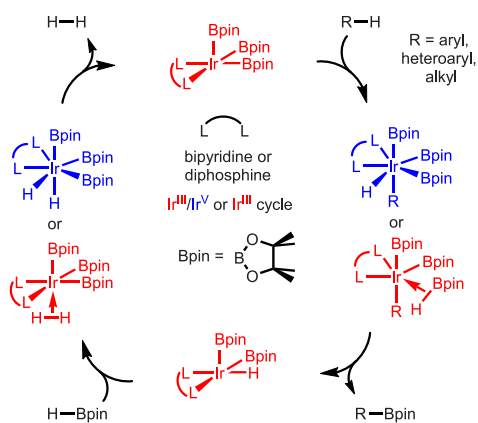


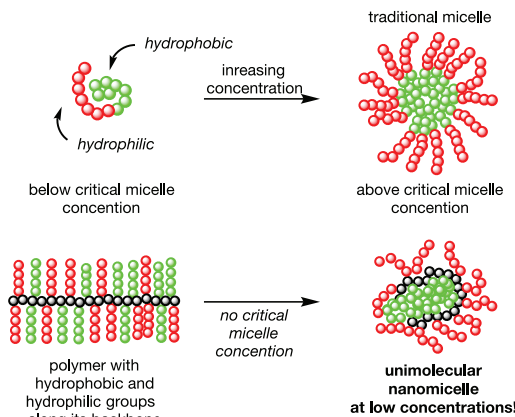
Our research ranges from developing metal-catalyzed reactions that act on organic and inorganic substrates, to designing polymers that interact in interesting ways with enzymes and drugs. The connecting theme is developing new chemistry and mentoring the next generation of scientists to tackle the challenge of sustainably meeting the needs of our species, which is predicted to number 9.5-13 billion people by the year 2100. We have several ongoing projects and frequently collaborate with scientists in academia and industry.

We have had long-standing interest in reactions of metal boryl complexes ( $M-BZ_2$ , where Z is an anionic substituent such as alkoxide) with organic molecules. Organoboron compounds are used extensively in pharmaceutical, agrochemical, and advanced materials industries. Consequently, new chemistry within this molecular class can eliminate steps and reduce waste streams associated with synthesis of these valuable intermediates. In this regard, we have developed new catalytic reactions, such as additions of B-B bonds to olefins and synthesis of B-C bonds from hydrocarbons and boranes, etc. The first thermal example of the latter catalytic reaction, now commonly referred to as C-H borylation, was discovered in our group. More recently, mechanistic studies integrating experimental and computational approaches have given us a deeper understanding of C-H borylation. The computational work is inspiring the design of new catalysts and boron reagents that are tailored to specific substrate classes.



#### The catalytic cycle for Iridium C-H borylation.

Our early polymer work focused on synthesis of biodegradable polymers with controllable properties. This evolved into the design of monomers with functional groups, which gave polymers that could readily be modified through chemical reactions. Recently, we have found that by incorporating combinations of hydrophobic and hydrophilic groups along the backbone, polymers that behave as nanomicelles can be prepared. Since the length of the initial polymer, and the sizes

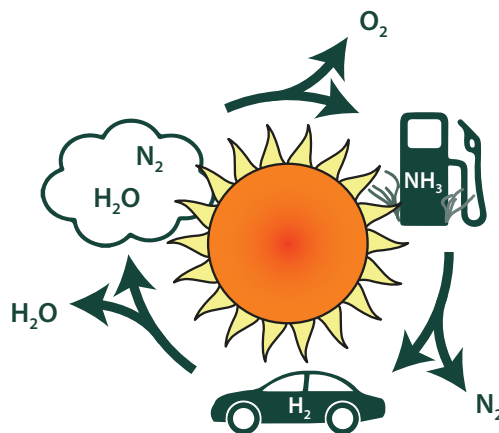


#### Design principles for controlling micelle size and assembly through polymer synthesis.

of hydrophilic and hydrophobic groups that are subsequently introduced, determine the sizes of the nanomicelles, we are exploring host-guest chemistry of these materials. For example, we have found that the nanomicelles can interact with enzymes to make them soluble in organic solvents with retention of enzymatic activity.

The newest project in our group explores the synthesis of ammonia and related nitrogen compounds using renewable energy. Ammonia synthesis via the Haber-Bosch process currently consumes approximately 2% of the energy we produce. The  $H_2$  that is required in the Haber-Bosch synthesis is produced by reacting methane or coal with water, which also generates large quantities of  $CO_2$ . Our goal is to develop new approaches for  $NH_3$  synthesis that can be coupled effectively to renewable energy sources like solar and wind, whose availability is intermittent.

The flip side of this project is that ammonia and other nitrogen compounds like hydrazine have been used as fuels. In fact, the X-15 aircraft that still holds speed and altitude records was fueled by  $NH_3$ . An example of a renewable nitrogen-based fuel cycle is shown below.



#### A cycle where nitrogen, water, and renewable energy could produce fuels with no $CO_2$ emissions.



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### Inorganic and Organic Chemistry for Sustainability in the 21<sup>st</sup> Century

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