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Ab initio study of Structural, energetic, electronic, and mechanical properties of Pmmn-V2O5 and Pnma-V2O5 polymorphs through Density Functional Theory Analysis

Research has increasingly shifted towards alternative battery chemistries due to the high costs, Lithium depletion and safety concerns of Li-ion batteries. Mg-ion battery chemistry has gained attention as a promising alternative in rechargeable battery technology due to the bivalency of Mg2+ ions. In this chemistry, Vanadium Pentoxide (V2O5) is projected to a suitable cathode material for rechargeable Mg-ion batteries due to its structural coordination, which ensures fast 3-D Mg2+ ion diffusion paths and prospects of being reversible intercalating cathodes. This study employed ab initio computational simulations to examine the structural, energetic, electronic, and mechanical properties of the Pmmn-V2O5 and Pnma-V2O5 polymorphs. These properties were thoroughly analyzed using first-principles methods based on Density Functional Theory (DFT). All calculations were performed using the CASTEP simulation code integrated within the Materials Studio 2020 software, utilizing the Generalized Gradient Approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) functional. Geometry optimization was carried out to determine the structural properties, which were found to be more than 95 % in agreement with the experimental data. The electronic band structures along high-symmetry directions in the Brillouin zone for both spin-up and spin-down configurations revealed energy band gaps of 2.535 eV and 2.011 eV, respectively, around the Fermi level, indicating semiconductor behavior for both polymorphs. Furthermore, the elastic constants of the monocrystalline structure of Pnma-V2O5 satisfied Born Stability conditions, suggesting mechanical stability, while Pmmn-V2O5 polymorph exhibits instability. These findings provide a comprehensive understanding of the structural, electronic, and mechanical properties of the Pmmn-V2O5 and Pnma-V2O5 polymorphs.

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