Accelerating Materials Discovery and Design through Computational Modeling

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The discovery and design of new materials has long played an enabling role in technological advances across a wide range of industries. Over recent years, a variety of composite nanomaterials have been used/tested for next-generation energy storage and conversion devices. However, in many cases little is known about their properties and performance, although such fundamental understanding is essential for further advances in energy storage and conversion technologies. Experiments may yield many clues to the behavior of those materials, but the interpretations are often controversial due largely to the difficulty of direct characterization. Under such circumstances, first principles-based computational approaches have emerged as one of the most powerful tools for design and development of new energy materials. This talk will focus on introducing our ongoing efforts in first principles modeling of energy storage and conversion materials. In the first part of my talk, I will present recent progress in our collaborative theoretical and experimental efforts to explore photocatalysts with the requisite band gaps, stability, costs, and abundance for solar-powered hydrogen production. Bismuth vanadate ($BiVO_4$) has received much interest as a promising visible-light-active photocatalyst for water splitting and pollutant decomposition. However, some fundamental aspects of its photocatalysis remain still unclear, including phase-dependent activity, doping effect, and surface reactivity. This talk will highlight the effects of crystal structure and doping on the photocatalytic performance of $BiVO_4$. In the second part, I will discuss the properties and performance of silicon-based nanomaterials for lithium-ion rechargeable batteries, particularly the impacts of surfaces, interfaces and alloying elements. From systematic first principles studies, we have found that the lithiation behavior of Si nanostructures and composites is considerably different from the case of bulk Si because of surface, interface, and/or alloying effects. The improved understanding can contribute to the rational design of Si-based anode materials to maximize capacity retention and rate performance.