Dr. Charles B. Musgrave  
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University of Colorado, Boulder  

"Computational Design of Organic Catalysts and Photocatalysis"  

Inorganic catalysts have been workhorses in many important industrial processes while many biological systems, such as photosynthesis, rely on organic catalysts. Dr. Musgrave 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, deamination 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.

**Required Graduate Student Seminar for ChE 5971**  
Refreshments served before Seminar

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Accommodations on the basis of disability are available by contacting the office.