COMPUTATIONAL AND EXPERIMENTAL STUDIES OF HALLOYSITE MODIFIED SURFACES FOR EFFICIENT FUNCTIONALIZATION

Lorenzo Lisuzzo, Marco Bertini, Chiara Ferlito, Francesco Ferrante, Giuseppe Cavallaro, Giuseppe Lazzara and Dario Duca

Dipartimento di Fisica e Chimica Emilio Segrè, Università degli Studi di Palermo, Italy

The surface functionalization is one the most crucial step for the design of novel materials with improved performance in a wide range of technological applications. Among them, Halloysite Nanotubes (HNTs) hold a certain importance due to their peculiar properties. HNTs are naturally occurring aluminosilicates with a hollow nanotubular shape that makes them eligible in many fields. However, their use strictly depends on the chemistry of functional groups on the inner and/or outer surfaces. In this work, the treatment of halloysite in alkaline medium was investigated in order to enlighten the formation of actives sites which can act as anchoring points for the grafting with organic molecules by chemical reactions. Computational studies, carried out by a cluster approach within density functional theory, provided atomistic details about the formation and the configuration of silanol groups on the surface of the inorganic solid and the promotion of covalent bonding with aminosilanes, such as APTES and AEAPTMS. Experimental analysis was carried out to assess the efficiency of the surface grafting, which is higher for the modified nanoclays compared to the neat aluminosilicates, as suggested by computational findings. Also, the modification of the inner surface by acidic treatment was evaluated to have more detailed insights about the appearance of acidic sites embedded in the clay nanostructure. These results pave the ground for the development, among others, of halloysite based materials to be exploited in catalytic processes.