DIFFUSION IN IONIC CONDUCTORS FROM AB INITIO MOLECULAR DYNAMICS

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Even if diffusion in ionic conductors could be rather fast, to study it from accurate ab initio equilibrium molecular dynamics (MD) is usually impossible due to prohibitively long simulation times. The use of the nonequilibrium color-diffusion algorithm [1] allows one to substantially speed up the simulations. The algorithm has been implemented in the widely used Vienna Ab Initio Simulation Package (VASP) and applied to the problem of oxygen diffusion in doped ceria, a promising electrolyte material for intermediate temperature solid oxide fuel cells (IT-SOFCs). The application of the methodology speeds up the simulated oxygen transport by a factor 60 compared with standard equilibrium MD. The calculated conductivity values agree with the available experimental data, and the experimental temperature trend is well reproduced [2,3]. If time allows we also discuss the finite-temperature lattice dynamics and superionic transition in ceria and show how they can be treated despite all the difficulties [4].

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