European XFEL Workshop – Theory of X-ray spectroscopies

Theoretical approaches of X-ray spectroscopies

October 6th - 7th 2025

In-person meeting – Auditorium of Lighthouse Visitor Center

Over the last 15-20 years we have witnessed major breakthroughs in X-ray spectroscopies with the increased exploration of X-ray spectrometers and applications in the ultrafast regime (< 100 fs). Pump-probe conventional XAS and XES experiments in the hard X-ray regime are now routine at XFELs. Thanks to the high repetition rate of European XFEL and a large suite of high-resolution spectrometers available at FXE more advanced X-ray spectroscopies have become a reality. These new techniques combined with a constant improvement in data quality and the increased complexity of the science cases have led to challenges in simulating and interpreting the data. In this workshop a diverse group of researchers, including experimentalists and theory/computational scientists will gather to discuss the existing methodologies, challenges and limitations in simulating different X-ray spectroscopy data in view of ultrafast dynamics. This workshop will also address future directions in the theory of X-ray spectroscopy.

Organizers: Frederico Lima
Chris Milne

Contact: *frederico.lima@xfel.eu*
christopher.milne@xfel.eu

Monday, October 6th 2025 - Agenda

Time	Session	Speaker	Institution
09:00-09:30	**Registration**	- - -	European XFEL
09:30-09:45	Introduction	Chris Milne/ Sakura Pascarelli	European XFEL
09:45-10:15	X-ray spectroscopic capabilities at FXE	Fred Lima	European XFEL
10:15-10:30	*Coffee break*		
10:30-11:00	Expt. 1 – tba	Michal Nowakowski	U. Paderborn
11:30-12:00	Calculation of the x-ray absorption spectral shapes of transition metal oxides	Frank de Groot	Uni Utrecht
12:00-12:30	Time-resolved Computational Spectroscopy: First Principles to Machine Learning	Tom Penfold	U. Newcastle
12:30-14:00	*Lunch*		
14:00-14:30	Challenges in calculating platinum valence to core resonant x-ray emission spectra	Chis Pollock	CHESS
14:30-15:00	Modelling X-ray spectra for evolving molecules in liquid solutions	Michael Odelius	U. Stockolm
15:00-15:30	X-ray Spectroscopy simulations on the basis of Ab initio Quantum Chemical Calculations and Modern Ligand Field Theory: Turning “Forgotten” Art to Routine Analysis Tools	Dimitrios Manganas	MPI-CEC
15:30-16:00	Excited-state RIXS of a cobalt coordination complex: A tale of three photons	Marcus Lundberg	U. Uppsala
16:00-16:30	The Simulation of Ultrafast Dynamics in Iron(II) Complexes	Dániel Buzsáki	HUN-REN Wigner RCP
16:30-17:00	Flash presentations (3-5 min each)		
17:00-18:00	Poster session & coffee break		
18:00-21:00	Dinner (Beam Stop)		

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Tuesday, October 7th 2025 - Agenda

Time	Session	Speaker	Institution
09:00-09:30	Recent advances in quantum chemical approaches to X-ray spectroscopy	Frank Neese	MPI-KOFO
09:30-10:00	Expt. 3 – tba	Camila Bacellar	SwissFEL
10:00-10:30	Modelling of X-ray spectra of biological systems	Juan Nogueira	U. A. Madrid
10:30-10:45	*Coffee break*		
10:45-11:15	The Electronic Structure of Fe-corroles: X-ray Probe of the Ligand Non-Innocence from the Metal Perspective	Meiyuan Guo	U. Uppsala
11:15-11:45	Expt. 4 – tba	Kyle Barlow	U. Basel
11:45-12:30	Advanced X-ray spectroscopic studies of bioinspired high-valent iron complexes	Serena DeBeer	MPI-CEC
12:30-14:00	*Lunch*		
14:00-15:30	Round table discussion (limitations and new expt.?)		
14:30-15:30	Visit to FXE		