CFEL SCIENCE

SEMINAR

25th April 2018 - 2:00 p.m.

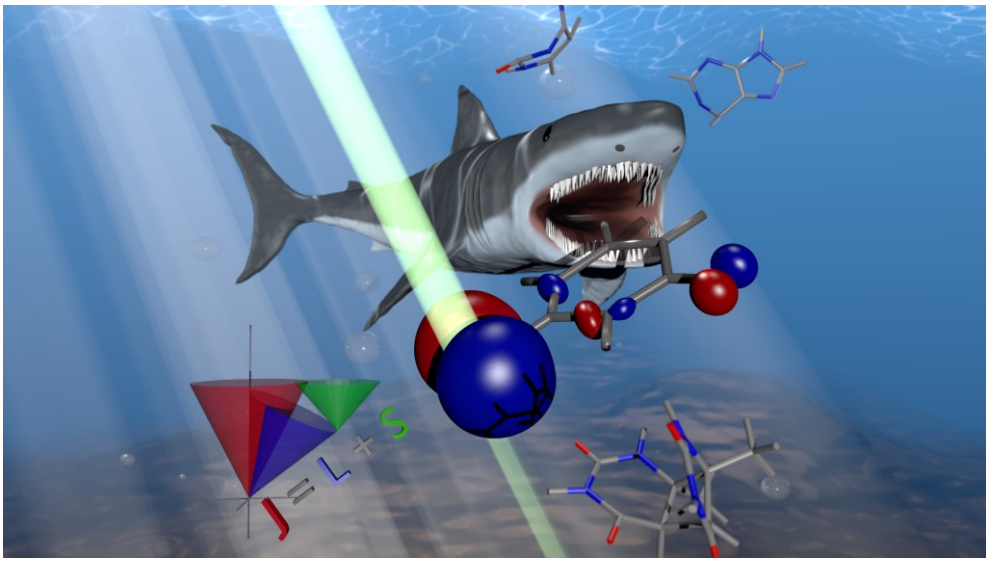
CFEL-bldg. 99, seminar rooms II-III

Leticia Gonzalez

University of Vienna, Institute of Theoretical Chemistry

Dancing with SHARCs, a theoretical view of molecular excited state dynamics

When molecules are electronically excited they can explore different regions of the excited potential energy surfaces. I will show how theoretical methods can be used to unravel the pathways molecules take after light irradiation. To this aim, we employ a locally developed ab initio molecular dynamics code, coined SHARC, which allows the simultaneous inclusion of non-adiabatic and spin-orbit couplings, and can therefore describe internal conversion and intersystem crossing on the same footing. Prototype examples discussed will include organic molecules but also transition metal complexes, the latter presenting extraordinary efficient femtosecond time scale intersystem crossing.



Host: Robin Santra – CFEL-DESY Theory Division