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Computational Modelling Study on Stability of Li-S/Se System

Lithium Sulphur batteries suffers from the low conductivity of S and the solubility of intermediary polysulfide species during cycling. It has been reported that Se and mixed SexSy represent an attractive new class of cathode materials with promising electrochemical performance in reactions with both Li ions. Notably, unlike existing Li/S batteries that only operate at high temperature, these new Se and Li/SexSy electrodes are capable of room temperature cycling. To study large systems and impact of temperature effectively, empirical interatomic potentials of Li2S were derived and validated against available experimental structure and elastic properties. Complex high temperature transformations and melting of Li2S was reproduced, as deuced from molecular dynamics simulations. Li2S was found to withstand high temperatures, up to 1250K each which is a desirable in future advanced battery technologies. Cluster expansion and Monte-Carlo simulations were employed to determine phase changes and high temperature properties of mixed Li2S-Se. The former generated 42 new stable multi-component Li2S-Se structures. Monte Carlo simulations produced thermodynamic properties of Li2S-Se system for the entire range of Se concentrations obtained from cluster expansion and it demonstrated that Li2S-Se is a phase separating system at 0K but changes to mixed system at approximately 350K.

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