

Quantum Chemical Approach to X-ray Spectroscopy: application to small molecules and surfaces

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Modern experimental methods allow us to obtain reliable spectroscopic data for free and adsorbed molecules as well as for local sites at substrate surfaces and in the bulk. Corresponding theoretical results, based on quantum chemical methods, can help to interpret these experimental spectra and can provide an understanding of excitation phenomena and other physical behavior on a microscopic scale. This applies, in particular, to electron spectroscopy experiments using synchrotron radiation such as X-ray absorption (XAS/NEXAFS), X-ray emission (XES), and X-ray photoemission (XPS). In this talk we describe our quantum chemical approach to evaluate energetics and (angle-resolved) transition matrix elements for photon absorption and emission involving electronically excited states. Our methods are based on modern Density-Functional Theory (DFT) together with gradient corrected functionals as implemented in the StoBe code (**S**tockholm-**B**erlin collaboration). In this talk approaches and computational strategies will be illustrated by examples of recent theoretical studies on C₆ ring containing hydrocarbons in gas phase, on larger hydrocarbons adsorbed at the Cu(111) surface, as well as on differently coordinated oxygen in vanadium oxide, V₂O₅ and V₂O₃. In all examples we compare our theoretical data with corresponding experimental results derived from electron spectroscopy using synchrotron radiation.

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