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# A topology-based investigation of the Ti-doping effects on the K+ conductivity in doped K(Fe,Ti)O2 solid electrolyte

Nowadays whole variety of electronic gadgets surround us in everyday life. Electricity-driven cars are being taken over the modern car industry. All of them rely strongly on the electrochemical energy storage devices. In the batteries and accumulators, one of the main part that governs their performance is the solid electrolyte material that separates the electrodes and provides the ion migration. At present, the lithium-based solid electrolytes are the most studied type of such materials due to their widespread application in the lithium-ion batteries. Nevertheless, due to the depletion of the lithium deposits and high demand by industry, its cost increased markedly. Therefore, an alternatives have being extensively searched among potential Na- and K-conducting compounds.

The control and tuning of the solid electrolytes conductivity can be achieved by means of deliberate introduction of dopant atoms in the pristine lattice of the modifying substance. Recently, we have developed an approach that combines the DFT calculations and machine learning methods for modeling the configurational space of the doped Li(Ni,Co,Al)O2 cathode materials [1]. In this study we have applied the mentioned topology-based approach for the Ti doped KFeO2 solid electrolyte exploration, which was extensively studied both experimantally and computationally [2]. The energetic characteristics for the vacancy formation and K-ion migration barriers were obtained. The topology-based analysis revealed the influence of the Ti distribution in the modelled cell on both the vacancy formation and ion migration characteristics. The obtained result can serve as a basis for the creation of the general approach for prediction of the dopants influence on the solid electrolyte and cathode materials performance.

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