Combined First-principles and Experimental Studies of a V-doped LiFePO₄/C Composite as a Cathode Material for Lithium-ion Batteries

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As a promising cathode material for lithium-ion batteries (LIBs), olivine-structured LiFePO₄ has been increasingly studied due to its high capacity, excellent thermal stability, cycling stability and environmental friendliness. Nevertheless, the main challenge of LiFePO₄ is its poor conductivity and Li⁺ diffusion coefficient. Herein, a V-doped LiFePO₄/C composite is prepared via a solid-state method. The electronic structures of the samples are obtained by first-principles calculations based on density functional theory. V₂ exhibits enhanced electrochemical performance, demonstrating discharge capacities as high as 155.6, 150.2, 136.0, 122.4 and 93.1 mA h g⁻¹ at 0.1, 0.2, 0.5, 1.0 and 3.0C, respectively, and approximately 100% capacity retention after 100 cycles at 1.0C.

Keywords: Lithium-ion battery, LiFePO₄/C, First-principles, V-doped

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