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P.S.A.16.

SYNTHESIS OF F-DOPED $LiFePO_4$ VIA PRECIPITATION METHOD

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Fluorine-doped, olivine-structured $LiFePO_4$ suitable for cathode material in rechargeable lithium batteries was prepared by aqueous precipitation followed by high temperature treatment at 700°C under slightly reductive atmosphere (Ar+5%H_2). The starting materials were equimolar quantities of $(NH_4)_2HPO_4$, $FeSO_4 \cdot 7H_2O$ and LiF. LiF served as both lithium and fluorine source. Besides the lattice parameters and the primitive cell volume reductions, compared to the undoped sample synthesized under the same conditions using $LiNO_3$ as lithium source, the Rietveld refinement also shows that fluorine ions preferably occupy specific oxygen sites. Particularly, the best refinement is accomplished when fluorine ions occupy O(2) sites exclusively. By means of up-to-date electronic structure and total energy calculations this experimental finding is theoretically confirmed. Such fluorine doping also produces closing of the gap in the electronic structure and consequently better conductivity properties of the doped compound. In addition, the morphological and electrochemical performances of the synthesized powders are fully characterized.

P.S.A.17.

CRYSTAL STRUCTURE REFINEMENT OF Li_2FeSiO_4 CATHODE MATERIAL

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Recently lithium iron orthosilicate, Li_2FeSiO_4, has been found to display attractive electrochemical properties when used as cathode material. Because its constituent elements are non-toxic, low-cost and abundant, it is also attractive system from the standpoint of environmental sustainability. Li_2FeSiO_4 compounds are known to exhibit a rich polymorphism and several crystal structures have been reported in the literature. Due to its complex polymorphism it is still a challenge obtaining a phase pure material. Here we report the properties of pure Li_2FeSiO_4 obtained by solid-state reaction at 750 °C. It was found that Li_2FeSiO_4 crystallizes in monoclinic $P2_1/n$ space group. In this structure one set of LiO4 tetrahedra are arranged in edge sharing pairs with FeO4 tetrahedra, while the other set of LiO4 tetrahedra forms edge sharing pairs with itself. In addition, galvanostatically cycled material was characterized in terms of structural and transport properties.