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Diffusion of lithium in titanium oxide PATRICK SHEA, Dalhousie University, JIANCHAO YE, BRANDON WOOD, STANIMIR BONEV, Lawrence Livermore National Laboratory — Titanium oxide has generated interest lately as a promising anode candidate for use in lithium-ion batteries. We report first principles calculations on the mobility of lithium atoms in both crystalline and amorphous phases of titanium oxide. Density functional theory calculations of structural properties and diffusion energy barriers are combined with rate theory and a lattice gas model to study diffusion of lithium over a range of concentrations. A summary of results, including significant differences in the mobility between amorphous and crystalline phases, will be presented and discussed.

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