Density functional approaches to the energy storage and environmental materials: Theory and applications

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Development of new advanced materials is a key to addressing many challenges in energy problem and future sustainability. However, usual procedure of discovering new materials from experiments in a trial-and-error fashion usually tak far too long, and accelerating this process using scalable computations would significantly reduce the time and cost of new discovery. In achieving this grand goal of high-throughput materials screening and design, density functional theory offers a sweet spot between the accuracy and feasibility for large scale computations, but the present day density functionals still have some significant errors for many systems and also require significant algorithmic advances to be applicable for massive screening purposes. In the first part, I will briefly talk about some of our recent theoretical efforts to make density functional calculations very accurate to have a predictive power and also scale favorably with system size. In the second part, I will then spend most of the time demonstrating the utilization of these tools by showing several examples of energy and environmental applications we have studied, including secondary battery and carbon capture materials, which have successfully guided the experiments in several instances.

Reference:

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4. Anomalous Manganese Activation of a Pyrophosphate Cathode in Sodium Ion Batteries: A Combined Experimental and Theoretical Study, *J. Am. Chem. Soc.* 135, 2787-2792 (2013)