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Biology Techniques to Tackle Heavy Metal

Adithi Raval*

Department of Biotechnology, Manipal Institute of Technology, Manipal, India

***Corresponding author:** Email: raval_a@gmail.com

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Description

Implementation of in-situ and operando experimental set-ups for bridging the pressure gap in characterization techniques based on monitoring of photoelectron emission has made significant achievements at several beamlines at Elettra synchrotron facility. These set-ups are now operational and have been successfully used to address unsolved issues exploring events occurring at solid gas, solid liquid and solid-solid interfaces of functional materials. The sections in the article communicate the research opportunities offered by the current set-ups at APE, BACH, ESCAmicroscopy and Nanospectroscopy beamlines and outline the next steps to overcome the present limits.

X-ray Raman Scattering

A study of the near-edge structure at the edge of elemental boron in its -rhombohedral phase is presented. Momentum-transfer dependent measurements of the B 1s core-electron excitation spectra were performed by X-ray Raman scattering (XRS) spectroscopy. Spectral features were interpreted based on calculations of the XRS spectra. A method to model a system with partially occupied sites (POS) was implemented based on FEFF simulations of XRS spectra. The inclusion of POS in the crystal structure of -rhombohedral boron in the calculations was essential in order to achieve agreement between simulated and measured spectra. Transitions from the core-level to exo-icosahedron orbitals were found to be sensitive to the presence of partially occupied sites in -rhombohedral boron. The origin and the momentum-transfer dependence of the spectral features are discussed. Characteristic spectral features from icosahedral units and from icosahedron clusters were identified. Activation of non-dipole transitions at high momentum transfers was detected.

Modular Soft X-ray Spectrometers

A momentum resolved resonant inelastic X-ray scattering (qRIXS) experimental station with continuously rotatable spectrometers and parallel detection is designed to operate at different beamlines at synchrotron and free electron laser (FEL) facilities. This endstation, currently located at the Advanced Light Source (ALS), has five emission ports on the experimental chamber for mounting the high-throughput modular soft X-ray spectrometers (MXS). Coupled to the rotation from the supporting hexapod, the scattered X-rays from 27.5° (forward scattering) to 152.5° (backward scattering) relative to the incident photon beam can be recorded, enabling the momentum-resolved RIXS spectroscopy. The components of this endstation are described in details, and the preliminary RIXS measurements on highly oriented pyrolytic graphite (HOPG) reveal the low energy vibronic excitations from the strong electron-phonon coupling at edge around σ* band. The grating upgrade option to enhance the performance at low photon energies is presented and the potential of this spectroscopy is discussed in summary.

Oscillator strengths and cross sections of the valence-shell excitations in CF_4 are of crucial importance in modeling the etching plasma and monitoring the greenhouse effect. In this work, generalized oscillator strengths of the valence-shell excitations in CF_4 were measured by using an angle-resolved electron energy loss spectrometer, operating at incident electron energy of 1.5 keV and a high energy resolution of 80 meV. The experimental GOSs are analytically fitted with the well-known Lassettre formula, and, thus, the optical oscillator strengths are determined at the limit of squared momentum transfer. The analytical GOS also enables integration over, determining the born cross sections with respect to the incident electron energy from the excitation threshold to 5000 eV. The BE-scaled integral cross sections for dipole-allowed transitions are obtained by adopting the BE-scaling method. Oscillator strengths and cross sections of the valence-shell excitations in CF_4 provide an independent cross-check to the previous experimental and theoretical works. Moreover, the cross-checked data supplement and benchmark the molecular database for use in plasma models.

A new method for the analysis of the scattering rates from angle-resolved photoelectron spectroscopy (ARPES) is presented and described in details. It takes into account experimental instrumental resolution and finite temperature effects. More accurate results are obtained in comparison with a standard, commonly used method. The application of the method is demonstrated for several examples commonly encountered in new quantum materials. Its usefulness is especially apparent in investigations of systems with strongly correlated electrons.

A method within the fully relativistic frame, based on the reconstructed Dirac–Coulomb Hamiltonian is suggested which applies to the plasma-embedded multi-electron atomic systems perturbed by applied magnetic fields. The proposal is a configuration interaction method and based upon a combination of two concepts, referred to as plasma screening and external magnetic field. An effective potential, derived by introducing a parameter dependent scaling of the radial dependence of free electron contribution in the ion-sphere, is adopted to model the interactions among the charged particles in dense plasmas, and also the range of external weak magnetic field B105 T is considered. In this instance, numerical calculations are performed for electronic structures and spectroscopic properties of the He atom and Fe ion as examples. The accuracy of the present approach is shown by comparison to previous theoretical calculations. The behavior of energies of low excited states and radiative transition probabilities for allowed transitions as a function of the plasma screening and field strength is classified. These results are developed in high energy density physics and astrophysics context.

The photoelectron angular distribution (PAD) of the Kr 4 and 4 fine structure states was measured with linearly polarized synchrotron radiation in the vicinity of the resonant excitations of the 3 subshell. Experimental dipole and non-dipole anisotropy parameters were determined from the measured angular differential cross sections. In order to interpret our experimental results we have used a theoretical model going beyond the dipole approximation considering the quadrupole and octupole terms for the direct photoionization. We have taken into account several autoionization channels relevant for the studied photon energy range. The photon energy dependence of the measured anisotropy parameters puts in evidence the importance of the channel interactions. Moreover, unexpectedly large non-dipole contribution has been observed..