

A guide to population, relatedness, and pedigree in conservation biology

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Description

Mechanisms of energy absorption in liquid water under 3–1000 Ry photon irradiation are studied by Monte Carlo simulation with accounting for the cascade decays of vacancies in inner electron subshells created by primary and secondary ionization processes. At incident photon energies above O1s ionization threshold, most of the energy is transferred to the medium by secondary electrons and photons produced in the processes of photoionization, electron impact ionization, and cascade decay of inner-shell vacancies. On the average, on the whole considered incident photon energy interval, 49.8% of the absorbed energy is transferred to the medium by high-energy secondary electrons and photons in inelastic processes of interaction with the atoms of the medium. Low-energy electrons and photons incapable of ionizing/exciting the atoms of the medium are responsible for 48.8% of energy absorption. Energy absorption in the processes of primary ionization by incident photons are significant only at small incident photon energies of a few Rydbergs, their average contribution to energy absorption on the whole considered energy interval makes only 1.4%. At incident photon energies above O1s-ionization threshold low-energy electrons are produced in large quantities; this can be important in radiotherapy since in the tissues of organisms, low-energy electrons may cause the DNA strand breaks via the mechanism of dissociative electron attachment.

X-ray photoelectron

X-ray photoelectron diffraction is a powerful spectroscopic technique in the direct legacy of C.S. Fadley that combines high sensitivity to the arrangement of atoms in crystals and element specificity providing unique fingerprints of selected atomic sites in matter. When used with kinetic energies between 500 eV and 1500 eV, its interpretation and description is based on the fact that the atomic scattering factors are strongly forward-peaked in such a way that low-angles scattering and backscattering events are respectively dominant and almost irrelevant in the photoemission process. In this paper we aim to demonstrate with the help of multiple-scattering simulations that energy scans of high-energy (500–

1500 eV) forward-scattering photoelectron diffraction can provide valuable structural and chemical information about thin epitaxial films or stacking of two-dimensional materials.

The valence and C 1s core photoelectron spectra of three carboxylic acids (butanoic, hexanoic and octanoic) as well as the near-edge absorption fine structure spectra and photo-electron photo-ion coincidence spectra have been measured. Changes in the valence spectra are related to the lengthening of the aliphatic chains, and the core spectra have been assigned. Small shifts of the carboxylic carbon 1s binding energy are related to screening of the core hole by the aliphatic group. The C K edge near-edge absorption fine structure spectra probe the unoccupied density of states and the main changes in the spectra are due to increasing length of the aliphatic chain and related Rydberg states. The coincidence spectra show that soft (near threshold) ionization of all compounds leads to parent ion formation for butanoic and octanoic acids. For hexanoic acid, both parent ions and fragments are produced for near threshold ionization. Fragmentation occurs at the C2C3 bond for all carboxylic acids at the lowest energies, and other channels open for higher internal energy.

Free Electron Laser

As the use of free electron laser (FEL) sources increases, so do the findings mentioning non-linear phenomena occurring at these experiments, such as saturable absorption, induced transparency and scattering breakdowns. These are well known among the laser community, but are still rarely understood and expected among the X-ray community and to date lack tools and theories to accurately predict the respective experimental parameters and results. We present a simple theoretical framework to access short X-ray pulse induced light–matter interactions which occur at intense short X-ray pulses as available at FEL sources.

Our approach allows investigating effects such as storable absorption, induced transparency and scattering suppression, stimulated emission, and transmission spectra, while including the density of state influence relevant to soft X-ray spectroscopy in, for example, transition metal complexes or functional materials. This computationally

efficient rate model based approach is intuitively adaptable to most solid state sample systems in the soft X-ray spectrum with the potential to be extended for liquid and gas sample systems as well. The feasibility of the model to estimate the named effects and the influence of the density of state is demonstrated using the example of CoPd transition metal systems at the Co edge.

We believe this work is an important contribution for the preparation, performance, and understanding of FEL based high intensity and short pulse experiments, especially on functional materials in the soft X-ray spectrum. Low energy elastic positron scattering from Zn and Cd atoms was studied using model correlation potential. Special attention is given to the study of polarization effects through the incorporation of quadrupole polarizabilities and hyperpolarizabilities in the scattering potential. Resonant p-wave shape structures are found for both systems. Results show that these become sharper and move to lower energies as the level of polarization of the potential is increased.

Resonance was suppressed in Cd when the second hyperpolarizability was taken greater than 46000 a.u. and true p-wave bound states were formed. Comparison to previous calculations and dependence of the results with the scheme adopted to match the correlation and polarization components of the potential is discussed. We find that the elastic cross sections and the resonant effects do not depend on the specific form of the correlation potential but strongly depend on the polarization parameters and the matching point determined by the crossing between the correlation and polarization components of the potential. The value for the dipole dipole quadrupole polarizability for Cd was specifically calculated using the relativistic coupled-cluster approach and is reported for the first time in this work.