronic properties of a MoS₂ monolayer are investigated. Calculations are performed using the projector augmented wave method (PAW) with the Perdew-Burke-Ernzerhof (PBE) for the exchange-correlation interactions. We find that the formation energy of the Ta substituting Mo (Ta_{Mo}) defect is negative whereas that of Re substituting Mo (Re_{Mo}) is positive. We observe that Ta_{Mo} induces non-spin-polarized states at 0.18eV above the valence band maximum(VBM), whereas Re_{Mo} yields spin polarized states at 0.25eV below the conduction band minimum(CBM). This reveals that Ta is a <i>p</i>-type dopant and Re is a <i>n</i>-type dopant. We find that one and three Re dopants yield a magnetic moment of 1µB but two Re dopants do not show any magnetic effects. Our results indicate that <i>p</i>-type (Ta) and <i>n</i>-type (Re) doped MoS₂ monolayers are promising materials for various electronic applications.

Apply to be
 considered for a student
 award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
 PhD, N/A)?

PhD

Main supervisor (name and email)
br>and his / her institution

Prof Nithaya Chetty, Nithaya.Chetty@up.ac.za, University of Pretoria

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Please indicate whether
this abstract may be
published online
(Yes / No)

Yes

Primary author: Ms ANDRIAMBELAZA, Noeliarinala Felana (University of Pretoria)Co-authors: Dr MAPASHA, Edwin (University of Pretoria); Prof. CHETTY, Nithaya (University of Pretoria)

Presenter: Ms ANDRIAMBELAZA, Noeliarinala Felana (University of Pretoria)

Session Classification: Poster Session (2)

Track Classification: Track G - Theoretical and Computational Physics

Yes