TRACKING THE REACTION COORDINATE OF ULTRAFAST SPIN-CROSSOVER IN Fe(II) COMPLEXES WITH FEMTOSECOND M-EDGE XANES

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Designing earth-abundant photosensitizers to replace rare-earth complexes is of high importance for the efficient collection and utilization of solar energy. The primary obstacle to using first-row transition metal complexes is the ultrafast dissipation of collected energy due to low energy metal-centered states.

Here, we study a series of Fe(II) complexes with different ligand frameworks in hopes to alter the intersection between various metal-centered states. Using femtosecond M-edge XANES, the involvement of triplet and quintet metal-centered states are identified. By decoupling the axial and equatorial stretching modes of an Fe(II) complex, we find that the lifetime of a triplet metal-centered state is significantly increased due to Jahn-Teller distortion in the excited state. This behavior is not observed in prototypical Fe(II) polypyridyl complexes, and provides a method to reduce energy losses in earth-abundant photosensitizers.