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TRANSITION METAL CARBONATE PRECURSORS AS CATHODE MATERIALS FOR LI-ION BATTERIES: COMPUTATIONAL AND EXPERIMENTAL STUDY

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Tebogo Morukuladi, Noko Ngoepe, Clifton Masedi and Phuti Ngoepe
Materials Modelling Centre, University of Limpopo, Department of Physics, Private Bag x1106, Sovenga, 0727
Email address: tebzamorukuladi@gmail.com

Abstract
The development of next generation cathode materials for lithium-ion batteries (LIBs) is critical to enable full implementation of energy storage into a grid and transportation sectors. The most common cathodes in today's LIBs are transition metal oxides with compositions LiNiaMnbCocO2 (referred to as NMCs). As a demand for new and improved technology continues to grow, critical factors such as cost and safety begin to play a significant role in lithium-ion batteries. Therefore, lithium and manganese-rich compounds are highly commended as sustainable candidates for the next generation of cathode materials due to their inherent safety, low cost and high reversible capacities of >250mAh/g. The electrochemical performances of these compounds depends mainly on the physical properties of the precursor materials. Precursors for NMC cathodes are generally synthesized via co-precipitation method. The two most common methods to synthesize precursors are carbonate co-precipitation and hydroxide co-precipitation. However, for this study carbonate co-precipitation method will be used to synthesize precursors because it is capable of keeping the valence state of 2+ for Mn-rich stable throughout the process. Cluster expansion methods were employed to determine the phase stability of Ni1-xMnxCO3 structures using the Universal Cluster Expansion (UNCLE) code. From the generated phase stability we further chose the stable structures and performed their preliminary first-principles density functional theory (DFT) calculations to investigate the structural, electronic and mechanical properties for transition metal carbonate using Vienna ab-initio simulation package (VASP) code. We further synthesized the Mn-rich transition metal carbonate precursors using the carbonate co-precipitation method whereby the tap density, morphology and particle growth for Mn-rich transition metal carbonates were calculated.
Keywords: Binary diagrams, electronic stability, mechanical stability, vibrational stability, morphology and particle growth.

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

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PhD

Primary author: Ms MORUKULADI, Mogahabo (Student)

Co-authors: Dr MASEDI, Cliffton; Dr NGOEPE, Noko; Prof. NGOEPE, Phuti

Presenter: Ms MORUKULADI, Mogahabo (Student)

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