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Design and optimization of energy materials through computational analysis

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Although batteries and fuel cells are generally considered electrochemical systems, a surprising amount of their performance stems from the physics of the materials that make up their basic components: anode, cathode and electrolyte. Ionic conduction, electronic conductivity, chemical stability and voltage can all be traced back to intrinsic materials properties which are governed by fundamental physics, and specifically by the quantum mechanical properties of their electronic structure. In this talk, I will discuss how computational simulation (mainly DFT) can be used to gauge how these microscopic and atomistic properties of materials enhance or detract from the macroscopic performance in an electrochemical environment.

First, I will contrast oxide and phosphate batteries to show how the energy nearness of the transition metal d-states to the oxygen p-states introduces a bonding-antibonding pair that determines both the voltage and the stability against outgassing which potentially leads to flammability. This necessarily induces a trade off between stability and performance, and I will suggest some methods of mitigating this intrinsic contradiction. I will show how computational analysis of oxide coatings pointed towards a method of stabilizing inherently unstable materials against degradation that is currently being used as industry standard. Finally, I will relate the concepts learned from Li^+ diffusion in batteries to p^+ diffusion in solid acid fuel cells and introduce a new family of phosphide materials that were developed using computational prediction and analysis.