Bond Valence Sum (BVS) Energy Maps as an efficient tool for high-throughput analysis of materials for discovery of new Li-ion conductors

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Li-ion conducting materials are a key component in Li-ion batteries. Desirable properties of these materials include high Li-ion conductivity and three-dimensional conduction channels in the bulk of the material. At the moment, there are a very limited number of known suitable materials used in commercially manufactured Li-ion batteries. The Inorganic Crystal Structure Database (ICSD) contains many Li-containing materials which could have potentially promising Li-ion conduction properties. However, synthesis and measurement of large numbers of samples is not a feasible method of investigation of these materials.

The BVS energy map method is an efficient computational method for approximating the conductivity of crystalline materials. We use this method to analyse a substantial proportion of the Li-ion containing materials in the ICSD to potentially discover new materials which possess promising properties for Li-ion battery applications. A description of the BVS Method will be presented as well as some preliminary results and details about the implementation of the program.

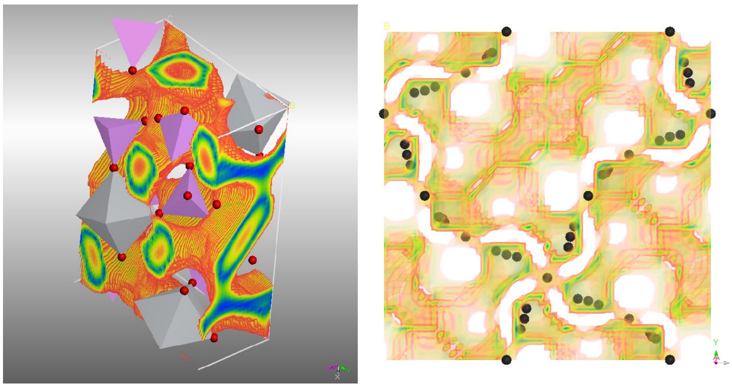

Figure 1. Examples of structures identified by BVS method with possess infinite connectivity of Li-ion pathways. Left: Isosurface showing volume containing likely positions of Li-ions according to BVS energy map. Blue region shows locations with highest probability of containing Li-ions. Note the continuous connectivity through the unit cell. Right: Shaded areas show likely occupation areas of Li-ions according to BVS energy map. Experimentally measured Li-ion positions (partially occupied) are shown as black spheres. Note the correlation between the BVS theoretical energy map and the experimentally measured Li-ion positions.