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Redox properties of VCo₂O₄ (001) surface in zinc air batteries

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The evolution and progress of humanity have a significant connection to our energy consumption practices. Reliable energy sources are essential for promoting economic expansion, particularly as modern society becomes ever more energy dependent. The rapid development of zinc-air batteries (ZABs) is leading them to be seen as promising alternatives to traditional lithium-ion batteries for energy storage. However, the kinetics of the air cathode are slow, resulting in a short life cycle and low energy efficiency for zinc-air batteries. First-principles calculations are used to develop the catalyst that promotes the nucleation of Zn-air batteries' most stable discharge products. The density functional theory (DFT) is used to determine the adsorption (Gamma;= +1, +2) and vacancy formation (Gamma;= -1, -2) energies of the oxygen atom on the (001) surface of VCo₂O₄. The Bader charge is used to determine how the system's atoms interact with one another. As oxygen atoms are reduced and adsorbed, it is observed that the V and Co atoms show negligible charge differences upon either reduction/oxidation as compared to the pristine phase. The interplanar distances indicate that when an oxygen atom is added and removed from the pristine state, the system expands and contracts, respectively. The work function aids in determining the level of reactivity within the system. Absorbing oxygen atoms decreases the system's reactivity, whereas the removal of oxygen increases it. The results will give insights into finding the catalyst that will enhance the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), thereby improving the performance of Zn-air batteries.

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Primary author: NGOBENI, Percy

Co-authors: Prof. NGOEPE, Phuti (University of Limpopo); Prof. MAENETJA, khomotso (University of Limpopo)

Presenter: NGOBENI, Percy

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