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Crystal structure and electrochemical properties of  $\text{LiFe}_{1-x}\text{V}_x\text{PO}_4\text{F}_{1-\delta}\text{O}_\delta$  cathode materials for lithium-ion batteries

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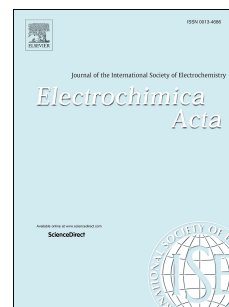
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# Crystal structure and electrochemical properties of $\text{LiFe}_{1-x}\text{V}_x\text{PO}_4\text{F}_{1-\delta}\text{O}_\delta$ cathode materials for lithium-ion batteries

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## ABSTRACT:

Tavorite-structured polyanion compounds such as  $\text{LiVPO}_4\text{F}$ ,  $\text{LiFePO}_4\text{F}$  and  $\text{LiVPO}_4\text{O}$  are promising cathode candidates of Li-ion batteries due to their structural stability as a result of strong covalent bonds. A few publications related to  $\text{LiVPO}_4\text{F}$ – $\text{LiFePO}_4\text{F}$  and  $\text{LiVPO}_4\text{F}$ – $\text{LiVPO}_4\text{O}$  solid solutions have been reported to date. In this work,  $\text{LiFePO}_4\text{F}$ – $\text{LiVPO}_4\text{O}$  solid solution, *i.e.*  $\text{LiFe}_{1-x}\text{V}_x\text{PO}_4\text{F}_{1-\delta}\text{O}_\delta$  ( $0 \leq x \leq 1$ ;  $0 \leq \delta \leq 0.36$ ) is first prepared by a two-step solid-state route using the pre-synthesized  $\text{FePO}_4$  and  $\text{VPO}_4\text{O}$  powders. Sloping discharge profiles shown in solid-solution cells indicate a single-phase behavior which is different from the two-phase reaction of end members. The structure determination, refinement and electrochemical properties are studied. The mechanisms are concluded involved in redox energies of cations. Redox energies are tuned within a wide range 1.5–4.5 V in polyanion-type cathodes, through the inductive effect introduced by cation (V for Fe) and anion (O for F) substitution.

**Keywords:**  $\text{LiFePO}_4\text{F}$ – $\text{LiVPO}_4\text{O}$ ; solid solution; tavorite; polyanion-type cathode; Li-ion battery

## 1. Introduction

$\text{LiVPO}_4\text{F}$  [1-6],  $\text{LiFePO}_4\text{F}$  [7-10] and  $\text{LiVPO}_4\text{O}$  [6, 11-18] are homeotypic with a tavorite-type ( $P\bar{1}$ , triclinic) crystal structure. As for unit-cell volume per molecular formula ( $V' = V/Z$ ),  $V'_{\text{LiV}^{\text{III}}\text{PO}_4\text{F}} > V'_{\text{LiFe}^{\text{III}}\text{PO}_4\text{F}} > V'_{\text{LiV}^{\text{IV}}\text{PO}_4\text{O}}$ . Considering the oxidation state and octahedral ionic radii of Fe/V cations while coordination number (CN) corresponds to 6,  $r_{\text{Fe}^{\text{III}}} = 0.645 \text{ \AA}$  (in high-spin state)

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