

	Monday 4 th	Tuesday 5 th	Wednesday 6 th
09:30	Arrival	Giacomo Ghiringhelli <i>“The charge transfer photoexcitations of NiO studied by high-resolution pp-RIXS at the European XFEL”</i>	Ian Wilkinson <i>“Steady-State & fs-Time-Resolved Photoemission Spectroscopy in the Aqueous Phase”</i>
10:00			
10:30		Manuel Izquierdo <i>“Femtosecond time-resolved photoelectron spectroscopy on solids at FELs”</i>	Andrea Trabatoni <i>“Quantum control of photo-induced electron dynamics in complex”</i>
11:00		Coffee break	Coffee break
11:30		Matteo Lucchini <i>“Attosecond virtual inter-band transitions in crystalline diamond”</i>	Kamal Abedin <i>“Advanced microfluid platforms for soft X-ray integrated photonics “</i>
12:00		Lorenzo Restaino <i>“Ultrafast nonadiabatic dynamics of NO2 probed by time-resolved X-ray absorption spectroscopy at N K-edge”</i>	Yann Amouroux <i>“Lighting our Future - The Impact of Optics and Photonics on a Global Economy”</i>
12:30	Lunch break	Lunch break	Lunch break
13:00			
13:45	Opening		
14:00	Massimo Altarelli <i>“X-ray Free-Electron Lasers and Electronic Properties of Materials”</i>	Angel Rubio <i>“Quantum materials engineering with high: a theoretical perspective”</i>	TRAINING <i>“How to Successfully Apply for Scientific Funding”</i> Alice Valkárová and Hannes Huebener
14:30			
15:00	Andrei Benediktovich <i>“Modification of x-ray absorption and scattering by transient changes of electronic populations”</i>	Chongxiao Fan <i>“Exciton Condensation in Strong Light-matter Coupling Regime”</i>	
15:30	Ettore Paltanin <i>“Ultrafast electronic and lattice dynamics in Al/Fe2O3 composite probed with the FERMI free electron laser”</i>	Benshu Fan <i>“Chirality-dependent Floquet Engineering of Topological Fermions in Chiral Crystal CoSi”</i>	
16:00	Coffee break	Coffee break	
16:30	Sangeeta Sharma <i>“Ultrafast light dressed exciton dynamics”</i>	Igor Tyulnev <i>“Strong-field Valleytronics in bulk MoS2”</i>	ESR social event
17:00		Masoud Lazemi	
17:30	Sam Shallcross <i>“Light control over valley polarization of charge and current”</i>	Emanuele Coccia <i>“Role of inner molecular orbitals in high-harmonic generation spectroscopy”</i>	
19:30		Social Dinner	

Massimo Altarelli

former director XFEL, MPSD, Hamburg, Germany

X-ray Free-Electron Lasers and Electronic Properties of Materials

Free-Electron Lasers in the EUV and X wavelength ranges have been operating for over a decade and have been used as very brilliant sources of ultra-short x-ray pulses, in the tens of fs range, most recently even in the few- and sub-fs regimes, with peak brilliances in the 10^{29} to 10^{32} photons/s/mm²/mrad² in a 0.1% bandwidth. The presently operating facilities and their key parameters shall be summarized, emphasizing spatial and temporal coherence properties. To exemplify how the ultrashort pulse duration and the high brilliance enable a new look at the electronic properties of quantum materials, the case of the mono- and few-layers transition metal dichalcogenides (TMD) shall be illustrated. These two-dimensional materials have attracted a lot of attention for their electronic structure, characterized by non-trivial topological features, such as non-zero Berry curvatures and Chern numbers associated to bands near the minimum gaps at the K⁺, K⁻ points of the BZ (the points of the Dirac cones in the related, but inversion symmetric, graphene case). One manifestation of these features is the “valley selective” optical population of either the K⁺ or the K⁻ valley at the direct band gap, depending on the sign of circular polarization of the incoming light. Recently, we investigated theoretically, with both group theory and DFT ab-initio calculations, whether this valley selectivity effect is also present in x-ray transitions from the core levels of the transition metal atom to the valence and conduction band K valleys(1). Valley selectivity with circularly polarized radiation is predicted for transitions from s, p_{1/2}, and p_{3/2} core levels to the valence bands in wide BZ regions around the K⁺,K⁻ points. Pump and probe IR – soft x-rays experiments at the FERMI FEL facility are being prepared; and the extension of the valley selectivity concept to Moiré heterobilayers of TMD is in progress; in these large-period compounds recent suggestions of a possible Anomalous Quantum Hall Effect phase with spontaneous breaking of time-reversal symmetry by asymmetric spin or valley occupation, were reported(2). As a second example, the extension to the x-ray region of non-linear optical experiments introduced in the optical domain after the invention of fs lasers, such as Four Wave Mixing is briefly discussed(3). The possibility to access new information via multi-dimensional spectroscopy and the study of temporal decay of population and coherence of excited states is described. (1) A. Geondzhian et al., Phys. Rev. B106, 115433 (2022) (2) Z. Tao et al., arXiv:2208.07452(cond-mat); arXiv2303.12881(cond-mat) (3) See for example F. Bencivenga et al., Advances in Physics X, 8, 1-90 (2023), and references therein

