Contribution ID: **21** Type: **Poster**

Structural and electronic properties of LiMnO2 doped with transition metals: A first-principles study

A spin density functional study of structural and electronic properties of LiMnO2 doped with different transition metals (Sc, V and Tc) is reported. The physical properties of LiMnO2 material are sensitive with the transition-metal dopants. Transition metal dopants increase the lattice parameters and their volumes, thus increasing the Li diffusion channel. The computations remark that the transition metals introduce the d orbitals around the Fermi level. Tc doping in LiMnO2 demonstrates the enhancement in the electronic conductivity because of the volumetric expansion. Finally, these results convey a valuable agenda for the future optimization of transition-metal doped LiMnO2 cathode materials for next-generation lithium batteries.

Keywords: LiMnO2, transition metal, dope, spin density functional calculations.

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Track Classification: Material Physics