Spin state and core level satellites
in the electronic structure of α- and ε-Fe₂O₃ nanoparticles

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We report on spectroscopic investigations on nanoparticles of α- and ε-Fe₂O₃ [1,2]. For both well-defined nanoparticles we analyze the electronic structure and we determine the partial density of states for the valence and conduction bands. From these data we derive a band scheme and compare it with recent band structure calculations [3].

The resPES data at the Fe2p absorption edge (Figure 1) are analyzed to unravel the spin states involved. We find that for the ε-Fe₂O₃ the majority is due to the Fe3d⁵ HS state. Contributions of the corresponding LS state are small and are found to be higher in the α-Fe₂O₃ prepared by ALD we in addition identify a LS 3d⁶L state [4].

Finally, we identify a loss process upon resonant excitation which appears predominately in the ε-Fe₂O₃ phase. We give a model to describe that loss process. It is used to also explain the appearance of the Fe2p core level satellites which are different for the α- and ε-Fe₂O₃ phases.


Figure 1.: Resonant photoelectron spectra of ε-Fe₂O₃ as recorded at around the Fe2p absorption edge.