



A Study of Fe_3O_4 @ Zigzag, @ Armchair and @ Chiral SWCNTs and α & γ Cyclodextrins

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ABSTRACT

Fe_3O_4 is used as a catalyst in the Haber process and in the water gas shift reaction. In this work we have investigated the physical and chemical properties of Fe_3O_4 @ Zigzag, @ Armchair and @ Chiral SWCNTs compare to Fe_3O_4 @ α & γ -Cyclodextrin in view point of chemical reaction and sensitizes. The electrical properties such as NMR Shielding, electron densities, energy densities, potential energy densities, ELF, LOL, ellipticity of electron density, eta index and ECP for Fe_3O_4 @ -Cyclodextrin shell and Fe_3O_4 @ Zigzag, @ Armchair and @ Chiral SWCNTs have been calculated for the simulations. Our Calculation indicate that the Fe_3O_4 @ (7, 7) and Fe_3O_4 @ (10,5) and Fe_3O_4 @ (9, 0) have physical and chemical properties close to Fe_3O_4 @ -Cyclodextrin and as well as the Fe_3O_4 @ (8,8) and Fe_3O_4 @ (11,6) and Fe_3O_4 @ (10, 0) are close to Fe_3O_4 @ -Cyclodextrin.

Keywords: Fe_3O_4 , Nano-Particles, electron density, SWCNTs, Cyclodextrin (α & γ).

INTRODUCTION

Fe_3O_4 nanoparticles (MNPs) are one of the most intensively studied magnetic nanoparticles and can be applied in a variety of areas, ranging from drug delivery¹ and bio-sensing², dynamic sealing³, and cell labeling⁴ to magnetic resonance imaging⁵.

Fe_3O_4 is ferromagnetic with a curie temperature of 858 K and The ferromagnetism of Fe_3O_4 arises because the electron spins of the Fe^{II}

and Fe^{III} ions in the octahedral sites are coupled and the spins of the Fe^{III} ions in the tetrahedral sites are coupled but anti-parallel to the former^{6,7}.

Fe_3O_4 is used as a catalyst in the Haber process and in the water gas shift reaction^{7,8}.

Moreover, MNPs are well suited for target capturing, enrichment, and isolation⁹. Accordingly, they can be used for isolating cells¹⁰ and bacteria¹¹ and for removing environmental toxins such as heavy metals and chemical waste¹².

The latter uses an HTS (high temperature shift catalyst) of iron oxide stabilized by chromium oxide⁶⁻⁸. This iron-chrome catalyst is reduced at reactor start up to generate Fe_3O_4 from $\alpha\text{-Fe}_2\text{O}_3$ and Cr_2O_3 to CrO_3 ⁵. Fe_3O_4 is an electrical conductor with conductivity significantly higher than Fe_2O_3 , and this is ascribed to electron exchange between the Fe^{II} and Fe^{III} centers⁶⁻⁹.

Magnetite (Fe_3O_4) is the earliest discovered magnet which crystallizes in the inverse cubic spinel structure. Each cubic spinel cell contains eight interpenetrating oxygen and the tetrahedral sites, occupied by one-third of the iron atoms, form a diamond structure. The remaining Fe atoms are located at the octahedral sites with the nearest-neighbor atoms lined up as strings along six different [110] directions. In other words Fe_3O_4 consists of a cubic close packed array of oxide ions where all of the Fe^{2+} ions occupy half of the octahedral sites and the Fe^{3+} are split evenly across the remaining octahedral sites and the tetrahedral sites^{6, 13, and 14}.

Nano sized magnetic particles are considered potential adsorbents for aqueous heavy metals due to their high surface area and the unique advantage of easy separation under external magnetic fields¹⁵⁻¹⁹. To further facilitate the adsorption affinity, surface modification, including physical coating and covalent binding, has often been explored to enable specific metal complexation²⁰⁻²⁵. For example, covalent attachment of carboxylic groups to the surface of magnetic nanoparticles was achieved by reacting hematite with 11-undecanoic acid, and the resulting material showed marked ability in adsorbing Cd (II)²⁰. The chitosan-coated Fe_3O_4 nanoparticles were reported to be efficient for the removal of Cu (II) ions²². Humic-acid-coated Fe_3O_4 nanoparticles prepared by the co-precipitation method were found to effectively sorb Hg (II), Pb (II), Cd (II), and Cu (II) from water²³. The thiol groups on the surfaces of Di-Mercapto-succinic acid-coated Fe_3O_4 nanoparticles also acted as binding ligands for Hg, Ag, Pb, Cd, and Tl metal ions²⁴. Recently, a magnetic nano-adsorbent prepared by coating a magnetite core with chitosan, followed by carboxylation with a keto-glutamic acid, was used to remove Cu (II) ions from aqueous solution²⁵.

