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Utilization of PAC of radioisotope trackers and DFT calculations to determine local environment of Hg(II) in dithiocarbamate functionalized particles for magnetic removal of Hg2+ from water

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Application of nanoparticles in water treatments attracts growing interest due to their high specific surface area and ability for chemical functionalization. In particular, functionalized iron oxide nanoparticles are promising sorbents because several pollutants (e.g. heavy metals) can be adsorbed and then removed from the solution by the application of an external magnetic field [1-2].
The present work aims to study the chemical mechanism behind the adsorption of the highly toxic mercury by magnetite particles with silica shells enriched in dithiocarbamate (DTC) groups [3-4], with total side diameters of approximately 50 and 100 nm.
Combining Perturbed Angular Correlations (PAC) Spectroscopy [5] of 199mHg with DFT calculations (LDA and GGA-PBE) we identify different local environments that characterize the position where the Hg is retained during the adsorption. For the non-enriched nanoparticles, we find that Hg mostly coordinates in a SiO2 environment, while for the nanoparticles functionalized with DTC groups Hg coordinates in an environment with two DTC units, at almost perpendicular HgS2 planes for each unit. In the functionalized nanoparticles which had been previously saturated with Hg, this environment is also predominant, but other fractions with SiO2 and SiO3 environments are now detected.
We also present an alternative method to determine the adhesion/uptake of Hg(II) by the different types of nanoparticles, resorting to direct tracking of the radioisotope. This method presents some advantages with respect to the fluorometry analysis [3], such as a lower detection limit (pg/L should be easily achieved, in comparison to tens of ng/L in typical fluorescence spectroscopy) and a direct detection in the nanoparticles. This paves the way to studies of recycling and manipulation conditions as well as studies of the path taken by heavy metals in flora and fauna.

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