Spin states of transition metal atoms in free clusters and organometallic complexes studied by x-ray magnetic circular dichroism spectrocopy

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While transition metals typically form high-spin states as free atoms, they might adopt high-spin or low-spin states when embedded into a host material, depending on the details of the interaction. The electronic ground states of endohedral transition-metal-doped silicon clusters have recently been discussed controversially, in particular with respect to high-spin [1] or low-spin ground states, [2] or to the presence of open-shell singlet states [3] with a local high-spin configuration on the transition metal atom that is counterbalanced by opposite spins in the silicon shell.

To resolve this controversy, we have studied a variety of size-selected transition metal atom doped silicon cluster ions by x-ray magnetic circular dichroism spectroscopy in a dedicated ion trap setup at the Berlin synchrotron radiation source BESSY II, [4–6] where we find a qualitatively similar behaviour of different transition metals. For a broader view, we have extended the range of samples to organometallic sandwich complexes of 3d transition metals with well-characterized ground states as simple model systems for spin states of endohedral clusters.

This talk will briefly summarize the spectroscopic technique of x-ray magnetic circular dichroism in cryogenic ion traps that has recently even been able to demonstrate ion temperatures as low as 7.4 ± 0.2 K of a cloud of approx. 10^7 ions in the space charge limit. [7] General findings on the interdependency of electronic and geometric structure of transition metal doped silicon and organometallic clusters will be discussed from the spectroscopic point of view.

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