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Theoretical investigation of one- two- and three-dimensional Li diffusion in solids

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Possible migration pathways for Li ions in solids are investigated theoretically at density-functional theory level. The activation energies and migration pathways for local hopping events between neighboring lattice sites are calculated with the nudged elastic band method [1] as implemented in the VASP program package [2].

The possibilities for two- and three-dimensional diffusion are investigated for h-$LiTiS_2$ by comparing the calculated activation barriers for lateral migration in the *ab* plane and along the *c* lattice vector. The concentration dependence of two competing mechanisms for *ab* migration, via octahedral edges and via tetrahedral sites, is investigated [3]. In $Li_2Ti_3O_7$ one-dimensional channels exist that may lead to one-dimensional Li diffusion. We calculated the activation barriers along these channels and in the vertical direction in order to decide if this is the case. Three-dimensional Li diffusion is studied for a number of components, e.g. $LiBO_2$ [4]

References

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