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EXPLORING THE POTENTIAL OF H-Zn2GeO4 AS AN LI-ION HOST

The demand for eco-friendly and efficient energy sources in industrial, portable, and wearable applications has driven extensive research into electrochemical storage devices. The lithium-ion batteries emerge as highly promising due to their exceptional physicochemical and electrochemical properties. To further enhance lithium-ion battery performance beyond conventional graphite-based anodes, there is ongoing exploration of advanced nanomaterials with specific chemical compositions and crystalline structures capable of facilitating reversible and rapid conversion and alloying reactions, thus enabling superior Li-ion storage capacity [1]. In this context, our study focuses on employing hexagonal Zn2GeO4 nanoparticles as a Li-ion host material. The synthesis of h-Zn2GeO4 in a willemite-like phase is done by using the facile Pechini method. the charge-discharge curves show that the h-Zn2GeO4 delivers a specific capacity of 900 mAh/g with a Coulombic efficiency of 97%. The experimental analyses were complemented by computational simulations using Density Functional Theory (DFT) and Ab Initio Molecular Dynamics (AIMD) to delve into atomic-scale interactions between Li ions and the h-Zn2GeO4 crystal structure. The results evidence the chemical reactions observed in the experiment; besides the theoretical gravimetric capacity is 1400 mAh/g in agreement with experimental measurements.

Keywords

Li-ion battery, DFT calculations, anode material, Zn2GeO4

Reference

[1] Chen, X., Ma, B., Li, W., Zhang, Y., & Tang, Y. (2014). ChemInform Abstract: Rational Material Design for Ultrafast Rechargeable Lithium-Ion Batteries. https://doi.org/10.1039/c4cs00442f

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Author approval

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