MO 12: Poster – Novel Experimental Approaches and Novel Theoretical and Computational Approaches

Time: Tuesday 17:00–19:00 Location: Philo 1. OG

MO 12.1 Tue 17:00 Philo 1. OG

Analysis of ultrafast structural dynamics based on single-shot XUV FEL data through deep learning — •Viktoria Chatrchyan[1], Alexander Magunia[2], Thomas Pfeifer[2], and Tiago Buckup[1] — [1]Physikalisch-Chemisches Institut, Ruprecht-Karls Universität Heidelberg, Germany — [2]Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Ultrafast time-resolved spectroscopy of core-electron excitation with extreme-ultraviolet (XUV) and x-ray free-electron lasers (FELs) is an effective approach to study structural dynamics and relaxation kinetics in atoms and molecules in real time. However, the kinetic analysis of such data is often accompanied by many challenges due to the complex, partially coherent nature of SASE FEL pulses. To compensate for the lack of control over exact machine parameters during a single experiment, the analysis is performed on averaged data from hundreds of single shot measurements described with statistical parameters. Thus, information about the direct impact of an individual laser pulse on a system is often lost. The goal of this work is to extract the exact correlation between single-shot laser pulse characteristics and the resulting changes in a molecular system. For this purpose, a deep neural network is being trained on transient absorption data and XUV FEL pulse spectra simulated using a partial-coherence method that predicts the structural dynamics of a system. This tool promises significant advantages for FEL science research allowing instantaneous and exact analysis of large amounts of data without omitting crucial information from single experiments.

MO 12.2 Tue 17:00 Philo 1. OG

Disentangling Nonlinear Signal Orders in Fluorescence-Detected Multidimensional Spectroscopy via Intensity Cycling — •Vishnu E. Krishnan, Stefan Mueller, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Ultrafast spectroscopic measurements inherently include contributions from higher-order terms of the perturbation series, which can obscure the interpretation of nonlinear signals. Recently, our group demonstrated that intensity-dependent measurements (intensity cycling) enable the recovery of clean nonlinear responses in transient absorption [1] and coherently detected multidimensional spectroscopy [2]. Herein, we extend this method to fluorescence-detected multidimensional spectroscopy, using CdSe-based nanoplatelets as model samples, and successfully extract clean nonlinear signals.

[1] P. Malý, J. Lüttig, P. A. Rose, A. Turkin, C. Lambert, J. J. Krich, T. Brixner, Nature 616, 280 (2023).

[2] J. J. Krich, L. Brenneis, P. A. Rose, K. Mayershofer, S. Büttner, J. Lüttig, P. Malý, T. Brixner, J. Phys. Chem. Lett. 16, 5897 (2025).