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Computational Study on Advanced Lithium – Sulphur Battery for Future Portable Energy Storage

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Abstract content
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Advanced energy storage systems are highly desired to meet the increasing demands of high energy density batteries. Rechargeable lithium batteries are expected to play a key role also in future energy storage, including both stationary and automotive applications.
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, for example, extended range electric vehicles. To go beyond the horizon of Li-ion batteries is a formidable challenge; there are few options. Here we consider a study on Li–S battery which holds the promise for the next generation of battery technology.

We investigated the stabilities and atomistic properties of discharge product Li< sub >2< /sub >S formed in Li- S batteries using density functional theory within the generalized gradient approximation and molecular dynamics. Their structural, mechanical, electronics and atomistic properties were determined. The lattice parameters were well reproduced and agree with the available experimental data. The heats of formation predicts that the structure are generally stable. The elastic constants suggest that all the structure is mechanically stable which was in good agreement with calculated phonon dispersions. The Buckingham interatomic potentials describing the interactions between lithium and sulphur were successfully fitted and validated since they produced same melting temperature same as experimental studies.

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