

# Defective SnS monolayer as a candidate for long-range ferromagnetism

Hamid Ullah, Mohammad Noor-A-Alam, Hye Jung Kim, and Young-Han Shin\*

Department of Physics, University of Ulsan, Ulsan 44610, Republic of Korea

\*E-mail : hoPONPOP@ulsan.ac.kr

We investigate the formation and migration of vacancies at both tin (Sn) and sulfur (S) sites in SnS monolayer using first principles calculations. Since the vacancy formation at the Sn site (4.75 eV/Sn) is more probable than that at the S site (6.03 eV/S), we expect that the Sn vacancies will be more likely to be observed in experiments. Due to the high vacancy migration energy barrier, we expect that the S vacancy will remain at the position where it is created, reducing the formation of vacancy clusters. SnS monolayer remains non-magnetic with the creation of both Sn and S vacancies. To induce magnetism in SnS, we replace Sn with transition metals (TMs = Mn, Fe, Co) and find a significant influence on the electronic and magnetic properties of monolayer SnS. The doping of TM alters the non-magnetic nature of SnS monolayer into magnetic one, but keeps it semiconducting. Additionally, long-range ferromagnetic behaviors are observed for all the doped systems. Hence, the addition of TM in monolayer SnS could be a promising process to realize two-dimensional diluted magnetic semiconductors. More interestingly, all the doped configurations show a high spin state, which can be used in nanoscale spintronic applications such as spin-filtering devices. [1, 2]

## References

- [1] L. C. Gomes and A. Carvalho, Phys. Rev. B 92, 085406 (2015).
- [2] Ullah *et al.* J. Appl. Phys. 124, 065102 (2018).

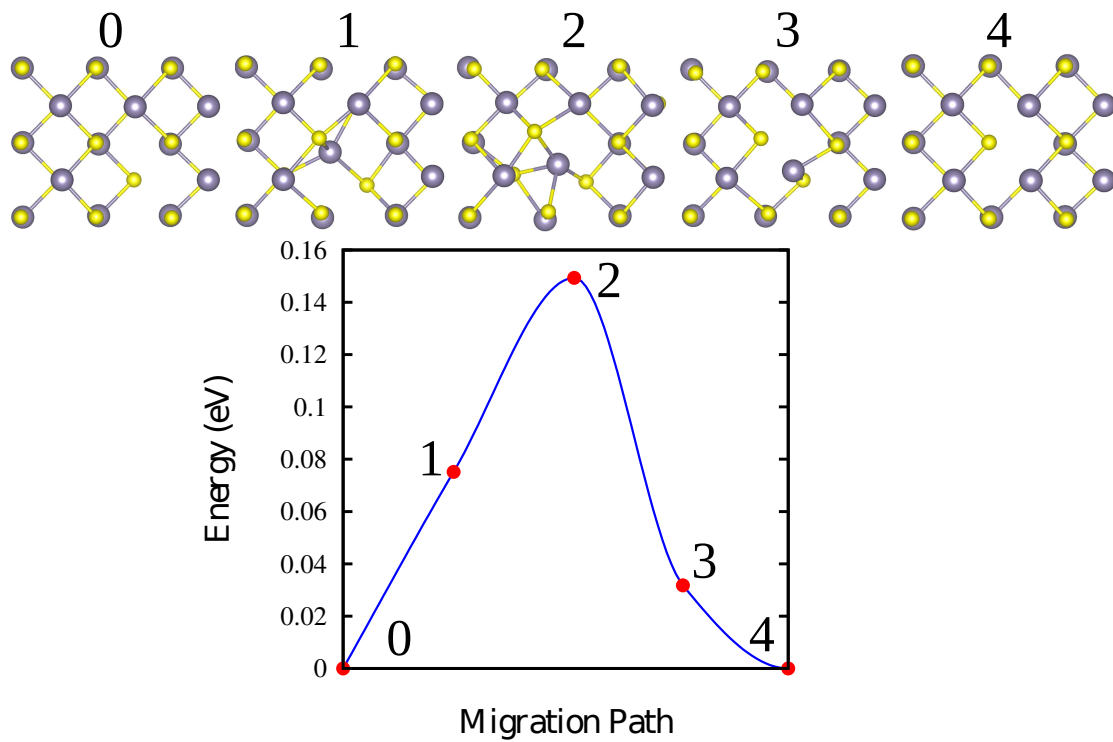


Figure 1: The schematic figures of the migration of the Sn-vacancy from initial position to final position from the top plane to the bottom plan. Energy profile for the corresponding vacancy migration is shown below the schematic view. The initial and final position are represented by 0 and 4, respectively. 1, 2, and 3 represent the images between initial and final position of vacancy. position.