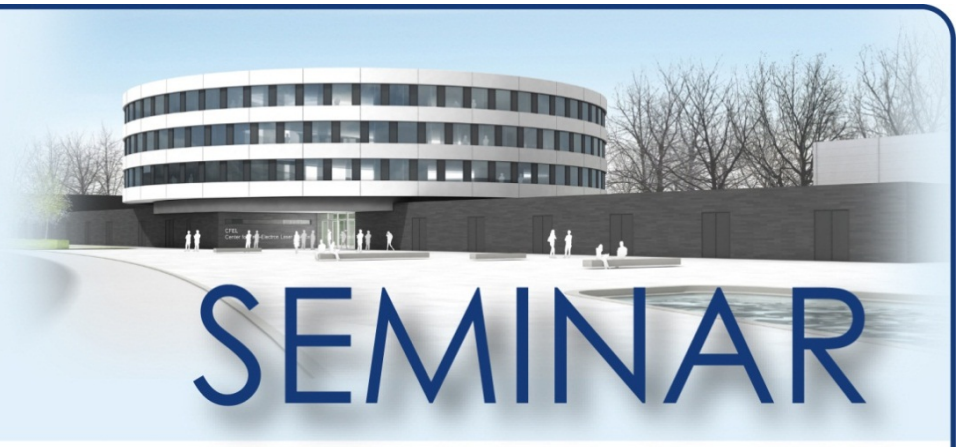
CFEL SCIENCE



# SEMINAR

***10th July 2024 - 2:00 p.m.***

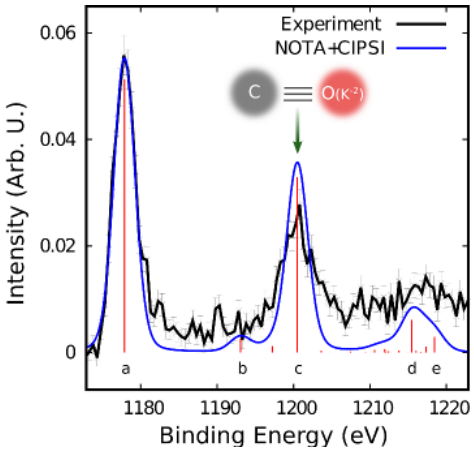
CFEL-bldg. 99, seminar room IV

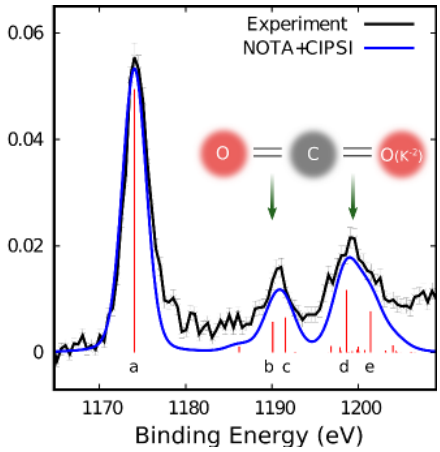

## Anthony Ferté

Center for Free-Electron Laser Science, DESY, Germany


# Advanced electronic structure calculation for double core photo-ionization spectroscopy


With the development of high-energy and high-intensity X-ray sources, inner-shell photoionization spectroscopy has greatly expanded, enabling the study of molecular systems with two core-shell vacancies. This enhances XPS by increasing its resolving power for chemical shifts, amplifying the relative signal of excited states, and offering new perspectives due to flexible positioning of the core vacancies. However, accurately describing double core hole states quantum chemically is challenging [1,2]. We developed a method using mutually non-orthogonal MO bases to address relaxation during double core vacancy formation, combined with a selected configuration interaction (CIPSI) method [1]. This approach faithfully reproduces experimental spectra [1,3,4] and provides a comprehensive theoretical framework for studying multi-electronic effects, showing in particular that satellites in double core hole spectra are signatures of the molecular structure [3].



[1] A. Ferté *et al.*, *J. Phys. Chem. Lett.* **11**, 4359 (2020).

[2] A. Ferté *et al.*, *J. Chem. Phys.* **159**, 144104 (2023).

[3] A. Ferté *et al.*, *Phys. Chem. Chem. Phys.* **24**, 1131 (2022).

[4] I. Ismail, A. Ferté, *et al.*, *Phys. Rev. Lett.* **131**, 253201 (2023).


Host: Robin Santra – CFEL-DESY Theory Division