SiO_2 is stable under acidic conditions and inert to redox reactions, as compared with the organic coating materials, and hence functions as an ideal shell composite to protect the inner magnetite core²⁶⁻²⁸. Silica-coated core-shell magnetite nanoparticles, i.e., $\text{Fe}_3\text{O}_4@ \text{SiO}_2$, have recently been investigated for potential biomedical applications^{27, 28}. Additionally, the SiO_2 coating shell has an abundance of surface hydroxyl groups, which offers ease of functionalization of magnetite nanoparticles.

Cyclodextrins, cyclic oligosaccharides obtained from the degradation of starch by *Bacillus macerans*, were first isolated in the late nineteenth century²⁹. Their ability to form inclusion complexes with suitable organic molecules was discovered soon thereafter³⁰. With the development of the field of Supramolecular Chemistry, their complexation properties have been extensively studied³¹. Applications for cyclodextrins and their derivatives are sought in various areas of chemistry, including the sensing of organic molecules³².

Carbon nanotube (CNT) is a representative nano-material. CNT is a cylindrically shaped carbon material with a nano-metric-level diameter³³. Its structure, which is in the form of a hexagonal mesh, resembles a graphite sheet and it carries a carbon atom located on the vertex of each mesh. The sheet has rolled and its two edges have connected seamlessly^{33, 34}.

Although it is a commonplace material using in pencil leads, its unique structure causes it to present characteristics that had not found with any other materials. CNT can be classified into single-wall CNT, double-wall CNT and multi-wall CNT according to the number of layers of the rolled graphite. The type attracting most attention is the single-wall CNT, which has a diameter deserving the name of "nanotube" of 0.4 to 2 nanometers. The length is usually in the order of microns, but single-wall CNT with a length in the order of centimeters has recently released.

SWCNTs have considered as the leading candidate for nano-device applications because of their one-dimensional electronic bond structure, molecular size, and biocompatibility, controllable property of conducting electrical current and reversible

response to biological reagents hence SWCNTs make possible bonding to polymers and biological systems such as DNA and carbohydrates.

$$\nabla\rho(r) = \left[\left(\frac{\partial\rho(r)}{\partial(x)} \right)^2 + \left(\frac{\partial\rho(r)}{\partial(y)} \right)^2 + \left(\frac{\partial\rho(r)}{\partial(z)} \right)^2 \right]^{\frac{1}{2}} \quad \dots(2)$$

Theoretical background

Electron density profile models

The electron density has been defined as

$$\nabla^2\rho(r) = \frac{\partial^2\rho(r)}{\partial x^2} + \frac{\partial^2\rho(r)}{\partial y^2} + \frac{\partial^2\rho(r)}{\partial z^2} \quad \dots(3)^{35-37}$$

$$\rho(r) = \eta_i |\varphi_i(r)|^2 = \sum_i \eta_i \left| \sum_l C_{li} \chi_l(r) \right|^2 \quad \dots(1),^{35-37}$$

Where η_i is occupation number of orbital (i), φ is orbital wave function, c is basis function and C is coefficient matrix, the element of i_{th} row j_{th} column corresponds to the expansion coefficient of orbital j respect to basis function i . Atomic unit for electron density can be explicitly written as e/Bohr³.

The positive and negative value of this function correspond to electron density is locally depleted and locally concentrated respectively. The relationships between $\nabla^2\rho$ and valence shell electron pair repulsion (VSEPR) model, chemical bond type, electron localization and chemical reactivity have been built by Bader³⁸.

Table1: All Electron Densities of non-bonded interactions for Fe₃O₄ - Cyclodextrin (γ)

Atom number	Density of all electron 10 ⁻³	Density of alpha 10 ⁻³	Density of Beta 10 ⁻³	Spin Density	Lagrangian kinetic [G(r)]energy(10 ⁻³)	Hamiltonian kinetic [K(r)] energy(10 ⁻²)
Fe(1)	0.14	0.07	0.07	0.0	0.22	0.32
Fe(2)	0.26	0.13	0.13	0.0	0.26	0.56
Fe(3)	0.32	0.16	0.16	0.0	0.11	0.24
O(1)	0.24	0.12	0.12	0.0	0.28	-0.12
O(2)	0.18	0.09	0.09	0.0	0.31	-0.22
O(3)	0.40	0.2	0.2	0.0	0.27	-0.11
O(4)	0.30	0.15	0.15	0.0	0.11	-0.22

Table 2: Laplacian, ELF, LOL and Local information entropy of non-bonded interactions for Cyclodextrin (γ)

