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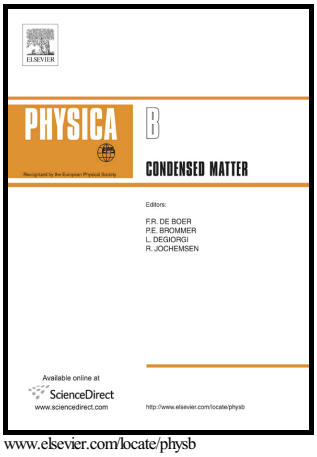

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E. Igumbor, R.E. Mapasha, W.E. Meyer

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Density functional theory calculation of monolayer WTe_2 transition metal dichalcogenides doped with H, Li and Be

E. Igumbor[a,b,*], R. E. Mapasha[a], W. E. Meyer[a]

[a] *Department of Physics, University of Pretoria, Pretoria 0002, South Africa.*
[b] *Department of Mathematics and Physical Sciences, Samuel Adegboyega University, Km 1 Ogwa-Ehor Rd, Ogwa Edo State Nigeria.*

Abstract

Results based on density functional theory modelling of electronic and structural properties of single layer WTe_2 dichalcogenides doped with X (X= H, Li and Be) were presented. The generalized gradient approximation functional of Perdew, Burke, and Ernzerhof exchange correlation was used for all calculations. Formation energies of X dopant substituted for W (X_W) were obtained to be between 3.59 and 2.61 eV. The Li_W defect with energy of formation of 2.14 eV was energetically the most favourable. For all dopants considered, while the H_W induced no magnetic moment, the Li_W and Be_W induced magnetic moments of 3.44 and 0.05 μ_B, respectively. The band gap of the WTe_2 as a result of the dopants was populated with several orbital ground states, and thus reduced within a few eV. While all X_W were spin polarised and behave as $p-$type dopant, the Li_W defect posses half metallic character.

Keywords: Electronic structure, dopant, formation energy

*Corresponding author
Email address: elgumuk@gmail.com (E. Igumbor)