Contribution ID: **36** Type: **Poster Presentation**

THE CATALYTIC ACTIVITY OF MO₂ (M= Ti, V, Mn) ON (110) SURFACE OF Na-AIR BATTERY

Tuesday, 4 July 2023 15:46 (1 minute)

Metal-air batteries have a far higher theoretical energy density than lithium-ion batteries and are frequently proposed as a possibility for next-generation electrochemical energy storage for applications like electric vehicles and grid energy storage. The Na-air battery is an energy storage system with moderate catalytic activity in the Oxygen Reduction Reaction (ORR) and Oxygen Evolution Reaction (OER). The current study uses the Density functional theory (DFT) to develop a deeper understanding of the catalytic activity of rutile types of MO₂ for the ORR and OER in Na-air batteries. As oxygen is adsorbed on Na/MO₂ (110) surfaces, the electronic properties of several configurations (dissociated, superoxide, peroxo on Na-M, and dissociated') are examined to determine the catalytic influence towards the generation of the discharge product in Na-O₂ batteries. Using the density of states analysis, the MnO₂ system was found to be more stable than TiO₂ and VO₂ systems. These discoveries are significant for the nucleation and development of Na₂O₂ and NaO₂, as well as for understanding the reactivity of Na/MO₂ (110) surfaces.

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

YES

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

PhD

Primary authors: NGOBENI, PERCY (UL); NGOEPE, Phuti (University of Limpopo); MAENETJA, khomotso (University Of Limpopo)

Presenter: NGOBENI, PERCY (UL)

Session Classification: Poster Session 1

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