Atom number	Laplacian of electron density (10 ⁻¹)	Electron localization function ELF (10 ⁻³)	Localized orbital locator (LOL) (10 ⁻¹)	Local information entropy (10 ⁻⁴)	Reduced density gradient(RDG) (10 ⁺¹)	Average local ionization energy
Fe(1)	-0.15	0.60	0.18	0.17	0.39	0.32
Fe(2)	-0.16	0.42	0.28	0.19	0.41	0.39
Fe(3)	-0.20	0.32	0.18	0.41	0.52	0.50
O(1)	0.38	0.32	0.24	0.18	0.44	0.34
O(2)	0.41	0.22	0.15	0.29	0.16	0.16
O(3)	0.35	0.26	0.34	0.31	0.47	0.83
O(4)	0.34	0.33	0.22	0.25	0.24	0.20

Hamiltonian kinetic energy density $K(r)$

The kinetic energy density is not uniquely defined, since the expected value of kinetic energy operator

$$\langle \varphi | -\left(\frac{1}{2}\right) \nabla^2 | \varphi \rangle \quad \dots(4)$$

can be recovered by integrating kinetic energy density from alternative definitions. One of commonly used definition is:

$$k(r) = -\frac{1}{2} \sum_i \eta_i \varphi_i^*(r) \nabla^2 \varphi_i(r) \quad \dots(5)$$

Relative to $K(r)$, the local kinetic energy definition given below guarantee positivizes everywhere; hence the physical meaning is clearer and is more commonly used.

Table 3: Lambada2, Wave function value, Ellipticity of electron density and Eta index of non-bonded interactions for Cyclodextrin (γ)

Atom number	Lambada2 (10^{-3})	Wave function value (10^{-3})	Ellipticity of electron density	Eta index	ESP from nuclear charge (10^4)	ESP from electron charge (10^2)
Fe(1)	-0.12	0.41	0.40	-3.15	0.10	-0.41
Fe(2)	-0.14	0.89	0.40	-3.65	0.10	-0.41
Fe(3)	-0.14	0.62	0.33	1.77	0.10	-0.42
O(1)	0.35	0.31	-0.44	1.47	0.11	-0.43
O(2)	0.15	-0.41	-0.27	0.90	0.11	-0.41
O(3)	0.31	0.35	-0.43	0.68	0.11	-0.42
O(4)	0.28	-0.38	-0.27	0.66	0.15	-0.41

Table 4: All Electron Densities of non-bonded interactions for Fe_3O_4 @ (11, 6) SWCNTs

Atom number	Density of all electron 10^{-3}	Density of alpha 10^{-3}	Density of Beta 10^{-3}	Spin Density	Lagrangian kinetic [G(r)]energy	Hamiltonian kinetic [K(r)] energy	Energy Density [E(r)]
Fe(1)	0.42	0.21	0.21	0.0	0.51	0.55	-0.41
Fe(2)	0.62	0.31	0.31	0.0	0.25	0.24	-0.23
Fe(3)	0.78	0.39	0.39	0.0	0.22	0.23	-0.21

Table 5: Laplacian, ELF, LOL and Local information entropy of non-bonded interactions for Fe_3O_4 @ (8,8) SWCNTs

Atom number	Laplacian of electron density 10^{-1}	Electron localization function (ELF) (10^{-3})	Localized orbital locator (LOL) 10^{-1}	Local information entropy 10^{-4}	Reduced density gradient (RDG) 10^{-1}	Average local ionization energy	ESP from electron charge 10^2
Fe(1)	-0.08	0.31	0.22	0.20	0.18	0.49	-0.68
Fe(2)	-0.08	0.30	0.12	0.14	0.35	0.51	-0.67
Fe(3)	-0.09	0.48	0.12	0.21	0.22	0.33	-0.68

The Lagrangian kinetic energy density, “G(r)” is also known as positive definite kinetic energy density.

$$G(r) = \frac{1}{2} \sum_i \eta_i |\nabla\varphi_i|^2 = \frac{1}{2} \sum_i \eta_i \left\{ \left[\left(\frac{\partial\varphi_i(r)}{\partial(x)} \right)^2 + \left(\frac{\partial\varphi_i(r)}{\partial(y)} \right)^2 + \left(\frac{\partial\varphi_i(r)}{\partial(z)} \right)^2 \right] \right\} \quad \dots(6)$$

K(r) and G(r) are directly related by Laplacian of electron density

$$\frac{1}{4} \nabla^2 \rho(r) = G(r) - K(r) \quad \dots(7)$$

Electron localization function (ELF)

Becke and Edgecombe noted that spherically averaged likespin conditional pair probability has direct correlation with the Fermi hole and then suggested electron localization function (ELF) [39].

