

Resonant Soft-x-ray Emission of *Molecular* Materials: Electronic Structure and Dynamics

Jinghua Guo

Department of Physics, Uppsala University, 751 21 Uppsala, SWEDEN

With high resolution monochromatized synchrotron radiation excitations, resonant inelastic soft-x-ray scattering has emerged as a new source of information about electronic structure and excitation dynamics. I will present a series of experimental counts, including the studies of small molecules i.e. O₂, N₂ and CO₂, to demonstrate the selection rules of energy, momentum, and symmetry in the resonant soft-x-ray emission process. In the molecule-like systems, such as C₆₀, C₇₀, benzene and its derivatives, π -conjugated polymers, symmetry selection rules have been established, and deviations from the symmetry selection rules have been interpreted in terms of dynamical symmetry breaking. In the studies of π -conjugated polymers, it has been found that the benzene-ring has a strong identity as building block in some of the conjugated polymers. Isomeric dependence was able to be clarified in the studies of polypyridine. The resonant soft-x-ray emission has been applied in the study of molecules in liquid phase. The symmetry dependence of resonant soft-x-ray emission is reflected in the gas phase spectrum, but in the liquid phase it has disappeared. Example data is shown later which compares pure water, isolated H₂O molecules in vapor, and various solutions for resonant soft-x-ray emission. Those changes which are observed in the fine structure are directly attributable to the chemical bonding of water molecules to each other and to ions introduced to the solution. In particular, the resonant measurements in K₃[Fe(CN)₆] reveal chemical-species-selected valence band features unique to those H₂O molecules bonded to [Fe(CN)₆]³⁺ clusters.