Atomic level simulation of oxide ion migration in stabilized zirconia

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An atomic level understanding of oxide ion transport and degradation mechanisms is needed to realize the potential of solid oxide fuel cells. Atomistic simulations can shed light on defect-dopant and defect-defect interactions and improve our understanding of fundamental phenomena that govern the performance of fuel cells.

In the present work, molecular dynamics simulations have been performed using reliable potentials to study the mechanism of oxide ion migration in yttria and scandia stabilized zirconia.

The activation energies for oxide ion migration in stabilized zirconia have been determined for various yttria and scandia mole fractions. The results shed light on migration pathways and defect interactions, and are in excellent agreement with experimental data.