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Resonant Inelastic Soft-x-ray Scattering (RIXS) in Probe of Electronic Structure of Matter

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Inner-shell x-ray absorption spectroscopy (XAS) is a powerful technique for gaining element specific information about the unoccupied orbitals. However, there are still issues in the interpretation and assignments of certain features in XAS spectra. Even for some smaller molecules there are absorption features that have not yet been conclusively assigned. Hence, there is a need for techniques that provide additional symmetry information for the assignments. The possibility to assign XAS spectra using resonant inelastic soft-x-ray scattering (RIXS) is demonstrated. The oxygen *K*-emission spectra of CO₂ are used to illustrate the possibility to assign core excitations through excitation-energy and angular dependence of RIXS spectra. The Rydberg associated structures just below the ionization threshold in the O *1s* absorption spectrum are assigned to be mainly due to excitations to orbitals of π_g character. The results, which contradict some previous literature assignments, are supported by quantum-chemical calculations. The bonding between titanium atom and C₆₀ has been examined by means of RIXS. Using the symmetry-selection rules in the scattering process the symmetry of the orbitals involved in the bond formation is determined. The lowest unoccupied states are due to hybridization between the highest occupied orbital of C₆₀ and Ti orbitals. A comparison between experimental and theoretical results indicates Ti bonding to the six-ring site. This method can be used to probe bonding between metal atoms and organic molecules in general.

15. Instrumentation and Measurements

Special Focus Topics

15.9.3 New Techniques, Applications and Instruments in X-Ray Absorption Spectroscopy (GIMS/DCP)