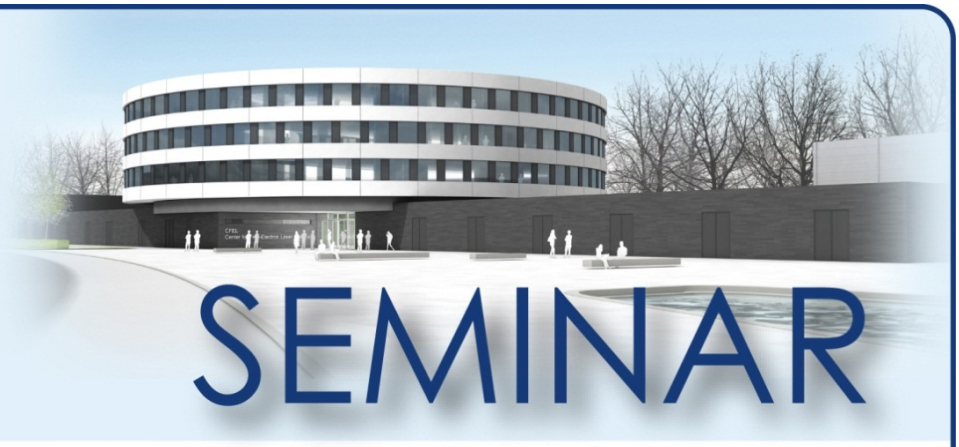
CFEL SCIENCE



SEMINAR

6th December 2023 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

Sergey I. Bokarev

Institute of Physics, Rostock University, Germany

Molecules in highly-excited states: a multi-configurational perspective on spectroscopy and dynamics

Molecules in highly excited states, such as those accessible by XUV and X-ray light excitation, attract much attention because of fascinating progress in experimental methodology, which has been made possible in tandem with theory. In my talk, I will discuss several computational protocols based on the multi-configurational electronic structure theory. First, I will describe approaches to computing valence and core photoionization and Auger decay in molecules employing different flavors of the central-potential method and beyond. Second, I will present our recent developments of the density-matrix-based time-dependent restricted active space configuration interaction method (ρ-TD-RASCI) to compute the ultrafast electron dynamics. The applications of these theoretical protocols will be exemplified by the simulations of the linear X-ray spectra, high harmonic generation, ultrafast charge migration, and spin-flip dynamics in molecules and transition metal complexes.

Host: Robin Santra – CFEL-DESY Theory Division