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Transition metal systems: a theoretical modeling of their $L_{2,3}$-edge X-ray absorption spectra

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X-ray absorption spectroscopy (XAS) of transition metal (TM) complexes is recognized as a tool able to probe, site-selectively, the empty frontier MOs, the TM coordinative environment, the ligand -field splitting, the oxidation states and, in general the nature and the strength of the TM–ligand bonding in TM complexes. Despite metal K and $L_{2,3}$-edges XA spectra contain a huge chemical information, a stiff theoretical analysis is needed to extract it. The $L_{2,3}$-edges XA simulated spectra herein presented have been obtained by using the restricted open shell configuration interaction with singles method, which includes spin orbit coupling and relativistic effects by employing the ORCA program package. Numerical experiments have been carried out to investigate the TM $L_{2,3}$-edges spectra of a huge number of systems that spread between single molecules (TM $(acac)_2$ (TM = Mn, Co) , TM $(acac)_3$ (TM = Cr, Mn, Fe), VPc and VXPc systems (X = O, I) Iron complexes (scorpionate, ferrocene and bridged carbonyl ones) and 2D complex systems (Ag supported FePc/FePc(η_2-O_2) and Cu supported THQ/THQ:Cu_4). Instead, K-edge spectra have been modeled by running time dependent density functional theory calculations and by using the ADF program package. Numerical experiments on the $^{O, C, F, N}$ K-edges have been performed on TM$(acac)_3$ and CuPc/CuTPP systems. The goals of these systematic studies is: i) to reveal the role played by the TM, by its oxidation state and its environment in determining the spectral features, ii) to provide an intimate understanding of the electron transfer pathway ruling the catalytic oxygen reduction reaction of FePc on Ag (110) and iii) to quantify the amount of different species that contribute to the same XA spectrum. Relevant trends for L_3-edge XA spectra are the lower energy side which is characterized by TM→TM transitions, while the higher energy one involves metal to ligand charge transfer transitions.

Recent Publications:

1. Carlotto S et al. (2017) Mn $(acac)_2$ and Mn $(acac)_3$ complexes: a theoretical modeling of their $L_{2,3}$-edges X-ray absorption spectra. Polyhedron. 135:216-223.
2. Carlotto S et al. (2017) The electronic properties of three popular high spin complexes [TM $(acac)_3$, TM = Cr, Mn and Fe] revisited: an experimental and theoretical study. Physical Chemistry Chemical Physics. 19(36):24840-24854.
3. Carlotto S et al. (2016) Theoretical modeling of the L 2, 3-edge X-ray absorption spectra of Mn $(acac)_2$ and Co $(acac)_2$ complexes. Physical Chemistry Chemical Physics 18(3):2242-2249.
4. Carlotto S et al. (2016) L 2, 3-edges absorption spectra of a 2D complex system: a theoretical modelling. Physical Chemistry Chemical Physics 18(40):28110-28116.
5. Mangione G et al. (2016) Electronic structures of CuTPP and CuTPP(F) complexes: a combined experimental and theoretical study I. Physical Chemistry Chemical Physics 18(28):18727-18738.

Biography

Silvia Carlotto is a Researcher at the University of Padua, Italy. She started her PhD research activity in the Theoretical Chemistry Group at the same university with a thesis devoted to the modeling of dynamic solvation effects. After her PhD, she participated as Postdoc in several national and international projects about the simulation of non-linear optical properties of multipolar chromophores in solution; the development of computational methods for micro fluidic devices and the theoretical study of the next generation, cost efficient, automotive catalysis in particular and the modeling of the catalytic properties of pure and doped perovskites. During the past years, she has worked on the simulation of X-ray absorption and photoemission spectra (K- and L-edges) of isolated and supported (Fe and FeO_2-phthalocyanine) systems to gain insights into their occupied and unoccupied electronic structures.

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