Contribution ID: **239** Type: **Poster Presentation**

First principles calculations study of O3 and P2 NaMn1/2Fe1/2O2 as potential cathode for Sodium ion battery application

Sodium oxides with mixed transition metals have received significant attention as positive electrode candidates for sodium-ion batteries, due to their high reversible capacity. To understand the relation between layered structures and electrochemical properties, it is necessary to understand layered compound phase transformations during electrochemical responses. Using first-principles calculations, we successfully investigate the electrochemical performance of the O3 and P2 NaMn1/2Fe1/2O2 for the sodium-ion batteries. We calculated the structural, electronic, and mechanical properties and both O3 and P2 NaMn1/2Fe1/2O2. The computational results are found to be well consistent with the experimental investigations. The electronic properties show that the metallicity of NaMn1/2Fe1/2O2 steadily increases during Na extraction, whereas the elastic properties show that adding 50% Mn NaFeO2 does not compromise the structure's stability.

Apply to be considered for a student ; award (Yes / No)?

YES

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

PhD

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Session Classification: Physics of Condensed Matter and Materials

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