UC RIVERSIDE UNIVERSITY OF CALIFORNIA | Materials Science and Engineering

WINTER 2020 COLLOQUIUM SPEAKER

Enabling a Sustainable Energy Future Through Theory and Computation

Fast growing economies, pollution concerns and climate change are fueling the search for new, sustainable sources of energy. A sustainable energy future requires the ability to generate, store and convert electricity for use at a desired time or place. At the heart of this effort is the need to identify and develop new materials for catalysis, energy storage and conversion. In recent years it has become clear that 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 structural phases, come together to determine whether a material will exhibit favorable properties under the required operating conditions. 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 that may aid in the realization of a truly sustainable energy future. This research was sponsored by the US DOE, Office of Science, BES, MSED and Early Career Research Programs.

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