Andrei Benediktovitch

DESY, Hamburg

Modification of x-ray absorption and scattering by transient changes of electronic populations

X-ray free-electron lasers (XFELs) are capable of driving solids into electronically highly excited states at fs time scales. The resulting transient state is electronically far out of equilibrium with the crystal structure still intact. The characterization of this “warm-dense matter” poses intricate experimental and theoretical challenges. In two recent experiments, our team investigated the early stages of formation of warm-dense copper by transient x-ray absorption spectroscopy and resonant elastic x-ray scattering. X-ray pulses of 15 fs duration are tuned to the Cu L3 edge at 932 eV and focused on a 100-nm thin foil of Cu (B4C/Cu/SiC multilayer in the 2nd experiment, respectively). Ionization followed by Auger-Meitner decay rapidly creates hot electrons. Subsequent electron collisions produce highly charged ions with vacancies in the Cu 3d shell. Measuring the transmitted x-ray spectra gives a snapshot of the electronic population averaged over the first 15 fs upon pulse arrival. Increasing the XFEL intensity, an absorption peak below the neutral Cu L3 edge appears in the spectra, assigned to 2p-3d resonant excitations of the created 3d vacancies. The total absorption is thereby increased (reverse saturable absorption). Increasing the XFEL pulse energy further, higher-charged ions are formed, eventually shifting the 2p-3d resonances out of the spectral window of the x-ray pulse and quenching ionization (saturable absorption). This interpretation is corroborated by simulations based on a kinetic Boltzmann approach that follows the interaction with the x-ray pulse and subsequent electron-electron and electron-ion collisions. The output of the kinetic Boltzmann approach is combined with real-space Green’s function code FEF10 to simulate the x-ray absorption near-edge spectra. Similarly to resonant absorption, the transient 2p-3d resonances are reflected in additional resonant elastic x-ray scattering channels, resulting in an enhanced scattering. In line with our first experiment, at XFEL intensities above 10^{13} W/cm² we observe a strong enhancement of the diffracted intensity in the pre-edge spectral region. This demonstration paves the way towards control of atomic scattering properties and, when implemented in hard x-ray spectral range, could have applications for x-ray crystallography and single-particle imaging.

Sangeeta Sharma

Max Born Institute, Berlin, Germany

Ultrafast light dressed exciton dynamics

Giacomo Ghiringhelli

Politecnico di Milano, Italy

The charge transfer photoexcitations of NiO studied by high-resolution pp-RIXS at the European XFEL

High repetition rate X-ray Free Electron Lasers (XFELs) offer the opportunity of performing time-resolved experiments in photon-hungry spectroscopy. This advantage is particularly significant for solid samples that are easily damaged by non-attenuated XFEL pulses. At the SCS instrument of the European XFEL [1], the hRIXS spectrometer [2] is the first end-station allowing high resolution pump probe resonant inelastic x-ray scattering (ppRIXS) experiments both on liquid jets and solid samples to come into operations. Already in the user-assisted commissioning of 2022, very exciting results were obtained on NiO and La₂CuO₄ by pumping the samples across the charge transfer electronic gap and measuring RIXS spectra at selected reciprocal space vectors and time-delays [3]. It was immediately clear that RIXS can provide unprecedented insight on the transient photoexcited states in Mott insulators. Inspired by those preliminary results, in October 2023 we performed a full official experiment on NiO pumped with 266 nm optical pulses and probed at the Ni L₃ absorption edge. We clearly detect a local charge transfer exciton that decays after few picoseconds into a delocalized state. In the two regimes the orbital and spin excitations are affected in different ways, and their evolution can be well followed by exciting the RIXS spectra at different points of the x-ray absorption multiplet [4].

I will present these unpublished results on NiO and La₂CuO₄ and discuss the opportunities of high-resolution ppRIXS as an advanced tool to study transient states in quantum materials.

