**Vacancy Formation in Monolayer Rhenium Disulfide**

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Recently, rhenium disulfide ($ReS_2$) monolayers were experimentally extracted by conventional mechanical exfoliation technique from as-grown $ReS_2$ crystals. Unlike the well-known members of transition metal dichalcogenides (TMDs), $ReS_2$ crystallizes in a stable distorted-1T structure and lacks an indirect to direct gap crossover. Here we present an experimental and theoretical study of the formation, energetics, and stability of the most prominent lattice defects in monolayer $ReS_2$. Experimentally, irradiation with 3-MeV $He^{+2}$ ions was used to break the strong covalent bonds in $ReS_2$ flakes. Photoluminescence measurements showed that the luminescence from monolayers is mostly unchanged after highly energetic α particle irradiation. In order to understand the energetics of possible vacancies in $ReS_2$ we performed systematic first-principles calculations. Our calculations revealed that the formation of a single sulfur vacancy has the lowest formation energy in both Re and S rich conditions and a random distribution of such defects are energetically more preferable. Sulfur point defects do not result in any spin polarization whereas the creation of Re-containing point defects induces magnetization with a net magnetic moment of 1–3μB. Experimentally observed easy formation of sulfur vacancies is in good agreement with first-principles calculations.

## References

[1] S. Horzum et al., Phys Rev B 89 155433 (2014)

## Figures