Role of cationic vacancies on the electrochemical storage properties of Hydroxy-Fluorinated TiO$_2$ 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 TiO$_2$, 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$_{1-x-y}$□$_x$O$_{2-4x+y}$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 TiO$_2$ 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 Mg$^{2+}$ ions.

References
