Figure 1. New Ionic liquids based on crown ether building blocks.

Keywords: Ionic liquids, electrolytes, battery, crown ether

MS19-P14 Can we predict Al ion conductors? A combination of crystallographic and energetic evaluation tools.

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Ionic conduction in crystalline oxides can be described as jumps of mobile ions between interconnected oxygen-coordinated crystallographic sites. Therefore, crystallographic evaluation tools can be utilised and combined into a high-throughput prediction method for crystalline ionic conductors. An energetic consideration in the end allows an in-depth analysis of the predicted ionic conduction process in order to verify the most-promising compounds.

Three approaches can be synergetically used to allow a time-efficient and consistent methodology for the identification of oxidic, crystalline aluminium ion conductors: Voronoi-Dirichlet partitioning (VDP) combined with data mining offers a fast high-throughput screening of crystallographic databases on the basis of a geometrical division of the crystal structure into domains assigned to each constituent of the structure, pointing towards possible void networks.

Bond-valence methodology (BVM) as a chemically motivated evaluation tool assists in the prediction process as the second step, determining the most probable migration ways by calculating bond-valence sums for each point in the crystal structure. Bond-valence energy landscape calculations then allow for an energetic estimation of jump energies.

The most promising structures are, eventually, fully electronically modelled by density functional theory (DFT) calculations *ab initio*. Calculating migration step energies subsequently enables a full assessment of jump energies from equilibrated structures as well as electronic conductivities and diffusion coefficients. As a very time-consuming method, DFT is applied as the final step.

This work presents the first results of the identification of promising oxidic Al-ion conductors involving all three approaches and their comparison.

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Keywords: Voronoi-Dirichlet, Bond-Valence, DFT, Ionic conductors, data mining