

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

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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 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. One 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 pro-crystal 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.

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[1] Meutzner, F., Münchgesang, W., Kabanova, N. A., Zschornak, M., Leisegang, T., Blatov, V. A., & Meyer, D. C. (2015). On the Way to New Possible Na-Ion Conductors: The Voronoi-Dirichlet Approach, Data Mining and Symmetry Considerations in Ternary Na Oxides. *Chemistry—A European Journal*, 21(46), 16601-16608.

[2] Yan, G., Mariyappan, S., Rousse, G., Jacquet, Q., Deschamps, M., David, R., Tarascon, J. M. (2019). Higher energy and safer sodium ion batteries via an electrochemically made disordered Na<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>F<sub>3</sub> material. *Nature communications*, 10(1), 585.

[3] V.A. Blatov, A.P. Shevchenko, D.M. Proserpio, Applied Topological Analysis of Crystal Structures with the Program Package ToposPro, *Cryst. Growth Des.* 14 (2014) 3576–3586

[4] N.A. Anurova, V.A. Blatov, G.D. Ilyushin, O.A. Blatova, A.K. Ivanov-Schitz, L.N. Dem'yanets, Migration maps of Li<sup>+</sup> cations in oxygen-containing compounds, *Solid State Ionics*. 179 (2008) 2248-2254.

[5] R.A. Eremin, N.A. Kabanova, Y.A. Morkhova, A.A. Golov, V.A. Blatov, High-throughput search for potential potassium ion conductors: A combination of geometrical-topological and density functional theory approaches, *Solid State Ionics*. 326 (2018) 188–199.

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