

Role of cationic vacancies on the electrochemical storage properties of Hydroxy-Fluorinated TiO₂ Anatase

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Introducing defects, particularly vacancies, into hosted intercalation compounds has been shown to be a viable way to modify the electrochemical properties of electrode materials. (1) The fundamental reasons for the improvement of the materials properties are particularly challenging since it's required a clear identification of the defects and a fine description of the local structural changes.

Recently, we reported on a novel methodology allowing modifying the chemical composition of titanium dioxide anatase, one of the polymorph of TiO₂, yielding the stabilization of cationic vacancies. (2) The latter were induced by the partial substitution of divalent oxides by monovalent fluorides and hydroxyl groups yielding the general chemical formula Ti_{1-x-y}□_{x+y}O_{2-4(x+y)}F_{4x}(OH)_{4y}, where □ represents a cationic vacancy. The concentration of the cationic vacancies can be synthetically controlled by tuning the reaction temperature, reaching an unprecedented deviation of the chemical composition respecting to the pure TiO₂ anatase. Indeed, up to 22% of cationic vacancies can be generated yielding Ti_{0.78}□_{0.22}O_{1.12}F_{0.4}(OH)_{0.48}.

Here, we propose to discuss the impact of cationic vacancies on the insertion properties of Ti_{0.78}□_{0.22}O_{1.12}F_{0.4}(OH)_{0.48} with respect to Li⁺ and Mg²⁺ ions.

References

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