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NANOSCIENCE SYMPOSIUM

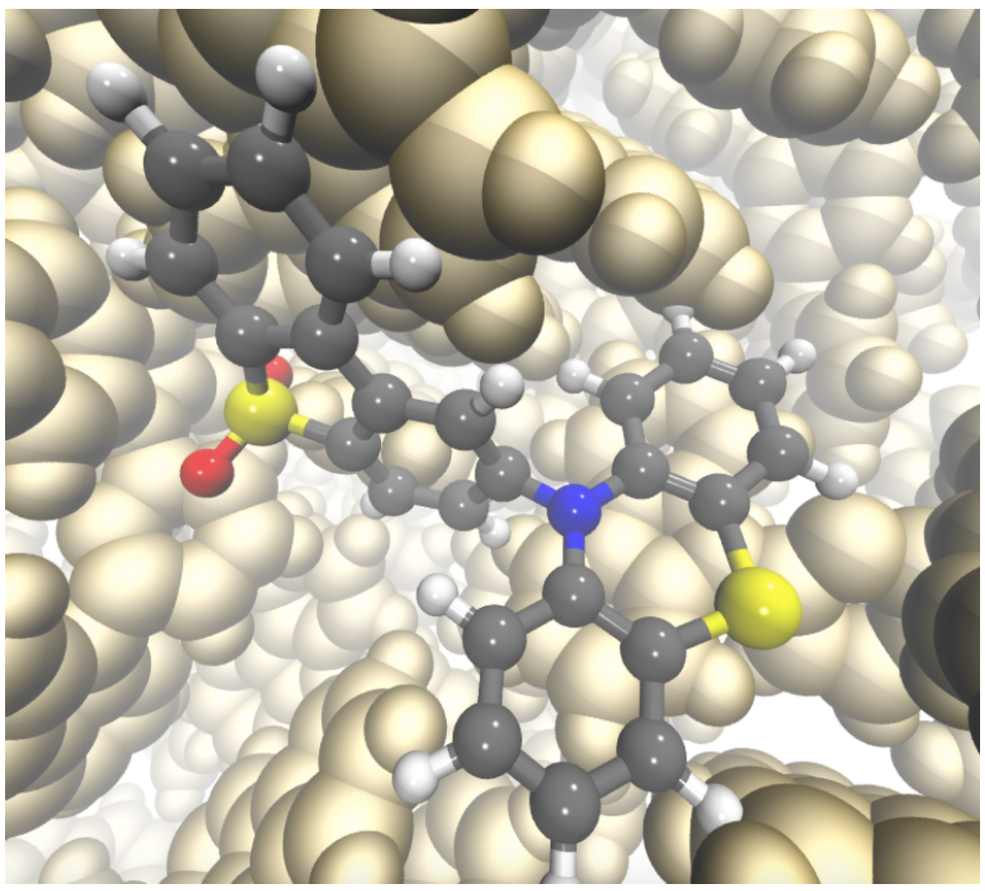
Understanding and Designing Photophysics Beyond the Born-Oppenheimer Approximation

Dr. Tom Penfold

Newcastle University, UK

Abstract:

The communication between low lying singlet and triplet excited states plays a fundamental role in determining key molecular and material properties. Consequently, a thorough understanding of the basic principles governing the interplay between these manifolds of spin states is of great importance. Herein I will present some of our recent results on spin-vibronic dynamics in the context of enhancing the communication between singlet and triplet states in organic and metal-organic molecules. I will show that in many cases intersystem crossing is dynamic, in the sense that it depends on specific molecular vibrations [1,2]. I will also discuss the importance of multiple coupled excited states, which can enhance the effect of the local environment. The understanding provided by these simulations, sets the foundations for advanced design rules beyond the Born-Oppenheimer Approximation.



References:

1. TJ Penfold, et al. Chem. Rev. 118:6975 (2018).
2. T.J. Penfold, et al. Chem. Comm., 54:3926, (2018).

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