Theoretical study of metal-DNA structure

Auto-organization, auto-recognition and selectivity are desirable features for new nanotechnological materials. Biological systems like proteins and DNA are candidates to technological devices. The possible applications range from biological sensors to electronic devices. The electronic transport though DNA have been studied from decades. It is known that some features have still to be improved in the electronic transport in DNA like those related with the chain hardness, substrate interaction and π-π orbital overlap [1]. In the last years modified DNA structures were developed towards improving these features. One class of these bases is the Cu-hydroxypiridone which is complexed with Cu [2] where EPR studies have shown ferromagnetic interactions among the Cu centers [2]. We study the electronic structure of a monomer and dimer Cu-hydroxypiridone with a theoretical approach in the Kohn-Sham scheme of the Density-Functional Theory using the CP-PAW code [3] including a non-collinear spin formulation. We show the differences in the magnetization in three approaches: influence of charge effects, backbone effects and in plane and inter-plane Cu coordination. We also discuss the magnetic interaction including up to five Cu-hydroxipiridone modified bases.

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Local structure of FePt thin films investigated by polarized X-ray absorption spectroscopy

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The structure of FePt films have been studied by X-ray Absorption Spectroscopy (XAS). The purpose of this work is to quantify the local structural anisotropy, correlating with the macroscopic magnetic anisotropy of these films. In the XAS measurements, the sample orientation was varied with respect to the linearly polarized X-ray beam. This procedure allows obtaining more precise information about the local structure around the absorber atom. The results show that the short range chemical order inside the samples is highly dependent on the deposition procedure, growth temperature and substrate.
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