First Principle Study of $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$ for Na Batteries Application and Experimental Investigation

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In this paper, we used first principle calculation and experimental investigation for exploring the application of $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$. The influence of insertion and extraction of Na was investigated using XRD analysis. Results indicated the $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$ owing a stable lattice structure with unit cell volume. The desodiated phase of the $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$ could remain a stable state until 700 °C, which provide an excellent stability for battery electrode fabrication. The experimental study showed the $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$ could serve as an excellent candidate for rechargeable Na battery fabrication.

Keywords: $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$; First priciple; Na battery; Electrode; XRD

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