

Abstract

This dissertation is concerned with the occupied and unoccupied electronic structure of lanthanide materials.

With surface sensitive electron-excited x-ray emission spectroscopy (XES) we could experimentally determine a surface and bulk partial density of states (p-DOS) for the metals Lanthanum, Lutetium and Samarium. The experimental bulk p-DOS agrees well with the theoretical ones by *Danzenbacher* [Dan98]. From calculations of the O₃-XE transition probability we anticipate a three times higher probability for s-like than for d-like electrons to fill the 5p_{3/2}-hole; this was confirmed experimentally. A surface state - known from PE measurements [WeK95] - could not be observed in any XE spectrum. The emission from this surface state of d_{Z²}-symmetry is suppressed by more than one order of magnitude relative to emissions from s-like valence states. In the case of Samarium we could identify satellite emission in XES. Photoemission (PE) measurements were needed to determine the binding energy of 5p⁻¹ hole states - including the 5p-replica shift* in Samarium. For the determination of the Samarium p-DOS we developed a model describing the generation of IPE background radiation in XES, caused by Auger electrons which are created in a radiationless decay of the 5p core-hole. The absence of O₂-XE in all metals could be explained with intense Auger decays of the 5p_{1/2}-hole. With the present work we have set the basics for further surface sensitive XE measurements, e.g. at 3d transition metals.

In the second part of this work we have measured the occupied and unoccupied electronic structure of LaS, LaSe and LaTe. PE spectra agreed well with theoretical band structures [SMP92]; in particular the binding energy shift of the 5p⁻¹ state in LaS and LaTe relative to Lanthanum metal could be determined. With measurements of the O₃-XE in the Lanthanum-Chalcogenides we could demonstrate the transfer of s-like valence electrons from the Lanthanum atom to the Chalcogen atom. Furthermore, the binding energy of the 4f¹ state at the Lanthanum atom was determined; it agrees very well with calculations in a thermochemical model [JoM87]. The surface core-level shift is smaller by 25 % in the Chalcogenides than in La-metal. We also describe a theoretical model, which qualitatively explains the observed larger shifts of the core-level binding energy in PE than in IPE from Lanthan-Chalcogenides. Our 4f¹-IPE results allow a correct assignment of transitions in MOKE measurement [PSH97,SWH99] which had aroused a controversy.

* This has been measured for the first time.