Contribution ID: **458** Type: **Oral**

A combined approach for solid electrolytes investigations: handling geometrical/topological screening datasets

Wednesday, 17 April 2019 17:30 (15 minutes)

Search for potential conducting materials with promising electrochemical properties is of increasing interest due to electronic gadgets of all kinds and modern electric vehicles demand reliable, robust and safe storage devices of electrochemical energy. Both theoretical [1] and experimental [2] ways are possible, nevertheless computer modelling is a powerful tool for high-throughput searching of conducting/intercalating materials that meet the requirements of safety, durability and cost. One of the existing methods for fast screening of the the crystal structure databases is based on Voronoi-partition approach and is implemented in the ToposPro program package [3].
By now, it was applied for searching for the promising (from the geometrical/structural point of view) lithium [4], sodium [1], potassium [5] solid electrolytes. Amount of the structures (several hundred structures or less) in the obtained datasets is much lower than the initial set of structures. However, the subsequent investigation of the proposed materials within the precise quantum chemical methods is still complicated by their computational complexity. On of the possible solutions is to apply bond valence landscape approach [1].
Another approach that is being developed currently rests upon topological analysis of model electron density distributions for the big sets of promising solid electrolytes. The main idea of the proposed approach is to find correlations between topological properties of the electron density distribution calculated using the procrystal method with the DFT-modelled migration barriers in tested compounds. The proposed approach can be used for making an initial guess for nudged elastic band method on the ion trajectory in the crystal field individually or in a combination with the existing approaches.
Present report summarizes the current results obtained for different sample sets of crystal structures, obtained by screening of Inorganic Crystal Structure Database.
The authors thank hardware and software facilities of the 'Zeolite'supercomputer at the Samara Center for Theoretical Materials Science and the 'HybriLIT'heterogeneous platform at the Laboratory of Information Technologies of the Joint Institute for Nuclear Researches (Dubna, Russia). The study was funded by Ministry of Science and Higher Education of the Russian Federation (project No.3.6588.2017/9.10) and Russian Foundation for Basic Researches (project No.18-33-00477).

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Session Classification: Condensed Matter Physics

Track Classification: Condensed Matter Physics