CFEL SCIENCE

SEMINAR

18th May 2022 - 2:00 p.m.

Virtual meeting room in ZOOM (ID: 895 1951 2902 / PW: 925239)

Laura Budewig

Center for Free-Electron Laser Science, DESY, and
Department of Physics, Universität Hamburg, Germany

Theoretical investigation of orbital alignment of x-ray-ionized atoms in exotic electronic configurations

Ultraintense x-ray pulses provided by x-ray free-electron lasers (XFELs) can induce highly charged atomic ions via multiple sequences of photoionization and accompanying decay processes. To investigate the orbital alignment occurring during x-ray multiphoton ionization, a suitable state-resolved electronic-structure framework is necessary. In this talk, I will present an implementation of improved electronic-structure calculations in the XATOM toolkit. Based on first-order many-body perturbation theory, first-order-corrected energies as well as individual state-to-state cross sections and transition rates are calculated. By using the improved electronic-structure calculations, I will present a theoretical study of the orbital alignment of transiently formed ions after single photoionization for initially neutral argon and two exotic electronic configurations that may be formed during x-ray multiphoton ionization dynamics induced by XFEL pulses. I will also demonstrate how the orbital alignment is affected by Auger-Meitner decay and a sequence of one photoionization and one Auger-Meitner decay. The presented work establishes a step toward state-resolved ionization dynamics calculations, and, thus, towards investigation of orbital alignment in atomic ionization driven by intense XFEL pulses.

Host: Robin Santra – CFEL-DESY Theory Division