Computational Design and Prototyping of Organic Catalysts for Photopolymerization and CO_2 Reduction

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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 the fundamental chemical mechanisms of organic catalysts and photocatalysts for reducing CO_2 into fuels and visible light activated atom transfer radical polymerization (ATRP). In both cases, dearomatization of the aromatic core of the catalysts leads to powerful reducing agents capable of challenging reductions either by electron transfers or hydride transfers. Using various substituents, we can tune the thermodynamic and kinetic properties of these catalysts to optimize them for various reductions to make them fast, yet energy efficient. Our ATRP photocatalyst designs were synthesized, characterized and tested in ATRP experiments by our collaborators for their efficacy. They confirmed that our 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.

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