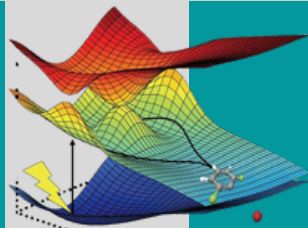


"SIMULATION OF EXCITED-STATE DYNAMICS OF TRANSITION METAL COMPLEXES"



ABSTRACT

Simulation of Excited-State Dynamics of Transition Metal Complexes

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The simulation of photodynamics of molecules is based on the description of coupled movement of the atomic nuclei in the molecule on the potential energy surfaces generated by the electrons. For transition-metal complexes, the description of these dynamics is particularly challenging due to their large number of vibrational degrees of freedom and many close-lying electronic states. When quantum dynamics is used to simulate transition-metal complexes, this imposes the use of truncated models with typically only few degrees of freedom and electronic states, where the electronic potentials are often described in parameterized vibronic coupling models. An alternative to quantum dynamics that can include all degrees of freedom and large number of electronic states is given by on-the-fly surface hopping (SH) methods. However, the repeating cost of the underlying electronic structure calculations in SH restricts the range of possible simulation times for molecules the size of transition-metal complexes severely.

By using SH on vibronic-coupling potentials, we can now lift the simulation-time restriction in SH and enable full-dimensional nonadiabatic dynamics simulations of transition-metal complexes on picosecond time scales. This is demonstrated for two examples. First, using CASSCF-derived linear vibronic-coupling (LVC) potentials, we can unravel the relaxation mechanism to the phosphorescent singlet state of a near-infrared emitting vanadium(III) complex with an open-shell triplet ground state, allowing us to establish a clear model to improve luminescence. Second, combining SH on LVC potentials with SH on ab initio potentials, we can capture both ultrafast bond breaking as well as long-time dynamics populating emissive states of a closed-shell rhenium(I) carbonyl diimine complex used in photoactivated redox reactions.

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September 10, 2021 (Friday)
12pm (BRT time) - Google Meet

ORGANIZATION:

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with the words "Patrick Zobel - Virtual" on the "subject"

Deadline: September 09, 2021 (Thursday), 06pm (BRT time)