Excited state dynamics of transition metal complexes using efficient trajectory surface hopping methods.

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Modelling excited state dynamics of transition metal complexes is challenging for different reasons: the many degrees of freedom, the large number of near degenerate electronic excited states, and last but not least, the difficulties of electronic structure methods to describe accurately the energy and character of different electronic excited states. In this lecture I will describe our most recent efforts to use trajectory surface hopping (SH) methods [1] to model the photophysical dynamics of several transition metal complexes. To alleviate the huge costs of such calculations, we have recently coupled SH to linear vibronic coupling (LVC) models [2]. The combination of LVC within SH offers extreme computational efficiency [2], allowing even to run SH for these large systems with different setups. Besides time-resolved chemical insight, this marriage offer opportunities for methodological benchmarks. On the one hand, SH can be used to identify essential degrees of freedom and electronic states that could be employed in a quantum MCTDH wavepacket propagation in reduced dimensionality. On the other, a comparison of SH with MCTDH dynamics with the same LVC model allows to question the validity of several assumptions of SH.

References

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