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Ab Initio Hyperfine Interactions as a Powerful Tool to Identify the Metal Binding Site in Biological Systems: Cd²⁺ in DNA Bases.

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Hyperfine interactions can be a powerful tool to identify local environments in many different systems. Recently it has been drawn attention to the possible application of the Time Differential Perturbed Angular Correlation (TDPAC) technique to study differences in the Nuclear Quadrupole Coupling constants (νQ) at Cd probes in mouse DNA infected with the Trypanosoma Cruzi. The electric contribution to the hyperfine interaction is usually expressed as the nuclear quadrupole coupling frequency νQ which is given by the product of the nuclear quadrupole moment Q and the Electric Field Gradient (EFG) at the nucleus. The EFG can be theoretically obtained from an ab initio electronic structure calculation. The $^{111}\text{In} \rightarrow ^{111}\text{Cd}$ β decay can be used in a TDPAC measurement to investigate the Cd metal binding to DNA. The interaction of the metal with the DNA bases can change many aspects of the base pairing [1]. Here we study electric hyperfine properties of Cd bound to some DNA bases. The methodology used for the electronic structure calculations is based on the Kohn Sham [2] scheme of the Density Functional Theory (DFT) and the Car-Parrinello [3] method. We use the Projector Augmented Wave [4] method as embodied in the (CP-PAW) computational code. The results of EFG and energies are discussed as function of water molecules present in the Cd²⁺ environment and compared with TDPAC measurements at Cd probes in mouse DNA infected with the Trypanosoma Cruzi. References [1] J. V. Burda, J. Sponer, J. Leszczynski, P. Hobza, J. Phys. Chem. B., 101, 9670 (1997). [2] W. Kohn, L. J. Sham, Phys. Rev. B., 140, 1133 (1965). [3] P. E. Blöchl, Phys. Rev. B., 50, 17953 (1994). [4] R. Car e M. Parrinello, Phys. Rev. Lett. 55, 2493 (1985).

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Oral presentation

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