Contribution ID: **488** Type: **Oral**

DFT-based study of the disordered solid electrolytes

Nowadays, the most of the 'green' technologies, such as power stations based on renewable energy sources and electromobiles, require new types of low-cost and at the same time large-scale energy storage systems. In turn, Li-ion batteries do not meet these requirements because of their high price and short maintenance interval. For this reason, searching for possible alternatives that are based on more abundant elements (Na- and K-ion batteries) and cheaper/robust technologies attracts both theoreticians and experimentalists in the field of electrochemistry and materials science.

Theoretical methods for electrochemical property predictions in big sets of known crystal structures, such as Inorganic Crystal Structure Database, allow one to perform screening for the prospective materials without any necessity of synthesis, treatment and experimental measurements. For instance, geometrical-topological approach, bond valence landscape method and other techniques are used widely for this purpose. Nevertheless, for many well-known solid electrolytes the conductivity is caused by doping and related disordering in the structure. Thus, a tool for efficient investigation of the doping effects on the electrochemical properties of solid electrolytes and electrode materials can become a starting point for the further high-throughput screening of materials and hopefully design of new ones.

Recently, we have developed an approach based on the geometrical-topological analysis, DFT calculations and machine learning methods for modeling the configurational/compositional spaces of cathode materials [1] and testified it for the well-known LiNiO2 and Li(Ni,Co,Al)O2 structures also studied by means of in situ neutron diffraction. In this work, we extend the proposed approach for disordered/doped solid electrolytes. Particularly, the current contribution concerns the K(Fe,Ti)O2 potassium conductor series (with respect to Ti content) studied comprehensively both from the electrochemical and computational standpoints [2].

We are obliged to computational facilities of the Samara University computing complexes 'Sergey Korolev'and 'Zeolite'(Samara Center for Theoretical Materials Science). The study was funded by the Russian Federation Government (project No.3.6588.2017/9.10) and Russian Foundation for Basic Researches (project No.18-33-00477).

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Track Classification: Condensed Matter Physics