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Phase stability prediction of mixed Li2S1-xSex system

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Recent rechargeable batteries are mainly based on conventional lithium intercalation chemistry, using lithium transition metal oxides as cathode material with typical capacities of 120-160 mA.h/g. The low energy density and/ or high cost of these cathode materials have limited their large scale production and application in Li ion batteries. Exploration of new cathode materials is consequently necessary to realise more efficient energy storage systems. Lithium sulphur cells have a promise of providing 2-5 times the energy density of Li-ion cells, however, they suffer poor cycling performance. Improvements that are effected by using Li/SeSxsystem in different electrolytes have been reported.
In the current study we employ computational modelling methods to explore stability, structural and electronic properties of discharge products formed in the Li/SeSx battery, which has potential to offer higher theoretical specific energy and remedies the challenges that Li-S battery encounters. First principle methods were used to calculate thermodynamic properties of Li2S and Li2Se, which agreed with available experimental results. A cluster expansion technique generated new stable phases of Li/SSex system and Monte Carlo simulations determined concentration and temperature ranges in which the systems mix. Interatomic Born Meyer potential models for Li2S and Li2Se were derived and validated and used to explore high temperature structural and transport properties of mixed systems.

Apply to be considered for a student ; award (Yes / No)?

No

Level for award;(Hons, MSc, PhD, N/A)?

N/A

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