Interaction of Amino Acids on Montmorillonite Clay Surfaces and its Effect on Electro-Magnetic and Biomedical Properties

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Abstract

The interaction of amino acids with clay minerals results in formation of novel biomaterial nanocomposite system promising for pharmacological and biomedical applications. We consider representative models of organically modified montmorillonite clay (OMMT) having a chemical formula of $(FeMg)_{0.25}Al_{1.5}Si_4O_{10}(OH)_2.nH_2O$ functionalized by three derivatives of the valeric acid. DFT calculations results in the surface energy of the OMMT slabs of 152.72, 153.37, and 175.34 mJ/m^2, depending on the position of Fe and Mg dopants. Three different isomers of valeric acid: NH2-[CH2]4-COOH (5-Aminopentanoic acid), HOOC-CH(NH2)-[CH2]4-COOH (2-Aminoheptandioic acid), and HOOC-CH(NH2)-[CH2]5]-CH3 (2-Aminooctanoic acid) are physisorbed on the OMMT along (001) plane at various distances with respect to Fe and Mg dopants. The calculated negative value of the acid-OMMT binding energies indicates the substantial electrostatic interaction between the acid molecules and OMMT slab. We have noticed a strong ferromagnetism due to dopant Fe that imparts the total magnetic moment of 9.76 μ_B, 9.73 μ_B and 7.99 μ_B for our proposed slab models, respectively. The varying magnetic order of antiferromagnetic, ferrimagnetic and ferromagnetic after the adsorption of acid molecules is a surprising result which indicates that OMMT can be a potential candidate for electro-magnetic, bio-imaging and sensing applications.