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SURFACE MODIFICATION AND MOLECULAR CLUSTER MODELLING OF γ-Fe_2O_3 NANOPARTICLES AS A POTENTIAL CARRIER FOR DRUG DELIVERY

C. J. K. Wijekoon[1], S. Randiligamage[1], R. Weerasooriya[2], W. M. A.T. Bandara[1]

[1]Department of Chemistry, Faculty of Science, University of Peradeniya
[2]Department of Soil Science, Faculty of Agriculture, University of Peradeniya

Magnetic drug delivery is based on the fact that a drug can be encapsulated onto a magnetic nano core shell. When the magnetic carrier is intravenously administered the accumulation takes place within the areas to which the external magnetic field is applied. In this research the suitability of casein - γ-Fe_2O_3 core shell nanoparticles as a magnetic drug carrier under controlled fashion was determined.

Unmodified γ-Fe_2O_3 particles are unstable in physiological fluids tending to agglomerate and precipitate quickly. A surface coating of casein was used to prevent this. Casein also provides chemical handles for the conjugation of drug molecules. It also enhances the bio compatibility and controls the hydro dynamic radius of the core shell.

Diffuse Reflection Infrared spectroscopy (DRIFT) data were used to interpret the binding of casein onto γ-Fe_2O_3. To effectively analyze the experimentally found data, molecular modelling calculations were done for γ-Fe_2O_3 and surface modified γ-Fe_2O_3 with Gaussian 03 code. All the models were built with Gaussview. Optimized molecular structures were determined by searching in the potential energy surface for minima with respect to each atomic coordination using Density Function Theory (DFT) calculations under DFT hybrid B3LYP function with 6-31G (d,p) basic set. The γ-Fe_2O_3 nanoparticles were modelled using $Fe_6(OH)_{18}(H_2O)_6$ ring cluster. The adsorption of casein onto γ-Fe_2O_3 surface sites was also modelled using the derived cluster and the vibrational frequencies for the clusters were calculated.

Combination of the experimental and calculated data showed that casein binds to γ-Fe_2O_3 through the carboxylate group (COO^-). COO^- shows two asymmetric vibrations (AS) (1610-1550 cm^{-1}) and one symmetric vibration (S) (1420-1300 cm^{-1}). By calculating AS-S (Δ) the binding modes of the COO^- group was determined. If $\Delta>200$ cm^{-1} monodentate, $140<\Delta<200$ cm^{-1} bridging and $\Delta<140$ cm^{-1} bidentate. The binding modes changed with the pH. At pH 3 and 5 both bridging and bidentate bindings were observed. At pH 10 and 13 only monodentate binding was observed and at pH 7 monodentate and bidentate bindings were observed.

Hence the COO^- group of casein binds very effectively to γ-Fe_2O_3 in acidic conditions. Thus the surface modification of γ-Fe_2O_3 can be conveniently carried out using casein.