Comparing structure and dynamics of solvation of different iron oxide phases for enhanced MR imaging

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Abstract: Cancer is a global epidemic that significantly affects all ages and socioeconomic groups[1]. One of the great difficulties of cancer is its diagnosis, mainly in the initial phase. Currently, the most used and effective technique for cancer diagnosis is Magnetic Resonance Imaging (MRI)[2]. For a better visualization of MRI images, it is necessary to use contrast agents (CAs). The CAs are paramagnetic compounds which increase image contrast by preferentially influencing T1 and/or T2 relaxation times of water molecules in the vicinity of their compounds[3]. Currently, the CAs most used as MRI probes are gadolinium (Gd3+) complexes; despite being very effective, they are very toxic to the body, even in small concentrations. Thus, less toxic and more efficient CAs able to substitute Gd3+ complexes have been studied. The SPIONs (superparamagnetic iron oxide nanoparticles) have been investigated as novel contrast agents in MRI, due to a combination of favorable superparamagnetic properties[4]. Following this line, the aim of this study is to analyze water coordinates in the face 100 of different phases of iron oxides (δ-FeOOH, α-FeOOH, Fe2O3, Fe3O4), in order to replace Gd3+ complexes. For this purpose, calculations of molecular dynamics (MD) with the FEOCH force field, were performed and the main conformations were selected using the OWSCA method[5] for subsequent quantum calculations of the hyperfine coupling constant (Aiso). The Aiso calculations were performed using the Gaussian 09 program[6]; functional PBE1PBE with the basis set aug-cc-pVTZ-J was used for oxygen and hydrogen atoms, and Lanl2dz for iron atoms for all structures. The results show a large increase in Aiso values. This increase in Aiso values was mainly due to the H bonds between water molecules and between water molecules and the oxides; this fact was proven by QTAIM and NCI calculations. At last, we strongly affirm that all the iron oxides studied are great candidates as promising ACs in MRI.

Key-words: MRI, Contrast Agents, Iron Oxide, SPIONs, OWSCA
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