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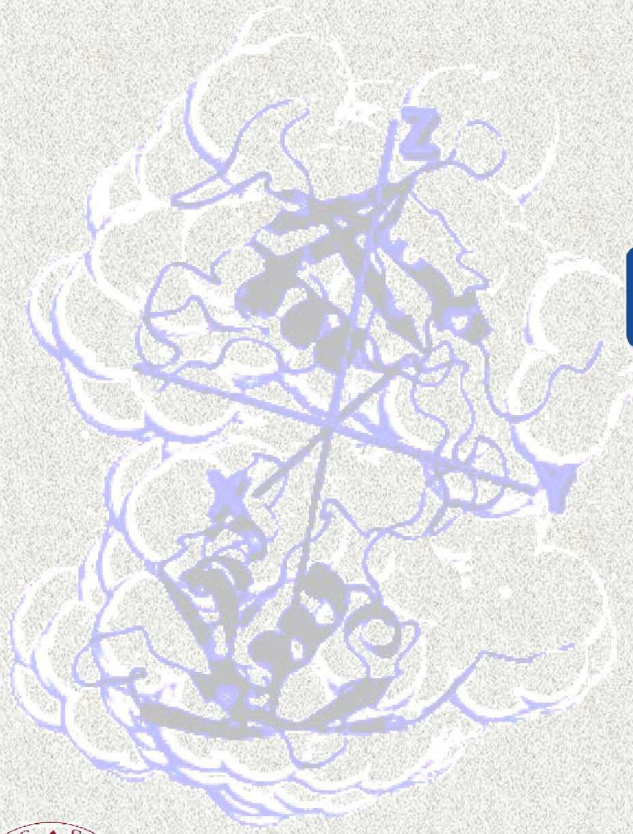
II Congresso Nazionale della divisione di Chimica teorica e Computazionale della Società Chimica Italiana



Padova, Centro Culturale S. Gaetano

20-22 febbraio 2013

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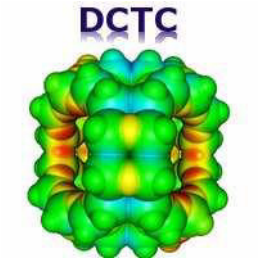

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POSTER

MODELING OF SPIRAL HALLOYSITE NANOTUBES

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Halloysite is an economically viable clay mineral, belonging to the kaolinite group and occurring in nature with a hollow tubular shape. The size of halloysite nanotubes are between 500 and 1000 nm in I and 15-100 nm in inner diameter, depending on the deposit. The general stoichiometry is $Al_2Si_2O_5(OH)_4 \cdot n\ H_2O$ with n=0 for the anhydrous (Halloysite 7Å) and n=2 for the fully hydrated halloysite (Halloysite 10Å). The crystal structure is described as a layer formed by two building blocks: $[SiO_4]$ tetrahedra and $[AlO_6]$ octahedra. Water molecules in Halloysite 10Å are sitting between two consecutive layers. This material finds application in ceramics, cements and fertilisers industry and, recently, as template in nanotechonology. In fact, thanks to its peculiar shape, halloysite is considered a promising entrapment system for loading, storage and controlled release system for various species [1].
The modeling approach is an helpful tool in the prediction and interpretation of the interactions occuring between adsorbed species and inner and/or outer nanotube surfaces. Even though a preliminary study on the adsorption process could be obtained from a flat monolayer of kaolinite model or single-walled halloysite nanotube [2], it is necessary to build up a more realistic model of the hollow spiral nanotube. To this aim the starting geometries of Halloysite 7Å and Halloysite 10Å have been generated by means of a program based on the analitycal properties of Archimedean spiral. Geometry optimization of the supercells so obtained (some of which exceed 2500 atoms) has been perfomed by means of Self Consistent Charges Density Functional Tight Binding employing the DFTB+ program [3]. These investigations, which represent the first attempts to model the hydrated halloysite spiral nanotube, allowed to obtain information on the $[SiO_4]$ tetrahedra and $[AlO_6]$ octahedra distortions necessary to the spiral formation and on the water molecules organization on the Halloysite 10Å outer surfaces and between the arms of its spiralling geometry.

[1] Lvov, Y. M., et al. *ACS Nano* **2008**, *2*, 814-820.
[2] Guimarães, L., et al. *J. Phys. Chem. C* **2010**, *114*, 11358-11363.
[3] Aradi B., et al. *J. Phys. Chem. A* **2007,** *111*, 5678-5684.