

Abstract

Toward Efficient Catalysts for Energy Conversion: From Enzymatic Function to Functional Mimics

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Enzymes represent an invaluable source of inspiration for improving catalytic processes. In this talk, I will highlight how theory and computation, tightly integrated with experiment, help elucidate enzymatic functionalities germane to activating energy-relevant small molecules and how these concepts can help design selective, efficient, and sustainable bio-inspired catalysts. In the first part of the talk, I will discuss how hydrogenase enzymes finely regulate electron and proton movements and how this understanding can drive the design of new electrocatalysts for H₂ oxidation and production. Taking a step further, in the second part, I will illustrate a few examples of how enzymes can be redesigned to obtain control of product outcomes.