First-Principles Study of Vacancy Effect on Electronic and Magnetic Properties of Iron Sulfide (FeS)

°Muhammad Alief Irham [1], Fahdzi Muttaqien [1], Satria Zulkarnaen Bisri [2], Ferry Iskandar [1]
Department of Physics, Institut Teknologi Bandung, Indonesia[1], RIKEN CEMS[2]
E-mail: ferry@fi.itb.ac.id

Troilite ion sulfide (FeS) is a metal-insulator transition material that naturally found in the Earth's crust. This material has an antiferromagnetic (AFM) configuration in its z-direction. Moreover, this hexagonal phase of FeS was recently predicted to exhibit magnetoelectric behavior.[1] However, the compound tends to have Fe vacancy, either synthesized or found in nature (i.e., meteorite). Despite the hurdles in finding its stoichiometric, FeS holds great potential in many different applications, such as spintronics devices and energy storage devices.[2] Therefore, a complete study of the vacancy effect on FeS is needed to understand this material's property.

In this present study, we analyze the effect of Fe vacancy on FeS by first-principles calculation. The Hubbard correction was also introduced to the density functional theory (DFT) calculation to accommodate the strong-correlation effect in the Fe atom. With the optimized structure, we found out that mid-gap states exist near the valence band maximum as an effect of the dangling bond. The band-gap of the Fe vacancy FeS decreased to 0.05 eV compared to pristine structure (0.64 eV). This band-gap value confirmed the experimental band-gap of Fe-vacancy FeS. Interestingly, the magnetization of the FeS was also increased with higher vacancy concentration. In higher vacancy concentration, the band-gap of FeS was closed and change the behavior to more metallic. Moreover, the defect structure observed in the same spin-state layer results in the mid-gap states only in one side of the spin region, which confirms the magnetization properties' finding. In many applications, these mid-gap states could enhance device performances and the ability to control magnetic states provides a higher chance for many applications, including quantum computer.

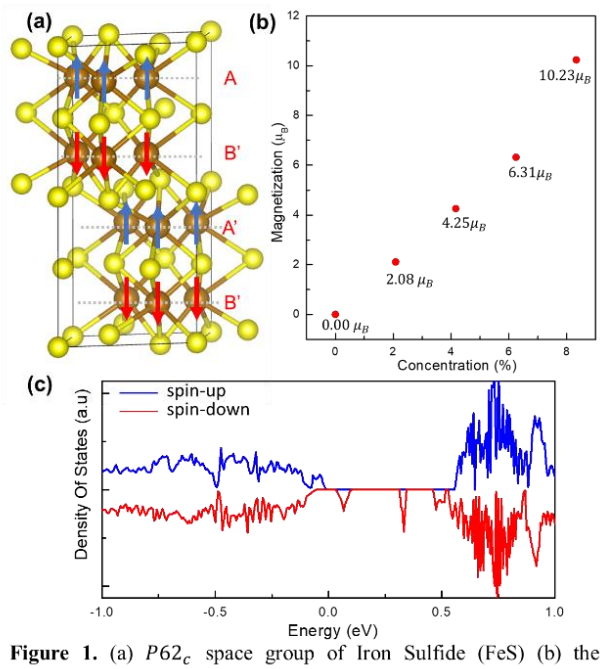

Figure 1. (a) $P62_c$ space group of Iron Sulfide (FeS) (b) the moment magnetic value of different vacancy concentration. (c) the calculated density of states of Fe-deficient FeS

Refs.:[1] F. Ricci, et.al., *Phys. Rev. Lett.* (2016), 116, 227601 [2] D. Bansai, et.al., *Nat. Phys.* (2020), 16, 6, 669-675