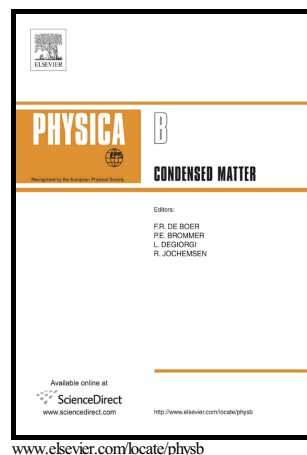


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Density functional theory calculation of monolayer WTe₂ transition metal dichalcogenides doped with H, Li and Be

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Abstract

Results based on density functional theory modelling of electronic and structural properties of single layer WTe₂ 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 WTe₂ 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

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