Conference Abstract

Defect chemistry of α-Spodumene; an atomistic simulation-based study

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Abstract

Naturally occurring lithium rich α-Spodumene (α-$LiAlSi_2O_6$) is a technologically important mineral that has attracted considerable in rechargeable lithium ion batteries (LIBs), ceramics and polymer industries [1, 2]. The defect chemistry and dopant properties of this material are studied using well-established atomistic simulation techniques. The calculated lattice parameters are in good agreement with the experimental values [3] within a range of 2% showing the efficacy of the potential parameters used in this study. Isolated point defects (vacancies and interstitials) were considered and their energies were combined to calculate Schottky, Frenkel and isolated anti-site defect disorders. The most favourable intrinsic defect process is the Li Frenkel (1.40 eV per defect) ensuring the formation of Li vacancies required for the Li diffusion via the vacancy assisted mechanism. The second most stable defect energy process is calculated to be the Li/Al cation anti-site, in which Li and Al ions exchange their positions (2.31 eV/defect). The anti-site defect has been found in many oxide based materials including Li-ion battery materials. The present theoretical prediction require experimental verification.

Keywords: α-Spodumene, Defects, Atomistic simulation.

References

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