References [1] N. Gerasimova, D. La Civita, L. Samoylova, M. Vannoni, R. Villanueva, D. Hickin, R. Carley, R. Gort, B.E. Van Kuiken, P. Miedema, L. Le Guyarder, L. Mercadier, G. Mercurio, J. Schlappa, M. Teichmann, A. Yaroslavtsev, H. Sinn, A. Scherz, "The soft X-ray monochromator at the SASE3 beamline of the European XFEL: from design to operation", J. Synchrotron Radiat. 29, 1299 (2022) [2] Justine Schlappa, Giacomo Ghiringhelli, Benjamin Van Kuiken, Martin Teichmann, Piter Miedema, Jan Torben Delitz, Natalia Gerasimova, Serguei Molodtsov, Luigi Adriano, Bernard Baranasic, Carsten Broers, Robert Carley, Patrick Gessler, Nahid Ghodrati, David Hickin, Le Phuong Hoang, Manuel Izquierdo, Laurent Mercadier, Giuseppe Mercurio, Sergii Parchenko, Marijan Stupar, Zhong Yin, Leonardo Martinelli, Giacomo Merzoni, Ying Ying Peng, Torben Reuss, Sreeju Sreekantan Nair Lalithambika, Simone Techert, Tim Laarmann, Simo Huotari, Christian Schroeter, Burkhard Langer, Tatjana Giessel, Stefan Neppel, Robby Buechner, Jana Buchheim, Vinicius Vaz da Cruz, Sebastian Eckert, Grzegorz Gwalt, Chun-Yu Liu, Frank Siewert, Christian Sohr, Christian Weniger, Annette Pietzsch, Friedmar Senf, Andreas Scherz, and Alexander Foehlich, "The Heisenberg-RIXS instrument at the European XFEL", in preparation [3] L. Adriano, A. Alic, D.R. Baykusheva, R. Carley, G.S. Chiuzbaian, M.P.M. Dean, O. Duros, A. Foehlich M. Först, B.K. Freelon, N. Gerasimova, G. Ghiringhelli, X. Jiang, D. Jost, M. Kusch, T. Laarmann, V. Lebedev, W.S. Lee, C.Y. Liu, L. Martinelli, L. Mercadier, G. Merzoni, M. Minola, M. Mitrano, S. Molodtsov, C.S. Pathiraja, S. Parchenko, J.N. Ranhili Pelige, Y.Y. Peng, Q. Qiu, T. Schmitt, J. Sears, A. Scherz, J. Schlappa, S. Sreenkatan Nair Lalithambika, S. Techert, M. Teichmann, S.F.R. Ten Huisen, B. van Kuiken, Z. Yin, unpublished [4] G. Merzoni, L. Martinelli, transfer metastable state of NiO", in preparation, "The photo-induced charge S. Dal Conte, L. Mercadier, Y.P. Chang, L.P. Hoang, G. Mercurio, F. Rosa, J. Schlappa, M. Teichmann, N. B. Brookes, R. Carley, G. Cerullo, M. Moretti Sala, A. Scherz, G. Ghiringhelli *

Acknowledgement(s) : the hRIXS project was funded by Helmholtz Association (Germany), European X-FEL, European Research Council, Italian Ministry of Research (Italy), FIRI (Finland) and supported by University of Potsdam, HZB and DESY (Germany), Politecnico di Milano (Italy).

Matteo Lucchini

Politecnico di Milano

Attosecond virtual inter-band transitions in crystalline diamond

The sudden response of an insulator to an intense few-femtosecond optical pulse is known to be mostly dominated by intra-band charge acceleration, an effect upon which are based diverse phenomena like high-harmonic generation and PHz field sampling. By studying monocrystalline diamond with attosecond transient reflection spectroscopy we showed that field-induced virtual inter-band transition can compete with intra-band motion and significantly alter the electro-optical properties of the material.

Angel Rubio

Max Plank Institute for the structure and dynamics of matter, Hamburg, Germany

Quantum materials engineering with high: a theoretical perspective

We will introduce our newly developed quantum electrodynamics density-functional formalism (QEDFT) as a first principles framework to predict, characterize and control the spontaneous appearance of ordered phases of strongly interacting light-matter hybrids. We will provide an overview of how well-established concepts in the fields of quantum chemistry and materials have to be adapted when the quantum nature of light becomes important. We will pursue the question whether it is possible to create these new states of materials as groundstates of the system. To this end we will show how the emerging (vacuum) dressed states resembles Floquet states in driven systems. A particular appeal of light dressing is the possibility to engineer symmetry breaking which can lead to novel properties of materials. We will discuss the potential to realize non-equilibrium states of matter that have so far been only accessible in ultrafast and ultrastrong laser-driven materials. We illustrate the realization of those ideas in molecular complexes and 2D materials and show that the combination of cavity-QED and 2D twisted van der Waals heterostructures provides a novel and unique platform for the seamless realization of a plethora of interacting quantum phenomena, including exotic and elusive correlated and topological phases of matter.