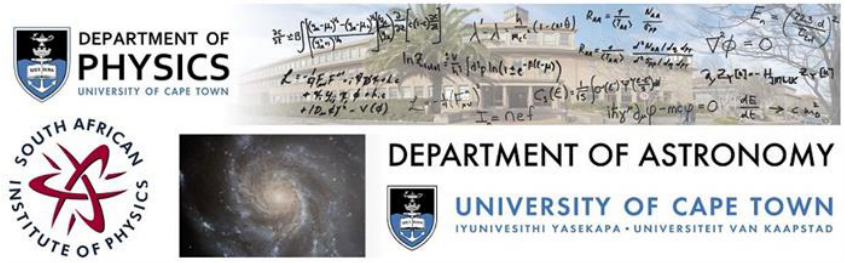

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First-principles studies of transition metal defects in a molybdenum disulfide (MoS₂) monolayer

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

Abstract content
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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 ab-initio 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 p-type dopant and Re is a n-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 p-type (Ta) and n-type (Re) doped MoS₂ monolayers are promising materials for various electronic applications.

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