Hard X-ray Core-hole Clock Spectroscopy of Adsorbates and Polymer Mixtures

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Resonantly exciting a core electron promotes it to an unoccupied electronic state. The core-excited state decays with the core hole filled by an electron. Excess energy may be emitted by another electron in a resonant Auger decay. In solids and adsorbates, the core-excited electron can tunnel away, which then leads to a normal Auger decay of the core hole at energies below the ionization potential.

Analysing spectral components' relative intensities in *e.g.* the KLL Auger kinetic energy region with photon energies near the resonance reveals insights into the electron's propensity to tunnel away as it is dependent on the energy landscape. This information aids the study of charge transfer processes in materials [1-3]. The tunnelling must occur within the core-hole lifetime to affect the spectral content, hence acting as a "core-hole clock".

In Xenon adsorbed on metal surfaces[1], polymer heterojunctions for organic electronics[2], and quantum dots (PbS) [3] the low excess energy part vary depending on composition whereas higher energy excitations share the same tunneling behavior. For adsorbed Xe core-excitation highlight channels present only in the core-excited state. It turns out that the material compositions that give best macroscopic performance with nanoparticles and in the polymer case conductivity in organic electronics built from these materials also have the swiftest charge transfer times measured via the core-hole clock method. The amount of molecular alignment also impact the charge transfer time.

An outlook with recent results on bilayer and heterojunction polymer systems will be given with an emphasis on evolution of the core hole clock spectrum upon X-ray exposure.

Keywords [optional]: Core hole clock spectroscopy; synchrotron based hard X-ray photoelectron spectroscopy; polymers; adsorbate

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[1] Fredrik O. L. Johansson, *et al.* "Resonant Auger spectroscopy on solid xenon on gold, silver, and copper substrates." Physical Review A **107**:3 (2023): 032802.

[2] Elin Berggren, *et al.* "Charge Transfer in the P (g42T-T): BBL Organic Polymer Heterojunction Measured with Core-Hole Clock Spectroscopy." The Journal of Physical Chemistry C **127**:49 (2023): 23733-23742.

[3] Tamara. Sloboda, *et al.*, "Unravelling the ultrafast charge dynamics in PbS quantum dots through resonant Auger mapping of the sulfur K-edge." RSC advances **12**:49 (2022): 31671-31679.