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Supporting information for article:

An investigation of the structural properties of Li and Na fast ion-conductors using high-throughput bond-valence calculations and machine learning

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Supporting information

S1. Computer programs description

See associated files po5136sup1.pdf and po5136sup2.pdf.

S2. Ranking lists of Li and Na compounds

See associated files po5136sup3.txt and po5136sup4.txt

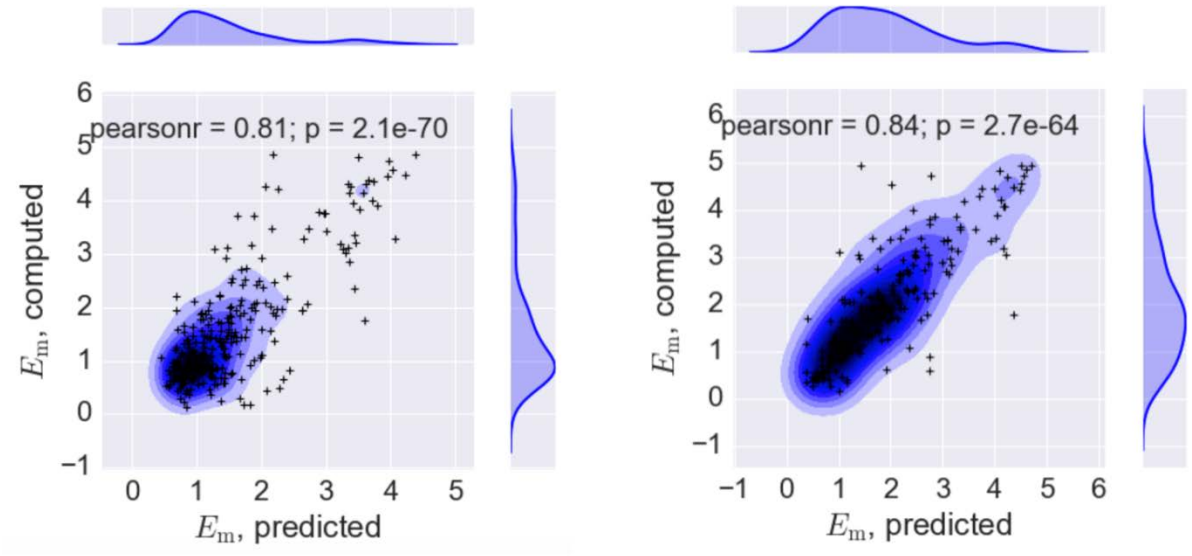

Fig. S1. Machine learning prediction of the migration energy (in eV) using three structural descriptors: the cation-anion coordination number, the percolation radius and the cation volume fraction. Left: Li compounds. Right: Na compounds.

