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Computational study of the magnetic behavior of metal DNA structures

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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]. In this work we study the electronic structure of Cu-hydroxypiridone with a theoretical approach in the Kohn-Sham scheme of the Density-Functional Theory using the CP-PAW code [3].

References

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