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First-Principle Study on Stabilities of Reactive Products of Sulphur and Oxygen in Lithium- and Sodium- air Batteries.

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Abstract content
   (Max 300 words)

Lithium-air batteries are potentially viable ultrahigh energy density chemical power sources, which could potentially offer specific energy up to 3000 Wh/kg being rechargeable. However, the realization of Li-air batteries has a number of difficult problems to overcome, the biggest shortfall exhibited with these systems is the formation of lithium dendrite which raises safety issues. We suggest here to replace the metallic lithium anode by sodium and operate the sodium-air cell, which could enable the development of a new generation of high specific energy rechargeable batteries.
We investigated the stabilities of insoluble discharge products of oxygen and sulphur in the Li-air and Na-air batteries(i.e.Li₂O, Li₂S, Li₂O₂, Li₂S₂ , Na₂O, Na₂S, Na₂O₂ and Na₂S₂ structures) using density functional theory within the generalized gradient approximation. Their structural, mechanical and electronic properties were determined. The lattice parameters were well reproduced and agree to within 2% with the available experimental data. The heats of formation predicts Li₂O and Na₂O to be the most stable structures whereas Li₂S₂ and Na₂S₂ are the least stable which is in good agreement with calculated phonon dispersions. The elastic constants suggest that all the structures are mechanically stable.

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