

SATELLITE STRUCTURE ACCOMPANYING PHOTOIONIZATION OF
TRANSITION METAL COMPOUNDS AND ADSORBATES

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ABSTRACT

The ionization of CO complexes and CO adsorbates is known to be accompanied by strong satellite structure due to intensity borrowing by excited states, i.e. two-particle-hole states derived from the hole state under consideration. This process is driven by electron-relaxation of the remaining electrons in the system leading to a screened hole state. For core ionizations the redistribution of electrons upon ionization is particularly significant due to the localized character of the hole. The electron distribution in the ion is calculated self-consistently and compared with the neutral molecular ground state distribution. This comparison allows a classification of the electron redistribution as "metal-to-CO", "CO-to-metal" if electrons are transferred accordingly or as "local-CO" and "local-metal" if only part of the molecular moiety is involved. The energy of those states, involving the transfer of electrons between the metal and the CO ligand is sensitive to the metal-CO bond strength in the neutral molecular ground state. The analogies between transition metal compounds and transition metal adsorbates in this respect is discussed in detail with emphasis on the question of how many metal atoms are sufficient to describe the ionization of an adsorbate.

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