



## James McCusker, Ph.D.

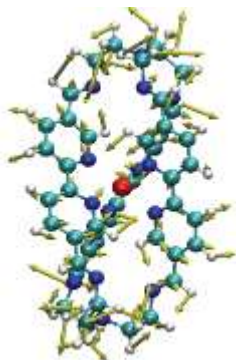
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### Tailoring the Photophysics of First-row Transition Metal-based Chromophores for Applications in Light-to-Chemical Energy Conversion: Challenges and Opportunities

#### ABSTRACT:

The interconversion of light and chemical energy is one of the most fundamental processes on Earth. Research on solar energy conversion, for example – which will ultimately lead to the next generation of solar energy technologies – has sought to replicate Nature's solution through the realization of artificial constructs that mimic various aspects of photosynthesis. Whether it is the creation of potential gradients to generate current (i.e., photovoltaics) or more recent efforts coupling photo-generated electrons and holes to catalysts (e.g., photoredox catalysis), the critical first step is the absorption of light and the subsequent separation of charge. Transition metal-based chromophores are particularly well-suited for use in such schemes by virtue of the charge-transfer excited-states that a majority of them possess. Indeed, tremendous advances have been made through use of compounds such as  $[\text{Ru}(\text{bpy})_3]^{2+}$  and  $\text{Ir}(\text{ppy})_3$  in areas ranging from solar energy conversion to photoredox catalysis. Despite the obvious advantages of ruthenium- and iridium-based chromophores, the fact that these elements are among the rarest in the earth's crust raises legitimate questions concerning cost and scalability of processes reliant on such chromophores. Such issues, coupled with the possibility of unlocking new chemistry, has motivated exploring the possibility of replacing these compounds with chromophores based on earth-abundant first-row transition metals that can carry out analogous excited-state reaction chemistry. With these



**Figure 1.** Nuclear displacements associated with the coherent oscillations accompanying excited-state evolution in an Fe(II)-based chromophore developed in our lab. These vibronic coherences were used as a guide for synthetic modification of the compound that altered its excited-state dynamics (*Nature*, **2020**, 582, 214-218)

opportunities come significant challenges due to inherent differences in the electronic structures of first- versus second- and third-row metal complexes that profoundly impact the ability of such compounds to engage in the desired chemistry. The focus of our research program is therefore to understand the factors that determine the dynamics associated with charge-transfer excited-states of first-row transition metal-based chromophores, with the ultimate goal of circumventing and/or redefining their intrinsic photophysics in order to make feasible their use in a variety of light-driven applications. This seminar will outline the key scientific issues defining this challenge as well as discuss recent examples from our lab illustrating how these challenges can be met and, ultimately, overcome.

#### BIO:

Jim McCusker was born in New Haven, Connecticut in 1965. A graduate of Bucknell University (where he majored in Chemistry with minors in Physics and Music), Jim enrolled in the doctoral program at the University of Illinois at Urbana-Champaign in 1987 and carried out research in physical-inorganic chemistry under the guidance of Professor David N. Hendrickson. Jim was awarded a two-year post-doctoral fellowship from the National Institutes of Health in 1992 to work with Professor Thomas J. Meyer at the University of North Carolina, then began his independent academic career at the University of California at Berkeley as an Assistant Professor of Chemistry in the fall of 1994. While at UC-Berkeley, Jim was awarded the Department of Chemistry Teaching Award in 1999 in addition to being named an Alfred P. Sloan Fellow (1998 – 2000) and a Hellman Faculty Fellow of the University of California (1997 – 1998). Jim moved his research group to Michigan State University in 2001 where he is currently MSU Foundation Professor of Chemistry. The central themes of his research group revolve around the light-induced properties of transition metal-containing molecules – in particular as they impact the development of solar energy conversion strategies and photoredox catalysis – as well as the interplay of spin, magnetism, and the excited-state dynamics of molecular systems. Jim has been recognized at Michigan State with the 2014 Junior Faculty Mentoring Award, the 2016 College of Natural Science Outstanding Faculty Award, and the 2018 William J. Beal Outstanding Faculty Award by the President of Michigan State University. Named a Fellow of the Royal Society of Chemistry in 2016 and recipient of their Chemical Dynamics Award in 2020, Jim has published nearly 100 articles in journals including *Science*, *Nature*, *Chemical Science*, and the *Journal of the American Chemical Society*, and has given in excess of 300 invited seminars at universities and conferences in more than 20 countries around the world. He is currently Associate Editor for Physical-Inorganic Chemistry at *Chemical Science*, the flagship journal of the RSC.