Computational Design of Energy Relevant Materials: From Electrons to New Technologies

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Theory and computation are critical aspects of the materials discovery process. Electronic structure methods, such as density functional theory, excel at the characterization of macroscopic properties in materials that have yet to be realized. In this realm, a myriad of factors, such as strain, operation temperatures and pressures, as well as the stability of competing phases, come together to determine whether a material will exhibit favorable properties under the required operating conditions. Our efforts have focused on the prediction of materials with enhanced properties that can be synthesized and remain active under device relevant conditions. In this presentation, I will discuss our three-pronged approach which emphasizes synergies between (i) density functional theory calculations for properties predictions, (ii) empirical models for examining phase stability, and (iii) experimental validation. As an example, I will discuss our recent work towards the discovery and understanding of bifunctional catalysts (i.e. catalysts that can simultaneously accelerate the evolution and reduction of oxygen), advanced materials for the absorption of gases for applications such as carbon capture and hydrogen storage, and the discovery and design of Pb-free piezoelectrics (materials that convert mechanical stress into electrical current). Together, these examples illustrate a framework for accelerating the design and experimental realization of novel functional materials. This research was sponsored by the US DOE, Office of Science, BES, MSED and Early Career Research Programs.