

Distinguished Lecture Series

presents

“Catalyst Discovery for Metal-Free, Photoredox CO₂ Reduction”***Professor Shaama Sharada***

University of Southern California

Abstract

Organic photoredox catalysis will be an important part of an energy-efficient, sustainable future as these catalysts can access highly reactive states upon excitation and quenching to carry out reactions that are otherwise thermally inaccessible or energy-intensive. Our group aims to identify sustainable photoredox routes for CO₂ utilization. Prior experiments show that a simple organic chromophore, p-terphenyl, can reduce and transform CO₂ into useful molecules such as amino acids. However, the steps of the photoredox cycle and reasons for low turnover numbers of these catalysts are poorly understood. Our goal is to utilize quantum chemistry methods to delineate mechanisms of key steps in this cycle and leverage these insights to drive discovery of novel chromophores that are both active and yield high turnover numbers. Thus far, we have demonstrated that the electron transfer (ET) step from the p-terphenyl radical anion to CO₂ is adiabatic, and ET barriers are lowered when electron-donating groups are substituted to p-terminal positions of the catalyst. To probe degradation pathways from the excited state, we are establishing a protocol for calculation and characterization of excited-state donor-acceptor charge transfer complexes in collaboration with the Dawlaty group (USC). We are also taking our first steps towards driving discovery of new chromophores by implementing a genetic algorithm (GA) whose fitness function factors in both catalyst activity and degradation resistance by means of simple descriptors obtained from routine DFT calculations. The GA yields several candidates that are more viable than experimentally studied terphenyls, highlighting the importance of automated computational tools in accelerating experimental efforts.

Biography

Dr. Shaama Mallikarjun Sharada is the WiSE Gabilan Assistant Professor in the Mork Family Department of Chemical Engineering and Materials Science and Assistant Professor in the Department of Chemistry at USC. Her research interests span the development and application of quantum chemistry methods to design catalysts for sustainable chemistry transformations. Her group is developing efficient algorithms, inspired from signal processing, for advancing sophisticated rate theories in catalysis. The group is also establishing frameworks for catalyst design and discovery towards efficient natural gas conversion and light-assisted carbon dioxide utilization. Dr. Sharada received her Bachelors and Masters in Chemical Engineering from the Indian Institute of Technology, Bombay (India) where she was awarded the Institute Gold Medal. She received her PhD in Chemical Engineering from UC Berkeley in 2015 for developing efficient reaction path search algorithms for catalysis. As a postdoctoral researcher at Stanford University, her work spanned the development of machine learning density functionals and surface chemistry benchmarking databases. She is a recipient of the 2022 inaugural Chevron Research Innovation Award (USC) and the 2020 ACS Petroleum Research Fund Doctoral New Investigator Award. She is also a Scialog Fellow for the Negative Emissions Science initiative.

**September 20, 2022****4:00P.M.****Location: ZHS 352**