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Selective adsorption of mercury (Hg^{2+}) on a metal-organic framework obtained from aluminium and mercaptosuccinic acid

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Water polluted with mercury represents a risk to the health of human beings and, in general, to all living beings that depend directly on these environments. It is then necessary to think about methods of capture and identification of chemicals species of mercury in water bodies. In this sense, the metalorganic frameworks (MOFs), hybrid crystalline materials, have a high potential to be used in the remediation of water contaminated with mercury. Through electronic structure calculations with Density Functional Theory (DFT), the mechanisms of the interaction between Hg^{2+} and organic ligands were evaluated. These ligands were derived from fumaric acid when functionalized with groups -SH, - SCH_3, -NH_2, or -PH_2. The interaction energy analysis, as well as the global reactivity indexes, suggest that the thiol group is the most selective to mercury compared to other water constituent metals such as calcium and lead (-56.40 kcal/mol, -48.99 kcal/mol, and -39.91 kcal/mol, respectively). This adsorptive capacity of the organic ligand was maintained by being part of a representative structure of the selected MOF. Through the analysis of charge transfer and non-covalent interactions index, it was verified that this adsorption was mediated by the tricoordination of mercury involving two oxygen atoms and the sulfur of the thiol group; these interactions are strong, mainly electrostatic, and not dispersive (see Figure 1). Taking as a basis the computational results, the Al-mercaptosuccinate MOF was synthesized and characterized. Its removal efficiency evidenced the high adsorptive capacity of this framework, reaching Hg^{2+} removal ratios of 99% at a concentration of the metal in aqueous solution of 10 μg/mL, in the same way this MOF shows to be selective against mercury in presence of other metals.

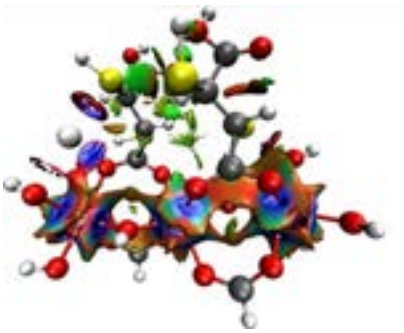

Figure 1: *Isosurfaces obtained from the Non-Covalent Interactions (NCI) index at the MOF---Hg^{2+}complex*

Recent Publications

1. Ha E, *et al.* (2017) Current progress on understanding the impact of mercury on human health. Environmental Research 152:419-433.
2. Jia J, *et al.* (2013) Metal–organic framework MIL53 (Fe) for highly selective and ultrasensitive direct sensing of $MeHg^+$. Chemical Communication 49:4670-4672.

3. Johnson E R, et al. (2008) Revealing Noncovalent Interactions. Journal of the American Chemical Society 132(18): 6498 - 6506.

Biography

Sol M Mejia is an Assistant Professor at the Chemistry Department of the Pontificia Universidad Javeriana in Colombia since 2014. She received her PhD from the Universidad de Antioquia in 2011. She did two postdoctoral researches, the first one at the University of Adelaide in Australia and the second one at the Universidad Autónoma Metropolitana in Mexico. She is the leader of the Computational Chemistry research line. Her major areas of interest are radical organic reactions, metal clusters, metal organic frameworks, and weak interactions (hydrogen bonds) as basic chemistry with possible applications in chemistry catalysis, biologic activity, new materials, and the like.

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