Contribution ID: **53** Type: **Poster Presentation**

Effects of Tin (Sn) doping on the layered LiMnO2 cathode material for Lithium-ion batteries

Abstract
Lithium transition-metal oxides, such as LiM2O2 and LiMO2 (where M = Ni, Mn, Co, etc.), are commonly used as cathode materials in lithium-ion batteries. These materials offer good capacity, low cost, high thermal stability, and energy density. However, they suffer from Jahn-Teller distortion, which leads to structural instability and decreased performance. One way to improve these materials is through cation doping, which has been shown to improve electrochemical performance, enhance electrical conductivity, and stabilize the crystal structure. This study focuses on the effects of doping with tin (Sn) in layered LiMnO2 (R-3m) and examines the changes using first-principles calculations combined with the cluster expansion technique. The cluster expansion approach generated several new Sn-doped phases of LiMnO2, resulting in 29 different phases, three of which were identified as stable and favourable. These stable phases Li4MnSn3O8, Li4Mn2Sn2O8, and Li4Mn3SnO8 all exhibited negative heats of formation, indicating that they are thermodynamically stable. Among these, Li4Mn2Sn2O8 was found to be the most stable phase, as it has the lowest heat of formation and lies at x = 0.5 in the binary phase diagram, with equal proportions of Sn and Mn. According to the heats of formation, Li4Mn3SnO8 was predicted to be the most thermodynamically stable of the phases, furthermore Li4Mn3SnO8 was also found to have no band gap, which leads to improved electron conductivity. All the generated structures are mechanically stable and are likely to with stand large amounts of plastic deformation before failure.

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Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials