PERCOLATION EFFECTS DURING IONIC MOTION

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Interest in materials exhibiting oxygen ion and/or proton conduction has increased during the last years owing to their great importance for energy and environmental applications.

Ceria-based oxides are regarded as key oxide materials because rare earth-doped ceria shows a high oxygen ion conductivity even at intermediate temperatures. Using density-functional theory (DFT), we have investigated defect interaction and oxygen migration energies as well. By means of Kinetic Monte Carlo (KMC) simulations we then investigated the oxygen ion conductivity. We show that all interactions between the defects, namely vacancy-dopant attraction, dopant-dopant repulsion and vacancy-vacancy repulsion as well contribute to the so-called conductivity maximum of the ionic conductivity [1].

BaZrO₃-based oxides are proto-type proton conductors. Using density-functional theory (DFT), we have investigated defect interaction and proton migration energies in Y-doped BaZrO₃. The macroscopic proton conductivity was then investigated by means of KMC simulations. We discuss the resulting proton conductivities concerning special percolation pathways for protons [2].

Finally, we compare our theoretical results with experimental ones and discuss similarities and differences for oxygen ion and proton conductors.

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