



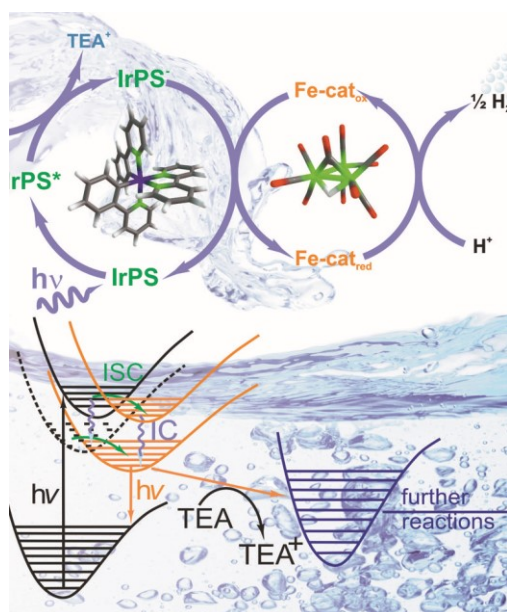
**19<sup>th</sup> February 2020 - 2:00 p.m.**  
CFEL-bldg. 99, seminar room IV

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## Unraveling the elementary steps of photosensitizer dynamics using methods across the spectrum from IR to X-ray

Transition metal complexes play an essential role as photosensitizers, photoemitters, and dyes. The theoretical description of mechanistic details of the associated processes are complicated due to (i) the nontrivial electronic structure with system sizes calling for density functional theory, which is challenged by correlation effects and charge transfer transitions, (ii) a pronounced spin-orbit coupling giving rise to spin forbidden mixing up to the point where a classification in terms of spin-free states ceases to make sense, and (iii) the practical use of photosensitizers as part of complex reaction schemes involving multiple reactants and products. All together these points are shaping the landscape of multidimensional nonadiabatic functional dynamics.



During the last years, we have applied electronic structure and theoretical spectroscopy methods to characterize the elementary steps of an exemplary hydrogen-generating photocatalytic cycle employing on an Ir-photosensitizer and a Fe-based water reduction catalyst. Our efforts comprised the electronic excitation and charge separation, the reduction of the photosensitizer as well as the electron transfer to the Fe-based catalyst. This talk will give an overview and address methodological challenges.

References: J. Phys. Chem. Lett. 2014, 5, 1355; PhysChemChemPhys 2014, 16, 4789; Coord. Chem. Rev. 2015, 304, 133; ChemCatChem 2016, 8, 404; Inorganics 2017, 5, 23; J. Chem. Theory Comput. 2018, 14, 5870; arXiv:1911.01254.