A Soft X-ray Emission Study of K_3C_{60}

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The alkali metal fulleride salts of composition A_3C_{60} (where A is an alkali metal) have attracted wide interest due to their metallic and superconducting properties. We present C 1s aborption (XAS) and resonant and nonresonant soft X-ray emission (SXES) spectra from a single phase crystalline thin film of K_3C_{60}.

The experiments were carried out on the Surface Endstation of BL511 at MAXLAB in Lund, Sweden. The RIXS spectra were recorded using the grazing incidence grating spectrometer on the endstation. The energy resolution was 0.2 eV in the X-ray emission spectra and 0.1 eV in the excitation channel (the monochromator). X-ray absorption spectra were acquired using a high-pass yield detector, set to accept C 1s Auger electrons.

Comparing the absorption spectra from K_3C_{60} and pristine C_{60} samples, it is seen that the lowest absorption resonance (corresponding to the LUMO of C_{60}) is broadened, compared to C_{60}, with the edge shifted slightly to lower energy. The next unoccupied energy levels have been lowered even further in energy, and broadened. The quite large modifications in the absorption spectrum have been a source of discussion considering even the assignment of the peaks. We have recorded resonant X-ray emission spectra from intermediate states of different parities, and used the inherent symmetry selectivity of the resonant X-ray emission process in try to identify the origin of the absorption peaks in terms of the C_{60}-derived electronic structure. We have reached the conclusion that it is correct to interpret the K_3C_{60} XAS as being directly analogous to that of pristine C_{60}.

The model of different surface and bulk electronic structures is consistent with the present results. This may also explain the increased widths of the absorption features, since electron yield spectroscopy is susceptible to mean free path effects.

The lines in the emission spectra are narrower than the corresponding valence band UPS-lines from K_3C_{60} (although the lines are broader than for C_{60}). As XES is sensitive to the bulk of the material, and UPS (and XPS) to a rather shallow surface layer, this again points to differences in the bulk and surface electronic structure of K_3C_{60}. This supports the idea that the surface region has a unique structure, and correspondingly unique electronic structure.