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Ultrafast intersystem crossing in nickel porphyrins JAVIER FERNANDEZ-RODRIGUEZ, JUN CHANG, A.J. FEDRO, MICHEL VAN VEENENDAAL, Department of Physics, Northern Illinois University, DeKalb, IL 60115 — We study the relaxation dynamics to the metastable state in laser-pumped nickel porphyrins. We use a ligand-field model which takes into account the crystal field created by the porphyrin ring and axial ligands. We propose different decay pathways in terms of charge-transfer and metal-center intermediate states. By accounting for the energy redistribution of the lattice vibrations we get an irreversible decay to the metastable state within the order of a few hundred femtoseconds. We show how non-equilibrium time-dependent x-ray absorption at the Ni K-edge measurements can elucidate the nature of the intermediate states involved in the decay. Understanding radiationless transitions in transition-metal complexes is of interest for their relevance for the design of photocatalytic systems and photothermal sensitizers for cancer treatment.

Javier Fernandez-Rodriguez
Northern Illinois University

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