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

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Li-ion batteries have transformed portable electronics and will play a key role in the electrification of transport. However, the highest energy storage possible for Li-ion batteries is insufficient for the long-term needs of society. Here we consider a study on rechargeable lithium–sulfur (Li–S) batteries which hold great potential for high-performance energy storage systems because they have a high theoretical specific energy, low cost, and are eco-friendly. This work employs computational modelling methods to explore stability, structural and electronic properties of discharge products formed in the Li-S/Se battery, especially Li₂S/Se, 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 Li₂S/Se 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 Li₂S/Se.

Apply to be
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Yes

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

PhD

Main supervisor (name and email)
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Yes

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