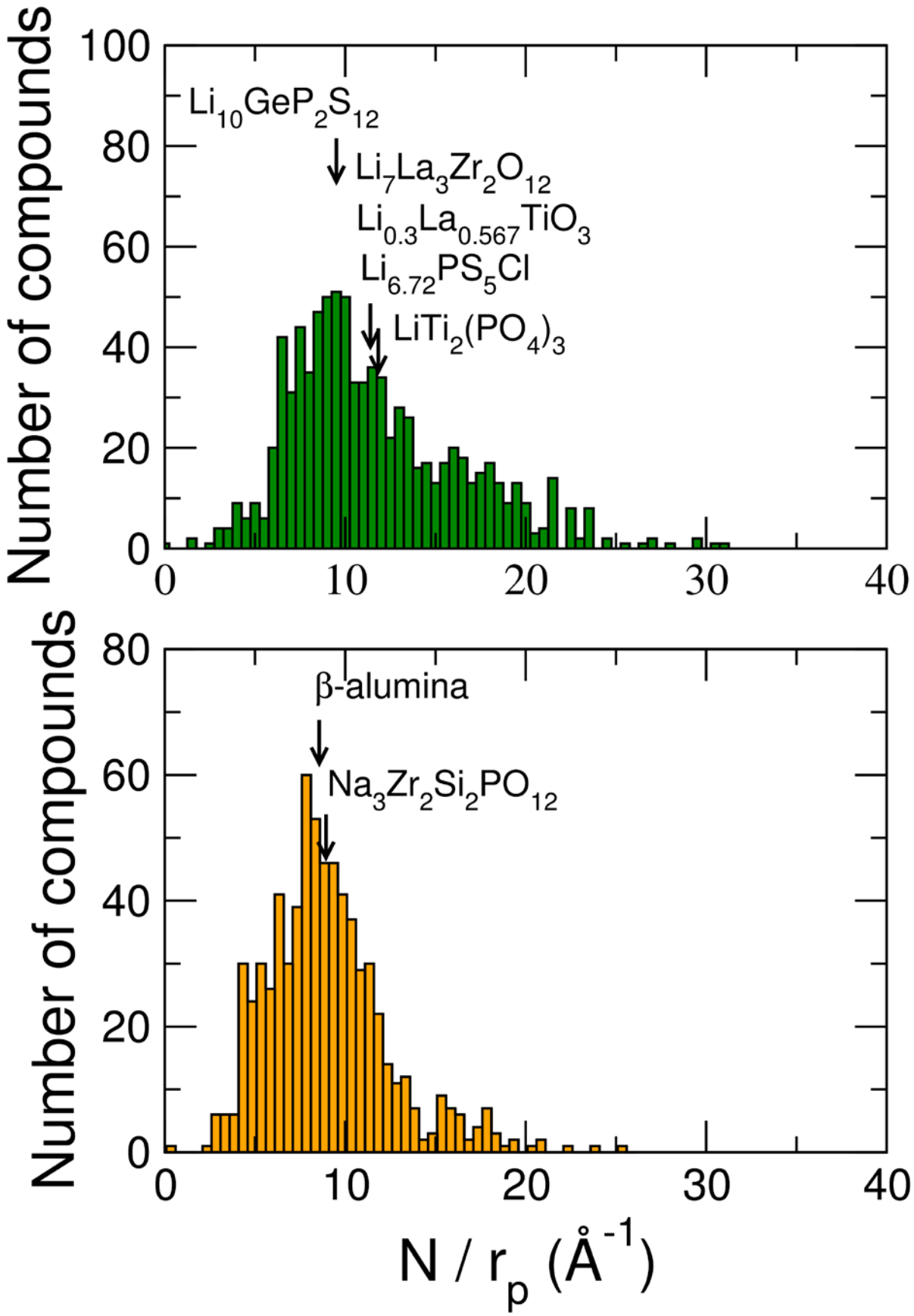

Fig S2. Number of scanned compounds as a function of the ratio between cation coordination number and percolation radius. Top: Li compounds. Bottom: Na compounds.

S3. BVEL vs density functional theory

It has been recently reported a study on the diffusion energy barriers of the layered oxide $Na_{2/3}Fe_{2/3}Mn_{1/3}O_2$ [Adv. Energy Materials, 7, 1601477 (2017)], using DFT calculations. It was observed that the Na diffusion path depends on the particular arrangement of Na ions. The Na ion diffuses across a tetrahedral site only if there is a di-vacancy next to it. If there is none, the ion migrates across a "dumbbell" of oxygen atoms, with a much greater energy diffusion barrier. In order to simulate these situations with BV theory, it must be removed only the Na ion that diffuses, and fix the rest. Fig. S3 shows the BV results. Yellow spheres represent the Na fixed ions, blue spheres the Na ion removed in the calculation of the BVEL. In the case where there is no di-vacancy (left figure), the diffusion path goes across the "dumbbell" of oxygen atoms. If we introduce a di-vacancy (right figure), then the diffusion path goes across the tetrahedral site, in agreement with DFT calculations.

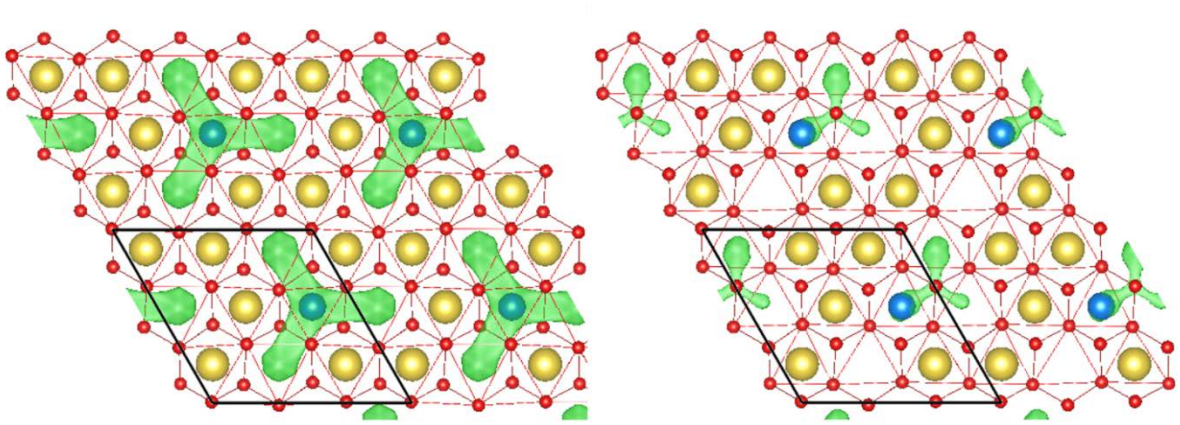

Fig. S3. Migration paths computed using the BVEL approach. Left (no di-vacancy): migration across the dumbbell of oxygen atoms. Right (di-vacancy): migration across the tetrahedral site.