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Simulating insertion and diffusion of lithium ions in V_2O_5

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Introduction

Vanadium pentoxide (V_2O_5) is a promising material to be used as cathode for lithium ion batteries due to its layered structure. We investigate the properties of Li ion insertion and diffusion in V_2O_5 using first-principles calculations on the base of density functional theory.

Development

For different phases of V_2O_5, our calculation reveal plateaus of the voltage curves, which represent very well the experimental data [1] of the using cylcles with respect to the reversible insertion of the lithium ions. This study is also used to evaluate the parameter set of the simulation.

In order to describe the diffusion processes, first-principle calculations are used to simulate diffusion pathways. The energetic barriers of those pathways are used to obtain the corresponding diffusion coefficients by employing two complementary methodologies: Kinetic Monte Carlo (KMC) simulations and a statistical thermodynamics approach. The KMC simulations for two different crystal planes give new evidence that the diffusion occurs mainly along the [010] direction, while the corresponding diffusion coefficients show a temperature dependence obeying the Arrhenius' Law. The necessity of considering concentration-dependent barrier heights in the KMC simulations is demonstrated by looking at the significant changes of the concentration-dependence of the diffusion coefficients [2]. The simulated diffusion coefficients of the combined approach show a good quantitative agreement with experimental data reported previously.

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References

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