

Electron transfer, Marcus theory, and Spin Chemistry

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Bob Cave had a deep interest in both theoretical and practical aspects of electron transfer theory. In this talk, I will attempt to highlight some of the big questions that my group is trying to answer nowadays regarding the fluctuations that lead to electron transfer, the time for decoherence, and the role of spin degrees of freedom.

I will also cover some of the practical means by which one can address these questions for realistic systems, with tools ranging from electronic structure all the way to statistical mechanics.