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Computational Study on Advanced Lithium – Sulphur Battery

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Abstract content
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Energy storage will be more important in the future than at any time in the past. Among the myriad energy-storage technologies, lithium batteries will play an increasingly important role because of their high specific energy and energy density.
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. The energy that can be stored in Li–S cells is compared with Li-ion; the operation of the cells is discussed, as are the significant hurdles that will have to be overcome if such batteries are to succeed. Fundamental scientific advances in understanding the reactions occurring in the cells as well as new materials are key to overcoming these obstacles.
In the current work we present a comparative study on stability, structural and electronic properties of discharge products formed in Li-S battery, using planewave pseudopotential methods. Structural parameters for the suggested materials were calculated and compare well with experimental results. The elastic constant of all the discharge products Li< sub >2< /sub >S and Li< sub >2< /sub >S< sub >2< /sub > formed in Li-S battery accord reasonably with experimental results, and the corresponding stability conditions are satisfied. Furthermore, the lattice dynamics of the products were calculated. The phonon dispersions also suggested that the structures are stable agree well with experimental studies using from neutron scattering experiments.

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MSc

Main supervisor (name and email)
and his / her institution

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