$$\text{ELF}(r) = \frac{1}{1 + [D(r)/D_0(r)]^2} \quad \dots(8)$$

where

$$D(r) = \frac{1}{2} \sum_i \eta_i |\nabla\varphi_i|^2 - \frac{1}{8} \left[\frac{|\nabla\rho_\alpha|^2}{\rho_\alpha(r)} + \frac{|\nabla\rho_\beta|^2}{\rho_\beta(r)} \right]$$

and

$$D_0(r) = \frac{3}{10} (6\pi^2)^{\frac{2}{3}} [\rho_\alpha(r)^{\frac{5}{3}} + \rho_\beta(r)^{\frac{5}{3}}] \quad \dots(22)$$

for close-shell system,

since $\rho_\alpha(r) = \rho_\beta(r) = \frac{1}{2}\rho$, D and D0 terms can be simplified as

$$D(r) = \frac{1}{2} \sum_i \eta_i |\nabla\varphi_i|^2 - \frac{1}{8} \left[\frac{|\nabla\rho|^2}{\rho(r)} \right] \quad \dots(10)$$

$$D_0(r) = \frac{3}{10} (3\pi^2)^{\frac{2}{3}} \rho(r)^{\frac{5}{3}} \quad \dots(11)$$

Savin *et al.* have reinterpreted ELF in the view of kinetic energy, ⁴⁰ which makes ELF also meaningful for Kohn-Sham DFT wave-function or even post-HF wave-function. They indicated that D(r) reveals the excess kinetic energy density caused by Pauli repulsion, while D0(r) can be considered as Thomas-Fermi kinetic energy density ⁴¹.

Localized orbital locator (LOL) is another function for locating high localization regions likewise ELF, defined by Schmider and Becke in the paper^{42, 43}.

$$\text{LOL}(r) = \frac{\tau(r)}{1 + \tau(r)} \quad \dots(12)$$

where

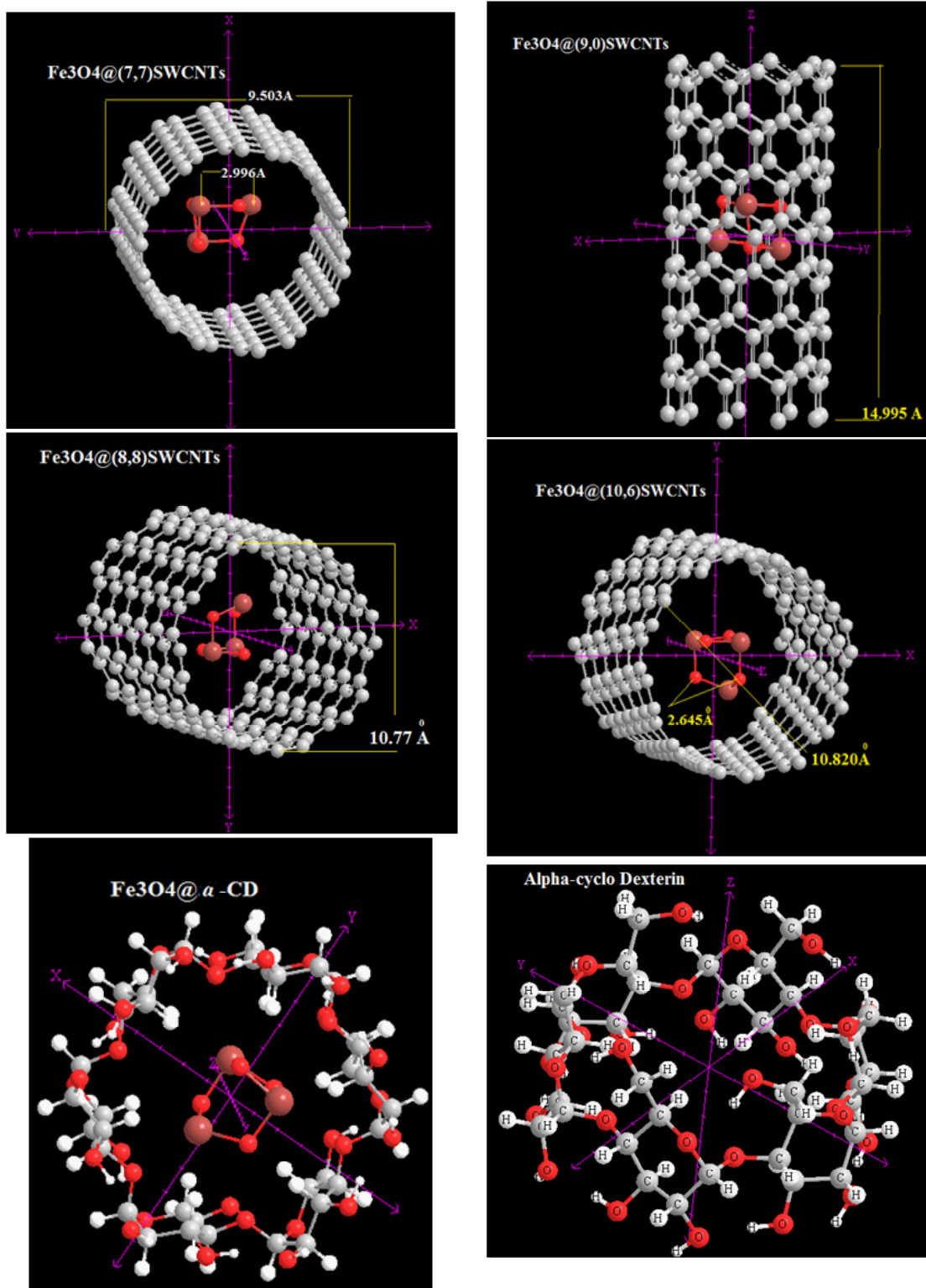
$$\tau(r) = \frac{D_0(r)}{\frac{1}{2} \sum_i \eta_i |\nabla\varphi_i|^2} \quad \dots(13)$$

