Spin-dipole moment in low symmetry structures

BIPLAB SANYAL, SUMANTA BHANDARY, SOUMYAJYOTI HALDAR, OLLE ERIKSSON, Dept. of Physics and Astronomy, Uppsala University — The spin-dipole contribution ($T_z$) is usually neglected in x-ray magnetic circular dichroism measurements for bulk systems, as the value is negligible compared to the spin moment. However, in the last few years, it has been demonstrated quite clearly from experiments and theory that $T_z$ can acquire relatively large values for systems with low dimensions, e.g., organometallic molecules like Fe porphyrine/phthalocyanine [1] or small inorganic clusters. In some cases, the large $T_z$ contribution can be opposite to the spin moment and hence, the effective moment $(2S+7T_z)$ turns out to be very small [2]. With the aid of first principles density functional calculations, the role of $T_z$ will be demonstrated for organometallic molecules and magnetite nanoparticles. The calculated effective moments follow the same trend as experimental measurements.


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