Plenary Talk PV XVIII Fri 9:15 B Audimax

The Role of Spin in the Photo-induced Ultrafast Dynamics of Transition Metal-based Chromophores — •James McCusker — Department of Chemistry, Michigan State University, East Lansing, Michigan USA

From fundamental issues concerning the interplay between geometric and electronic structure to their applications in energy conversion and chemical transformation strategies, the excited-state properties of transition metal complexes constitutes a very dynamic area of chemical research. This presentation will examine the role of spin and its influence on the photophysics of transition metal complexes through a discussion of three chemical systems. First, variable-temperature ultrafast time-resolved spectroscopic data acquired on a series of Fe(II) polypyridyl complexes will be presented that provide quantitative insights into the reorganization energies and electronic coupling involved in a conversion that is characterized by a two-quantum spin flip (i.e., $\Delta S = 2$); in this case, the dynamics are clearly dominated by the doubly spin-forbidden nature of this relaxation pathway. The role of spin becomes less well-defined when it comes to ultrafast excited-state evolution. This will be explored through a discussion of two chemical platforms that we have developed, one based on Fe(II) in which changes in spin-state appear to play no role whatsoever in dictating the kinetics of excited-state evolution, and a second based on Cr(III) in which spin not only influences these kinetics but can be controlled systematically through synthetic means. The possibility of leveraging these ideas toward problems in energy science will also be discussed.