D₀(r) for spin-polarized system and close-shell system are defined in the same way as in ELF⁴³.

This work has been studied based some previous works⁴⁴⁻¹⁶⁷ and has compared with the experimental data.

Table 6: Lambada2, Wave function value, Ellipticity of electron density and Eta index of non-bonded interactions for Fe₃O₄@(10,0)SWCNTs

Atom (number)	Lambada2 (10 ⁻³)	Wave function value (10 ⁻⁴)	Ellipticity of electron density	Eta index
Fe(1)	-0.31	0.14	0.98	1.2
Fe(2)	-0.54	0.15	0.92	2.1
Fe(3)	0.23	-0.34	0.90	0.5

Fig.1: Optimized Fe₃O₄@various nanotubes and cyclodextrin

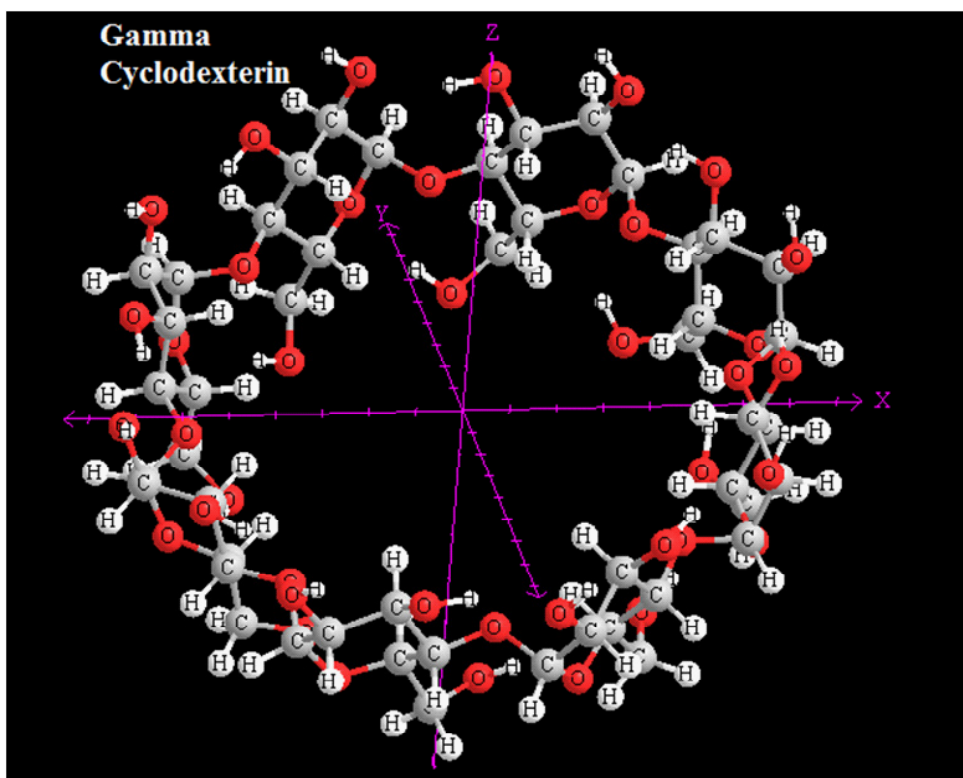


Fig. 2: Optimized of gamma cyclodextrin

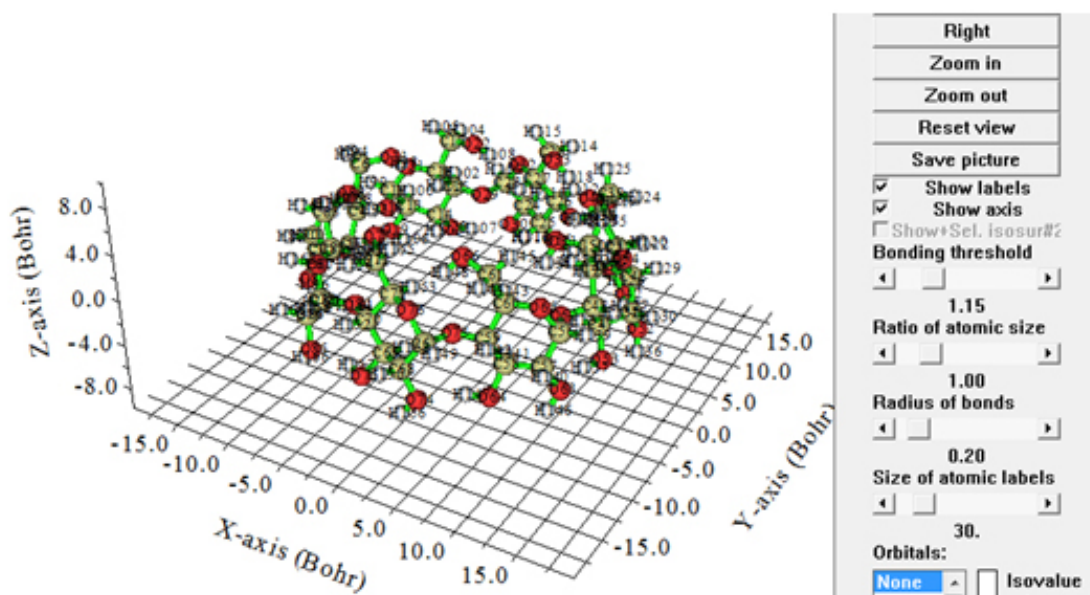


Fig. 3: The gamma CD versus Cartesian orientation

RESULT AND DISCUSSION

This study mainly focuses on the magnetic properties of Fe_3O_4 in a non-bonded system with Cyclodextrin (α and γ). Part of the systems including Fe_3O_4 @ α,γ -Cyclodextrin nanoparticles have been considered in this work. It has been exhibited that the Fe_3O_4 @ (7, 7) and Fe_3O_4 @ (10, 5) and Fe_3O_4 @ (9, 0) have physical and chemical properties close to Fe_3O_4 @ α -Cyclodextrin and as well as the Fe_3O_4

@ (8, 8) and Fe_3O_4 @ (11, 6) and Fe_3O_4 @ (10, 0) are close to Fe_3O_4 @ γ -Cyclodextrin.

The data are shown in tables 1-6 and figures 1-7 for a non-bonded interaction of the Fe_3O_4 with Gamma CD and various nanotubes.

This work has been modeled with QM/MM method and the calculations are carried out with the Advanced DFT methods. Gaussian 2009 and a HyperChem professional release 7.01 programs are used for the additional calculations. For non-covalent interactions between Fe_3O_4 and Cyclodextrins, the B3LYP method is unable to describe van der Waals by medium-range interactions. Therefore, the ONIOM methods including 3 levels of 1-high calculation (H), 2-medium calculation (M), and 3-low calculation (L) have been performed in our study for calculating the non-bonded interactions between Fe_3O_4 and Cyclodextrins.

The ab-initio and DFT methods are used for the model system of the ONIOM layers and the semi empirical methods of pm3mm (including pseudo=lan12) and Pm6 are used for the medium and low layers, respectively.

B3LYP and the most other popular and widely used functional are insufficient to illustrate

