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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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Abstract

Progress in energy-related technologies demands new and improved materials with high ionic conductivities. Na- and Li-based compounds have high priority in this regard owing to their importance for batteries. This work presents a high-throughput exploration of the chemical space for such compounds. The results suggest that there are significantly fewer Na-based conductors with low migration energies as compared to Li-based ones. This is traced to the fact that, in contrast to Li, the low diffusion barriers hinge on unusual values of some structural properties. Crystal structures are characterized through descriptors derived from bond-valence theory, graph percolation and geometric analysis. A machine-learning analysis reveals that the ion migration energy is mainly determined by the global bottleneck for ion migration, by the coordination number of the cation and by the volume fraction of the mobile species. This workflow has been implemented in the open-source *Crystallographic Fortran Modules Library* (*CrysFML*) and the program *BondStr*. A ranking of Li- and Na-based ionic compounds with low migration energies is provided.