ADSORPTION OF SULFONAMIDES ON PHYLLOSILICATE SURFACES AS MODELS OF SLOW RELEASE NANOMATERIALS BY DIFFERENT THEORETICAL APPROACHES

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Phyllosilicates can be considered as natural nanomaterials that can be funtionalized for therapeutic slow release of drugs. Sulfamides form a great group of antibiotics widely used since decades for human therapeutics and in veterinary for intensive livestock production. The efficiency of the administration of these drugs is very low and the presence of these antibiotics and their derivatives in soil can alter the bacterial resistance to animals and humans through the soil, water and food chains. Therefore, it is important to search environmental-friendly slow-release nanomaterials, in order to overcome these problems. Then, it is important to investigate the adsorption of these drugs on the surfaces of these nanomaterials. The adsorption of sulfonamides, Sulfamethoxypyridazine and Sulfamethoxypyrimidine, as models of sulfonamides, on pyrophyllite surface of (001) plane have been investigated by means of empirical interatomic potentials and quantummechanical methods based on Hartree-Fock and Density Functional Theory (DFT) approximations. Molecular Dynamic simulations have been also performed for this adsorption exploring the different configurations that these sulfonamides can adopt with respect to the surface. The adsorption energy calculated with different methods are compared and discussed on the application of empirical potentials and DFT methods for describing the weak interactions of this adsorption.

Keywords: modelling, adsorption, phyllosilicates