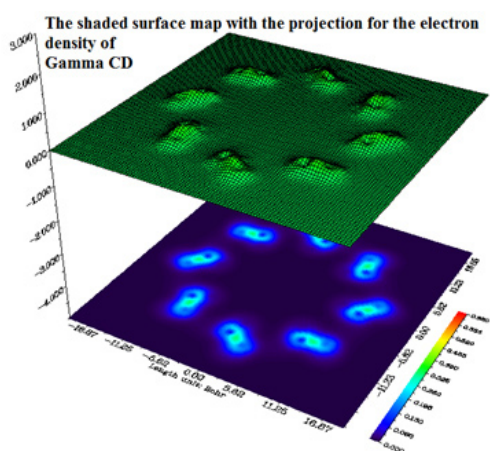


Fig. 4: The Shaded map of electron density for Gamma cyclodextrin

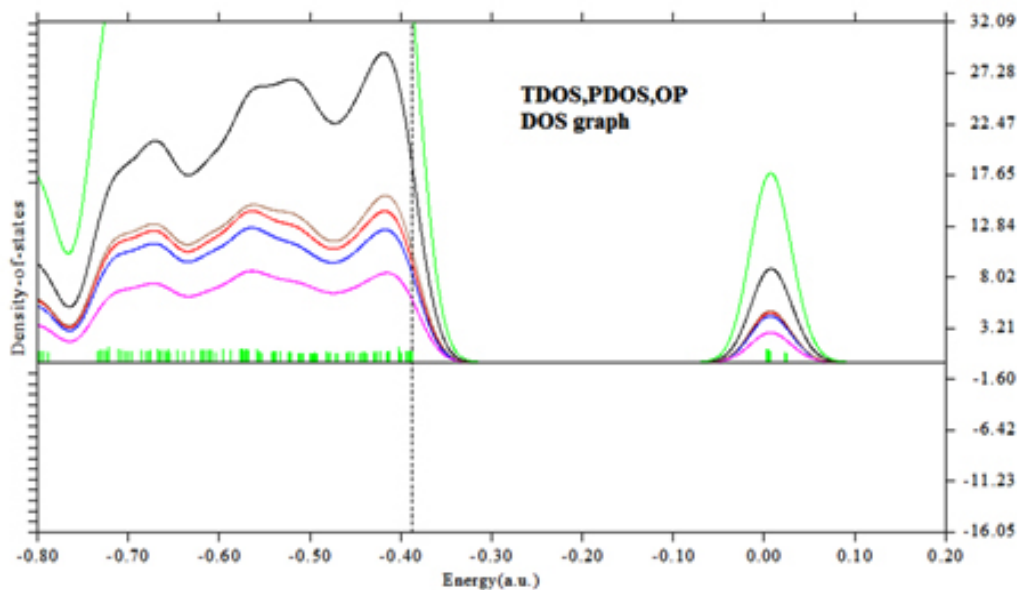


Fig. 5: TDOS, PDOS, OPDOS graph for Fe_3O_4 @GammaCD

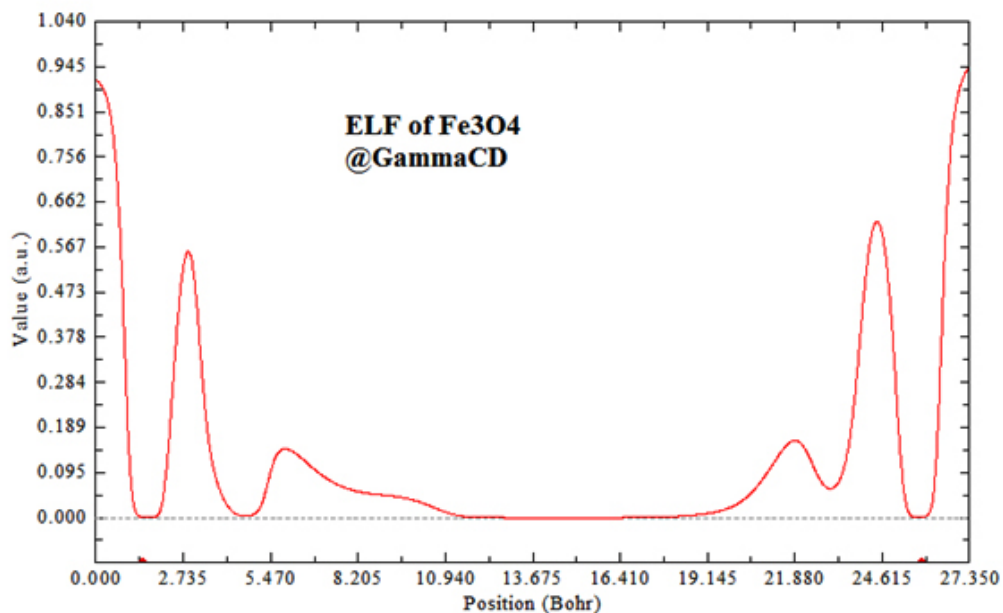


Fig. 6: Electron Localization Function of Fe₃O₄@Gamma Cyclodextrin

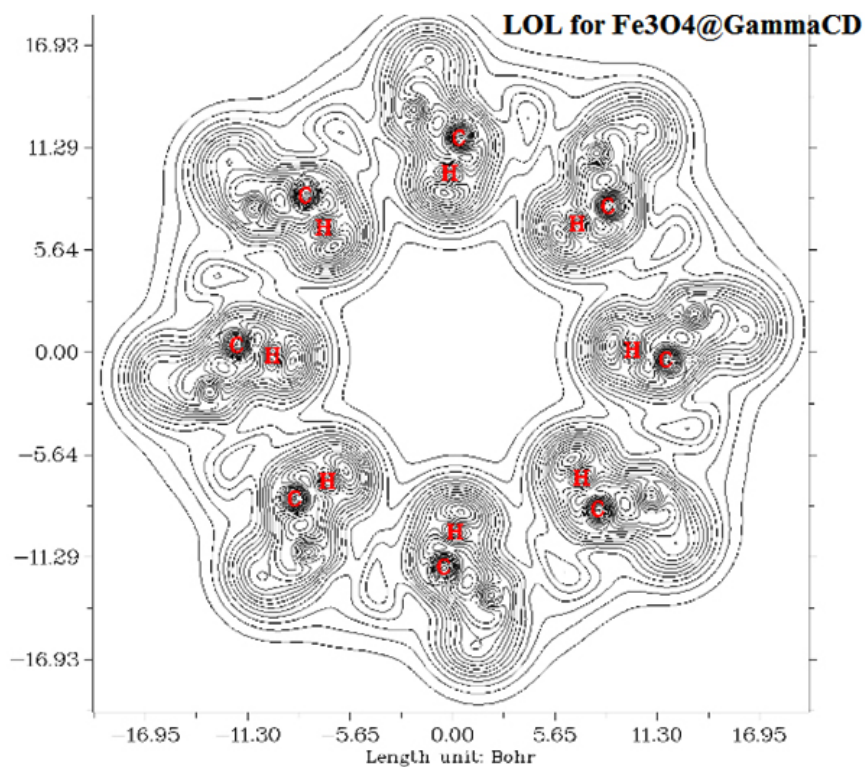


Fig. 7: Localized orbital Locator for Fe₃O₄@(7,7)SWCNTs

the exchange and correlation energy for distant non-bonded medium-range systems correctly. Moreover, some recent studies have shown that inaccuracy for the medium-range exchange energies leads to large systematic errors in the prediction of molecular properties¹⁶⁸⁻¹⁷⁰.

Geometry optimizations and electronic structure calculations have been carried out using the m06 (DFT) functional. This approach is based on an iterative solution of the Kohn-Sham equation¹⁷¹ of the density functional theory in a plane-wave set with the projector-augmented wave pseudo-potentials. The Perdew-Burke-Ernzerhof (PBE)¹⁷² exchange-correlation (XC) functional of the generalized gradient approximation (GGA) is also used. The optimizations of the lattice constants and the atomic coordinates are made by the minimization of the total energy.

The charge transfer and electrostatic potential-derived charge were also calculated using the Merz-Kollman-Singh chelp or chelpG¹⁷³⁻¹⁷⁶ the charge calculation methods based on molecular electrostatic potential (MESP) fitting are not well-suited for treating larger systems whereas some of the innermost atoms are located far away from the points at which the MESP is computed. In such a condition, variations of the innermost atomic charges will not head towards a significant change of the MESP outside of the molecule, meaning that the accurate values for the innermost atomic charges are not well-determined by MESP outside the molecule. The representative atomic charges for molecules should be computed as average values over several molecular conformations.

A detailed overview of the effects of the basis set and the Hamiltonian on the charge distribution can be found in references¹⁷⁵⁻¹⁷⁷. The charge density profiles in this study has been extracted from first-principles calculation through an averaging process as described in reference¹⁷⁵⁻¹⁷⁷. The interaction energy for capacitor was calculated in all items according to the equation as follows:

