

MIT Chemical Engineering Department

Spring 2018 Seminar Series

<http://cheme.mit.edu/seminar-series/>

Computational Design and Prototyping of Organic Catalysts for Photopolymerization and CO₂ Reduction



Charles B. Musgrave

Chair and Professor of Chemical and Biological Engineering and
Professor of Chemistry and Biochemistry, by courtesy
Joint Appointment, National Renewable Energy Laboratory
Fellow, Renewable and Sustainable Energy Institute
Fellow, Materials Science and Engineering
University of Colorado, Boulder

Friday, April 20, 2018

3:00pm (reception at 2:45pm)

66-110

Abstract:

Inorganic catalysts have been workhorses in many important industrial processes while many biological systems, such as photosynthesis, rely on organic catalysts. In this talk I will discuss the use of computational chemistry to examine organic catalysts and photocatalysts for visible light activated atom transfer radical polymerization (ATRP) and CO₂ reduction into fuels. In both cases, dearomatization of the catalysts leads to powerful reducing agents capable of challenging reductions either by electron transfers or hydride transfers. Using various substituents the thermodynamic and kinetic properties of these catalysts can be optimized for various reductions to make them fast, yet energy efficient. Our ATRP photocatalyst designs were synthesized and characterized for their efficacy, which confirmed that the best designs effectively photocatalyze polymerizations by ATRP using visible light and result in polymers and block copolymers with no metal contamination and properties that rival the best materials catalyzed with optimized, but expensive metal catalysts.