

Spectral Signatures of Water Activation by Ions & Radicals

Prof. Ryan P. Steele

Henry Eyring Center for Theoretical Chemistry

The University of Utah

ABSTRACT

Redox-active ions and radicals form the chemical core of catalysts, including those used for modern renewable-energy purposes. Water-splitting chemistry, in which the energy of the sun is stored in the chemical bonds of molecules, is one particularly attractive route for renewable-energy storage, but this process also exhibits as many unanswered questions for chemists as it does promises for renewable-energy solutions. In spite of considerable recent success in developing water-splitting catalysts, the inner-sphere mechanisms of these catalysts remain opaque to commonly used electrochemistry techniques, and computational analyses afford the opportunity to examine these pathways. This presentation will focus on these inner-sphere mechanisms and properties of water activation by ions and radicals. Importantly, these computational experiments will be combined with recent spectroscopic and mass spectrometric measurements in order to craft a cohesive picture of the electronic structure of these complexes. Copper-based complexes, for example, will be shown to exist between traditional oxidation states, an observation that explains their anomalous spectroscopic behavior, their simulation challenges, and their chemical flexibility in their catalytic roles.

