Contribution ID: **245** Type: **Poster Presentation**

First-Principles Study of sodium De-intercalation From Tri-Chalcogenide NaNbSe2

Thursday, 6 July 2023 16:15 (1 minute)

The importance of energy generation and storage cannot be overstated, given rising energy demands and the depletion of fossil fuels. Because of their low cost, abundance of elements, strong reversibility, and moderate energy density, sodium-ion batteries have piqued interest as a possible alternative for large-scale electrochemical energy storage. To provide critical fundamental insights into electrode materials and to ease the development of materials for sodium-ion batteries, computational techniques have been widely used in connection with experimental investigations. In this work we investigated the electrochemical performance of the transition metal chalcogenide NaNbSe2 as a material for sodium-ion batteries using systematic first-principles calculations based on density functional theory employing the generalized gradient approximation. The 2 × 1 × 1 super-cell is used for our research on NaNbSe2. Because of the slight distortion of octahedron, the simulation lattice was set to the P1 space group. The comparison of lattice parameters from the relaxation structure and previously experimental results was done and the calculated results were consistent with the experimental results.

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

YES

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

Hons

Primary author: SANA, Sana (University of Venda)

Co-authors: DIMA, Ratshilumela Steve (University of venda); RANWAHA, Tshifhiwa Steven (University of Venda); MALUTA, Nnditshedzeni Eric (University of Venda); MAPHANGA, Rapela (CSIR)

Presenters: SANA, Sana (University of Venda); RANWAHA, Tshifhiwa Steven (University of Venda)

Session Classification: Poster Session 2

Track Classification: Track F - Applied Physics