Contribution ID: **67** Contribution code: **S2 Condensed Matter Physics** Type: **Poster Presentation**

Electronic and magnetic properties of $MoTe_2$ monolayer doped with single and double transition metal configuration: spin density functional theory

The spin density functional calculations are performed to study the electronic and magnetic properties of $MoTe_2$ monolayer doped with single and double transition metal (V, Cr, Mn, Fe and Co) atoms. The electronic and magnetic properties are sensitive with the types and numbers of the doping transition metals. The semiconductor with narrow band gaps is shown in Cr and Co single-doped $MoTe_2$ monolayer. Mn single-doped $MoTe_2$ monolayer is metal. V and Fe single-doped $MoTe_2$ monolayers demonstrate the half-metallic behaviours with a 100% spin polarization. V and Co provide the first-two lowest formation energies which are used to the co-doping studies. $MoTe_2$ monolayers simultaneously doped with Co and V are characterized as metall. The p-d hybridization of d orbitals of transition-metal dopants and Mo host with Te-p orbitals and d-d hybridization between Mo-d states and d orbital of transition-metal dopants nearby the Fermi level induce the magnetism, called double exchange mechanism.

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Session Classification: Poster: S2 Condensed Matter Physics

Track Classification: Condensed Matter Physics