CFEL SCIENCE

SEMINAR

9th December 2020 - 2:00 p.m.

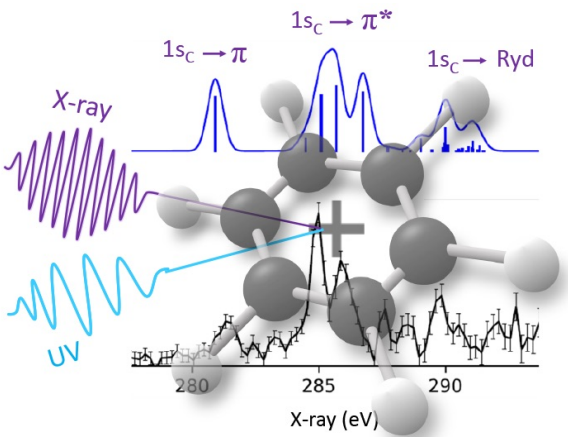
Virtual meeting room in ZOOM (ID: 951 6088 9833 / PW: 685729)

Sonia Coriani

Department of Chemistry, Technical University of Denmark, Denmark

Theoretical beamlines for local and ultrafast spectroscopies

The massive investments in advanced light sources operating in the X-ray and XUV regimes have increased the popularity of spectroscopic techniques exploiting these types of radiation to probe molecular systems. At the same time, it has stimulated the development of quantum-chemical theory and computational tools to simulate and elucidate the measured spectra. Theory and simulation tools are essential components to unambiguously relate experimental measurements to both structural and dynamical properties of the probed system. A key focus area of our research during the last decade has been the development of accurate electronic structure approaches, in particular rooted on the coupled cluster ansatz, to address X-ray spectroscopic techniques like X-ray absorption (XAS), emission (XES), circular dichroism (XCD), resonant inelastic x-ray scattering (RIXS), photoelectron (XPS), that are applied to probe both the electronic ground state and electronic excited states in a pump-probe set up, and at different absorption edges. More recently, we have addressed the accurate determination of XUV photoionization dynamic properties from the combined use of coupled-cluster Dyson orbitals and a B-spline DFT/TDDFT description of the continuum. An overview of the performance and capabilities of our methods will be presented.



A sketch of x-ray spectroscopy of benzene radical cation

Recent references: Vidal *et al.*, *J. Chem. Theory Comput.* **15**, 3117 (2019); Vidal *et al., J. Phys. Chem. A* **124**, 9532 (2020); Epshtein *et al.*, *J. Phys. Chem. A* **124**, 9524 (2020); Vidal *et al.*, *J. Phys. Chem. Lett.*, **11**, 8314 (2020); Faber & Coriani, *Phys. Chem. Chem. Phys.* **22**, 2642 (2020); Nanda *et al.*, *Phys. Chem. Chem. Phys.* **22**, 2629 (2020); Vidal *et al.*, *Phys. Chem. Chem. Phys.* **22**, 2693 (2020); *ibid.* **22**, 3744 (2020); Moitra *et al.*, *J. Phys. Chem. Lett.*, **11**, 5330 (2020).

Host: Robin Santra – CFEL-DESY Theory Division