From Twisting Motions to Function: Towards Design Principles for Photoactive Molecules

C. Müller, Erlangen/GER
Jun.-Prof. Carolin Müller, Friedrich-Alexander-Universität Erlangen-Nürnberg,
Computer-Chemistry-Center, Nägelsbachstraße 25, 91052 Erlangen

Understanding how photoexcitation reshapes a molecule's geometric and electronic structure is key for the rational design of responsive functional molecules and materials. In this talk, I will present theoretical studies on molecular systems that undergo pronounced conformational changes in the excited state, such as molecular switches and twisted intramolecular charge transfer (TICT) systems. The emphasis will be on the interplay between quantum chemical simulations and (time-resolved) spectroscopy, particularly (transient) IR and UV/Vis absorption techniques, examining how these methods jointly reveal how structural twisting influences transient spectroscopic features, and how this understanding can be translated into practical design principles.

Short Curriculum Vitae

I am a chemist passionate about unraveling the mysteries behind the behavior of photoexcited molecules using quantum chemical-, cheminformatical- and spectroscopic methods.

since 11/2023	Juniorprofessor for the Theory of Electronically Excited States, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
06/2022–10/2023	Feodor Lynen Postdoctoral Researcher, University of Luxembourg, Luxembourg
03/2021–05/2022	Postdoctoral Researcher, Friedrich Schiller University Jena, Germany
09/2018–02/2021	Dissertation (Dr. rer. nat), Friedrich Schiller University Jena, Germany
10/2013–09/2018	B. Sc. and M. Sc. in Chemistry, Friedrich Schiller University Jena, Germany