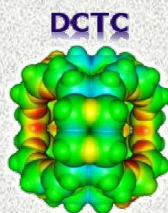
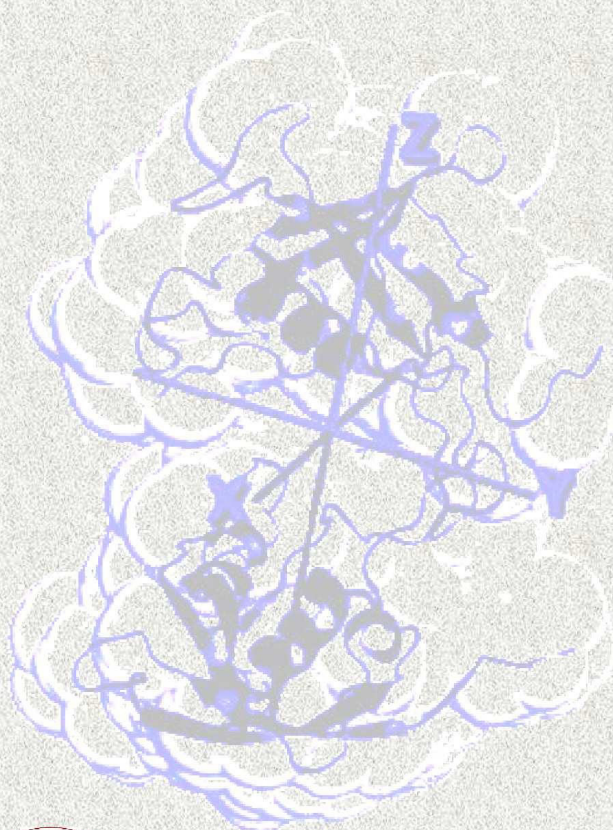


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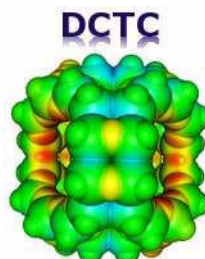


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POSTER

P01 FULLY AUTOMATED PROCEDURE TO EVALUATE ELASTIC AND PIEZOELECTRIC CONSTANTS 57

Elisa Albanese, Alessandro Erba, Bartolomeo Civalleri

P02 DFT AND TDDFT STUDY OF UNSYMMETRICAL SQUARAINES ADSORBED ON PbSe SURFACES 58

Mario Argeri, Claudia Barolo, Maurizio Cossi, Fabio Grassi, Leonardo Marchese

P03 MODELING OF SPIRAL HALLOYSITE NANOTUBES 60

Francesco Ferrante, Nerina Armata, Giuseppe Lazzara, Stefana Milioto

P04 IMPROVING THE COMPARISON OF COMPUTATIONAL DATA WITH EXPERIMENTAL ABSORPTION AND EMISSION SPECTRA. BEYOND THE VERTICAL TRANSITION APPROXIMATION..... 61

Francisco Avila, Javier Cerezo, Emiliano Stendardo, Roberto Improta, Fabrizio Santoro

P05 BERYLLIUM OXIDE NANOTUBES AND THEIR CONNECTION TO THE FLAT MONOLAYER..... 62

J. Baima, A. Erba, M. Rérat, R. Orlando, R. Dovesi

P06 THE NEAR-EDGE X-RAY-ABSORPTION FINE-STRUCTURE OF O₂ CHEMISORBED ON Ag(110) SURFACE STUDIED BY DENSITY FUNCTIONAL THEORY..... 63

Oscar Baseggio, Mauro Stene, Michele Romeo, Giovanna Fronzon

P07 FUNCTIONAL EFFECTS ON THE TDDFT INVESTIGATIONS IN ORGANOMETALLIC PHOTOCHEMISTRY 64

Luca Bertini, Maurizio Bruschi, Claudio Greco, Luca De Gioia, Piercarlo Fantucci, Giuseppe Zampella

P08 STUDY OF THE SPECIATION OF THE [Cu(HGGG)(Py)] COMPLEX IN WATER SOLUTION USING DFTB AND DFT APPROACHES 65

Maurizio Bruschi, Luca Bertini, Vlasta Bonačić-Koutecký, Luca De Gioia, Roland Mitrić, Giuseppe Zampella, Claudio Greco, Piercarlo Fantucci

P09 ARE THE NONADIABATIC TRANSITION RATES TRANSFERABLE AMONG DIFFERENT ENVIRONMENTS?..... 66

Valentina Cantatore, Giovanni Granucci, Maurizio Persico

P10 THEORETICAL ADSORPTION OF METHANE, HYDROGEN AND CARBON DIOXIDE IN POROUS AROMATIC FRAMEWORKS (PAFs)..... 68

L. Canti, A. Fraccarollo, M. Cossi, L. Marchese

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 length and 15-100 nm in inner diameter, depending on the deposit. The general stoichiometry is $\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4 \cdot n \text{H}_2\text{O}$ 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: $[\text{SiO}_4]$ tetrahedra and $[\text{AlO}_6]$ 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 nanotechnology. 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 occurring 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 analytical properties of Archimedean spiral. Geometry optimization of the supercells so obtained (some of which exceed 2500 atoms) has been performed 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 $[\text{SiO}_4]$ tetrahedra and $[\text{AlO}_6]$ 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.