

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

Mateus A. Gonçalves (PG)<sup>a</sup>, Mozarte Santos Santana (PG)<sup>a</sup>, Lizandro S. Santos<sup>b</sup>,  
Fernando C. Peixoto<sup>b</sup>, Teodorico C. Ramalho (PQ)<sup>a</sup>

<sup>a</sup>*Departamento de Química, Universidade Federal de Lavras,  
Lavras, Minas Gerais, Brasil.*

<sup>b</sup>*Department of Chemical and Petroleum Engineering,  
Federal University Fluminense, Niterói, Rio de Janeiro, Brasil.*

**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  $T_1$  and/or  $T_2$  relaxation times of water molecules in the vicinity of their compounds[3]. Currently, the CAs most used as MRI probes are gadolinium ( $Gd^{3+}$ ) 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  $Gd^{3+}$  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 ( $\delta$ -FeOOH,  $\alpha$ -FeOOH,  $Fe_2O_3$ ,  $Fe_3O_4$ ), in order to replace  $Gd^{3+}$  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 ( $A_{iso}$ ). The  $A_{iso}$  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  $A_{iso}$  values. This increase in  $A_{iso}$  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



# XIX SBQT

## Simpósio Brasileiro de Química Teórica 2017

12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

**Support:** The authors thank the Brazilian agencies FAPEMIG, CAPES, and CNPq for the financial support of this research the UFLA and UFF for infrastructure and encouragement in this work.

### References:

- [1] V. L. De Almeida, A. Leitão, C. Barrett, C. Alberto and C. Luis, *Quim. Nova*, **2005**, 28, 118–129.
- [2] J. Y. et al LI, *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2013**, 102, 66–70.
- [3] S. J. Dorazio and J. R. Morrow, *Eur. J. Inorg. Chem.* **2012**, 2006–2014.
- [4] S. Yoffe, T. Leshuk, P. Everett and F. Gu, *Current Pharmaceutical Design.* **2013**, 19, 493–509.
- [4] M. A. Gonçalves, F. C. Peixoto, E. F. F. da Cunha and T. C. Ramalho, *Chem. Phys. Lett.*, **2014**, 609, 88–92.
- [5] Frisch MJ, Trucks GW, Schlegel HB et al, Gaussian 09