How Well Do We Understand Ion Transport in Oxides?

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Ion transport in oxides plays an important role in energy and environmental applications and also in new concepts for data processing and storage. Examples are oxygen ion or proton conducting oxides for electrolytes in electrolyzers and fuel cells, lithium ion conducting oxides for electrolytes and electrodes in Li-ion batteries, and mixed conducting oxides in resistive switching devices.

I will present two approaches to understand these ionic transport processes. In the ab initio approach we use density-functional theory (DFT) to calculate on a microscopic level defect interaction energies and migration energies of defects. By means of Kinetic Monte Carlo (KMC) simulations we then predict macroscopic ion mobilities and ion conductivities on an ab initio level, i.e. without any adjustable parameters. As first example we will discuss rare-earth doped ceria. We show that all interactions between defects contribute to the so-called conductivity maximum of the ionic conductivity [1]. The second example concerns $BaZrO_3$-based oxides which are proto-type proton conductors. We show that the proton mobility is determined by nanoscale percolation of dopant ions which can enable high proton mobility [2].

In the model approach we use physical and chemical models to explain complex transport phenomena. We consider resistive switching where the electronic resistance of an oxide is determined by the redistribution of ions that are driven by an external voltage. We will discuss bulk switching in amorphous, non-stoichiometric gallium oxide, GaO_x [3,4], and filamentary switching in polycrystalline $SrTiO_3$ [5].

References

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