Contribution ID: **44** Type: **Poster**

Electronic band structures of MnS and Cr-doped MnS zinc blende materials using DFT+U

Electronic and magnetic calculations of zinc-blend (β) structure of MnS based on density functional theory were investigated using ultra soft pseudopotential. The spin orientation on Mn atoms was used to identify MnS magnetic phase. The DFT+U method was employed to predict underestimated band gap which obtained from standard DFT. In this calculation, Hubbard (U) energies are varied from 0 to 7.6 eV. Cr-doped MnS in its magnetic ground state and electronic band structure was also studied by considering only Hubbard energy at 0.0, 4.0 and 7.6. The results show that the β-MnS is anti-ferromagnetism and the band gap is raised up to 2.48 eV when Habbard energy is added by 4.0 eV into total energy calculation. The Cr dopant aligns at the Fermi energy level for Hubbard energy at 0.0 and 7.6 eV while at 4.0 eV, the Cr band is located at the donor level of the MnS structure.

Primary author: SRIPONGPUN, Nitat (Mahidol Wittayanusorn school)

Presenter: SRIPONGPUN, Nitat (Mahidol Wittayanusorn school)

Track Classification: Condensed Matter Physics