

CALCULATING LIFETIMES IN PHOTOACTIVE TRANSITION METAL COMPLEXES

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Transition metal complexes that are optically active are amenable to many fields, from clean energy research to photodynamical therapy. They can serve as photocatalysts, photosensitizers, luminophores, and much more. In order to tailor their properties, it is necessary to understand which processes take place after light irradiation, e.g. all the way to the luminescent state, or which deactivation pathways compete to each other in a particular reaction. Given the large number of electronic and nuclear degrees of freedom that can play a role after irradiation in metal complexes and the presence of simultaneous vibronic and spin-orbit couplings, an accurate theoretical description is challenging in most cases [1]. In this contribution, we showcase the power of theory to calculate lifetimes in two scenarios. In the first part, we show how temperature-dependent emission lifetimes can be quantitatively predicted. We use $[\text{Ru}(\text{bpy})_3]^{2+}$ to demonstrate that when multiple pathways involving Jahn-Teller isomers of the intermediate triplet metal-centered (^3MC) excited states are considered, lifetimes can be in excellent agreement to experimental values [2]. In the second part, we illustrate how to obtain relaxation lifetimes from excited-state dynamics, using trajectory surface hopping simulations on-the-fly [3] and with parameterized vibronic coupled potentials [4].

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