

# Probing Ultrafast Electron Delocalization Dynamics on Molecular Excited States in Solution

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Ultrafast photochemical processes result from a complex interplay between atomic and electronic motions on the timescale of a molecular vibration. Our ability to understand, predict and ultimately control the outcome of photoinduced chemical phenomena hinges on the continued development and use of novel femtosecond technologies. In this talk I will discuss a prototypical transition metal mixed valence system which undergoes rapid forward and back electron transfer. Femtosecond two-dimensional vibrational-electronic spectroscopy has revealed coherent couplings between the high-frequency cyanide stretching modes and the metal-to-metal charge transfer transition [1, 2]. Femtosecond Fe K-alpha X-ray emission spectroscopy directly measures the lifetime of the charge transfer excited state. Femtosecond XANES experiments coupled with *ab initio* molecular dynamics calculations on the electronic excited state reveal the transient electronic structure across the donor-bridge-acceptor interface on a sub-100 fs timescale.

## References:

- [1] T. L. Courtney, Z. W. Fox, L. Estergreen, and M. Khalil, *J. Phys. Chem. Lett.* **6**, 1286 (2015).
- [2] T. L. Courtney, Z. W. Fox, K. M. Slenkamp, and M. Khalil, *J. Chem. Phys.* **143**, 154201 (2015).