Effect of Protonation/Deprotonation of Intercalating Molecules on Electro-Magnetic Properties of Montmorillonite Nanoclay

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Layered clay minerals, such as montmorillonite (MMT) with a chemical formula $(FeMg)_{0.25}Al_{1.5}Si_4O_{10}(OH)_2.nH_2O$, belong to non-toxic, natural, low-cost, abundant materials. Usage of unnatural amino acids (AA) with COOH-CH-NH_2 moiety as intercalating agents results in formation of clay nanoplatelets of about 1 nm in thickness. Such organically modified MMT nanostructures (nano-MMT) have improved dispersion, mechanical, flame retardancy, thermal, transport, biocompatibility, and biodegradability properties, making them suitable for tissue engineering. Using first-principle calculations based on the density functional theory (DFT), we study structural parameters governing the interaction between AA molecules, such as 5-aminovaleric acid (AA1), 2-aminopimelic acid (AA2), and DL-2-aminocaprylic acid (AA3), and the nano-MMT. We investigate how these interactions are affected by the concentration of Fe(II)/Mg doping in the nano-MMT, protonation/deprotonation of amino acids, and water environment. Our calculations reveal high sensitivity of magnetic response of nano-MMT to the type of AA, its conformation at the nanocaly surface, and interactions with water molecules. Thus, transition in magnetic orders from ferromagnetism to antiferromagnetism or ferrimagnetism can be achieved by changing the alignment of the AA molecule on the surface. The introduced charge to the AA via its protonation increases the AA-nanoclay interaction, while the magnetization is reduced by about 1.5 times, compared to their neutral counterparts. The predicted tunability of magnetic properties may permit magnetic separation, visualization, and cell imaging and may also have a therapeutic benefit of these materials. Thus, our calculations show that the molecule-MMT interactions can be probed by electro-magnetic techniques, which extends experimental tools for studding these materials for bio-applications.