Contribution ID: **38** Type: **Oral Presentation**

Structural, thermodynamic, electronic and mechanical properties of MCO₃ (M: Ca, Mn, Fe, Co, Ni) precursor materials for Li-ion batteries

Tuesday, 9 July 2019 10:40 (20 minutes)

First-principles calculations were carried out on the structural, thermodynamic, electronic and mechanical properties of MCO₃ precursor materials at 0 K to investigate their possible application as cathodes in Li-ion batteries. Li-ion batteries are the most crucial power sources for portable electronic devices. However, their performance greatly depends on the cathode materials, which serves as a host structure for Li ions. We have employed the plane-wave pseudopotential method framed within the density functional theory (DFT) as implemented in the VASP code. The structural lattice parameters were calculated to 95% agreement with the experimental data, ensuring robustness of the approach employed. The calculated heats of formation are relatively low, suggesting thermodynamic stability. The electronic density of states showed that CaCO₃ and MnCO₃ are insulators, whereas CoCO₃ and NiCO₃ are semiconductors. Interestingly FeCO₃ is predicted to be metallic, suggesting good electric conductivity. The phonon dispersion curves showed negative vibrations in all MCO₃ systems, suggesting mechanical instability.

Apply to be
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Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

MSc

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Session Classification: Physics of Condensed Matter and Materials

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