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VCo2O4 (001) surface properties in zinc-air batteries

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The evolution and progress of humanity are closely linked to our ways of energy use. Reliable energy sources are vital for driving economic growth, especially as society's demand for energy keeps rising. The rapid development of zinc-air batteries (ZABs) makes them an appealing alternative to standard lithium-ion batteries for energy storage needs. However, the slow kinetics of the air cathode led to a short lifespan and low energy efficiency in zinc-air batteries. First-principles calculations help develop catalysts that promote the formation of the most stable discharge products in Zn-air batteries. Density functional theory (DFT) is used to examine the adsorption (Γ= +1, +2) and vacancy formation (Γ= -1, -2) energies of oxygen atoms on the (001) surface of VCo2 O4. The Bader charge analysis reveals how the atoms interact within the system. When oxygen atoms are reduced and adsorbed, it is observed that the V and Co atoms show minimal charge differences compared to the original phase, whether reduced or oxidized. Interplanar distances show that adding or removing oxygen causes the system to expand or contract, respectively. The work function helps assess the system's reactivity. Absorbing oxygen atoms decreases reactivity, while removing oxygen increases it. The calculations were executed concurrently on 24 of the 2400 available cores, leveraging CHPC with 2048 MB of memory. These findings provide insights into identifying catalysts that can enhance the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), thereby improving the performance of Zn-air batteries.

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No. Not a student nor Postdoc.

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Yes

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Yes

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