$$\Delta E_s (eV) = \left\{ E_c - \left(\sum_{i=1}^n (Fe_3O_4 - Cyclodextrin(\alpha \text{ and } \gamma))_i + \sum_{i=1}^n (Fe_3O_4 - Cyclodextrin(\alpha, \text{ and } \gamma))_j \right) \right\} \dots(14)$$

Where the " ΔE_s " is the stability energy.

The electron density (Both of Gradient norm & Laplacian), value of orbital wave-function, electron spin density, electrostatic potential from nuclear atomic charges, electron localization function (ELF), localized orbital locator (LOL defined by Becke & Tsirelson), total electrostatic potential (ESP), as well as the exchange-correlation density, correlation hole and correlation factor, and the average local ionization energy using the Multifunctional Wave-function analyzer have also been calculated in this study³⁵⁻³⁷. The contour line map was also drawn using the Multiwfn software^{35, 36}. The solid lines indicate positive regions, while the dash lines indicate negative regions. The contour line corresponding to VdW surface (electron density=0.001 a.u., which is defined by R. F. W Bader) is plotted in this study. This is specifically useful to analyze distribution of electrostatic potential on VdW surface. Such a contour line has also been plotted in gradient line and vector field map by the same option. The relief map was used to present the height value at every point. Shaded surface map and shaded surface map with projection are used in our representation of height value at each situation³⁵⁻³⁷.

Electrical properties can be obtained from changes in the non-bonded interaction situations. Electron densities, energy densities, Potential energy densities, ELF, LOL, Ellipticity of electron density, eta index and ECP for Fe_3O_4 -Cyclodextrin (α , and γ) shell and Fe_3O_4 @ (7, 7), Fe_3O_4 @ (10, 5), Fe_3O_4 @ (9, 0), Fe_3O_4 @ (8, 8), Fe_3O_4 @ (11, 6) and Fe_3O_4 @ (10, 0) were calculated for each of simulation (Table1-6).

We believe that this research has a great potential for the development of new multifunctional catalysts with high reactivity and selectivity. Another interesting development is using the SWCNTs on magnetic nanoparticles that enable effective removal of transition metal based catalysts from important pharmaceutical products in drug synthesis. This approach should find relevant industrial applications in biopharmaceutical, food additives, fragrances and other sectors.

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