

Quantum optics meets X-ray spectroscopy:

A mini-workshop on ultrafast AMO physics at the Mathematical Physics Division

Place: Mathematical Physics Division (C368)

Time: 09:00-11:00 Friday October 2nd (2026)

09:00-09:30

- Welcome! Mingle with coffee and tea in the kitchen area of the Mathematical Physics Division.

09:30-10:00 Speaker: *Markus Kowalewski, Stockholm University*
Title: *Molecular Photonics: From X-rays to Photochemistry in Nanocavities*

Abstract:

Over the past several years, our research has focused on advanced simulations that couple ultrafast and x-ray spectroscopic techniques to probe molecular electronic dynamics. A significant aspect of this work involves studying conical intersections and nonadiabatic dynamics in molecules. Furthermore, we have extensively investigated field quantization within nanocavities to understand modifications in chemical reactivity and polaritonic chemistry. In our current work, we integrate these two areas by proposing the use of x-ray spectroscopic techniques to study optical polaritons in organic molecules.

10:00-10:30 Speaker: *André Laestadius, Chalmers/Oslo Metropolitan University*
Title: *A Density-Functional Formulation of Quantum Electrodynamics*

Abstract:

Density-functional approaches offer a reduced description of interacting quantum systems in terms of selected observables rather than the full wavefunction. In this talk, I will discuss mathematical aspects of extending this perspective to coupled light-matter systems, focusing on the quantum Rabi and Dicke models. Topics include variational structure, density-potential relations, and representability.

10:30-11:00 Speaker: *Sang-Kil Son, CFEL, DESY, Hamburg*
Title: *Quantum-state-resolved X-ray multiphoton ionization dynamics*

Abstract:

Intense XFEL pulses can induce multiple sequences of inner-shell ionization events and accompanying decay processes in atoms, producing highly-charged ions. In general, X-ray multiphoton ionization dynamics have been so far described in terms of time-dependent populations of the electronic configurations visited during the ionization dynamics, neglecting individual state-to-state transition rates and energies. We extend our XATOM toolkit to study state-resolved dynamics based on time-dependent quantum-state populations, by combining a state-resolved electronic-structure method based on first-order many-body perturbation theory with a Monte Carlo rate-equation method. This allows us to explore spectroscopic detail in XFEL experiments that have been limited with electronic configuration or super-configuration approaches. Here we present recent studies of state-resolved X-ray multiphoton ionization dynamics of neon gas interacting with intense X-ray pulses generated by European XFEL. Several unexpected resonance features, for examples, emergence of pseudo-resonance feature and resonance-mediated double-core-hole formation, are identified with quantum-state-resolved ionization-dynamics calculations. Our study of quantum-state-resolved X-ray multiphoton ionization dynamics opens up new opportunities for high-resolution high-intensity X-ray spectroscopy.

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