

# Tuning the Electronic and Magnetic Properties of ReS<sub>2</sub> by Lanthanide Dopants Ions: A First Principles Study

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## Abstract

Using quantum mechanical calculations, we investigate the structural, electronic, magnetic and optical properties of lanthanide metal doped triclinic mono-layered rhenium disulfide (ReS<sub>2</sub>). The calculated electronic band gaps for pristine ReS<sub>2</sub> mono-layer is 1.43 eV with a non-magnetic ground state. The calculated dopant substitutional energies under both Re-rich and S-rich conditions show that it is possible to experimentally synthesize lanthanide metal doped ReS<sub>2</sub> mono-layer structures. We found that the presence of dopant ions (such as Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) in the ReS<sub>2</sub> mono-layer lattice significantly modifies their electronic ground states. Consequently, there is introduction of defect levels and modification of the density of states profile. Some of these dopant ions introduce magnetization in ReS<sub>2</sub> lattice. This implies that these group of materials would have possible application as spintronic materials. The calculated absorption and reflectivity spectra show that this class of dopants leads to a general increase in the absorption spectral peaks but only a minute influence on the reflectivity. These ordered doped ReS<sub>2</sub> monolayer can lead to designing effective ultra-thin spintronic materials with improved performance.

## References

1. KINGSLEY ONYEBUCHI OBODO AND CECIL NAPHTALY MORO OUMA AND JOSHUA TOBECHUKWU OBODO AND MORITZ BRAUN. Influence of transition metal doping on the electronic and optical properties of ReS<sub>2</sub> and ReSe<sub>2</sub> monolayers. PCCP. 19 (29) 2017 19050-19057.