

DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2018

DATE: TUESDAY, FEBRUARY 13, 2018
WHERE: CENTRAL KING BUILDING - 116
TIME: 1:30PM

GUEST SPEAKER

Dr. Ke Yang
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New Haven, CT

TOPIC

Mimic nature to utilize light energy: computational approach to alternative and renewable energy solutions

ABSTRACT

Photochemical processes, which involve interactions between light and molecules, are of paramount importance in nature as they are the basis of photoinduced electron transfer in photosynthesis, photoisomerization in vision, photoprotection in DNA base pairs, and etc. In this talk, I will first discuss a new approach to construct high-dimensional potential energy surfaces and state couplings and apply it to the study of the dynamics of photodissociation of phenol, a model system for photoprotection of DNA. Then, I will discuss one of the most important photochemical reactions happens on earth, the photosynthesis, which converts solar energy into chemical energy to power our planet. I will focus on the most energy demanding process of photosynthesis, the water oxidation reaction, catalyzed by the oxygen evolving complex (OEC) embedded in a large transmembrane protein photosystem II (PSII). The mechanisms of the O-O bond formation are studied computationally and the kinetic isotope effects (KIEs) of different mechanism are predicted. By comparing the theoretically predicted KIE with experimentally measured KIE, we find the water nucleophilic attack mechanism, a water molecule attacking onto an oxyl radical, is most likely to be the underlying mechanism of water oxidation in PSII. We then discuss the implication of the water nucleophilic attack mechanism in artificial photosynthetic systems and how to develop efficient catalysts for water oxidation. Finally, the combination of water oxidation catalysts with semiconductor surfaces will be discussed in the context of solar water splitting and strategies to develop more robust and efficient photoelectrochemical systems for solar fuels will be discussed.

BIOGRAPHY

Dr. Ke Yang was born in Chenxi, China. He earned his B.S. degree in chemistry from Tsinghua University under the supervision of Professor Jun Li. He went to the United States for his graduate study in Professor Donald Truhlar's group at the University of Minnesota, where he obtained his Ph. D. degree in 2014. He has worked in Professor Victor Batista's group at Yale University since August, 2014. He is interested in excited states and dynamics of photochemistry, as well as the computational approaches to develop renewable energy solutions.

Committee members:

Dr. Lev Krasnoperov, Dr. Alexei Khalizov, Dr. Yong Yan