Supporting information

Fabrication of chromium imprinted polymer: A real magneto selective sorbent for chromium Cr (VI) removal in a real water sample

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Preparation of Magnetic Fe_3O_4 Nanoparticles

Magnetic iron oxide Fe_3O_4 (MNPs) were prepared with some modification following reported method Luo et al., [49]. Initially solid amount of 0.597g and 0.975g of ferrous chloride tetrahydrate and anhydrous ferric chloride was weighed in 250mL reaction flask and completely dissolved in 100mL ultrapure Milli-Qwater with the help of ultra-sonication. Afterward, the reaction was carried out at 80°C vigorous mechanical stirring for 15 min on the hot plate. To obtained fine black, small particle size the 20 ml of (NH_4OH 33%) was poured dropwise to the precursor solution, and the reaction was further processed for 20 minutes. The fine black precipitates were then separated using an external magnet and washed once with (0.002M) NaCl solution and several times with ultrapure water and dried in an oven at 60°C.

Silica Modification of Magnetic Nanoparticles (Fe3O4@SiO2)

Silica coating of iron oxide nanoparticle was carried out following shah et al., [50] method with minor modification. Briefly, Silica coating was done by taking 0.5g of freshly prepared Fe_3O_4 nanoparticles in H_2O/Ethanol solution of 80ml of (HPLC) grade Ethanol and 20ml of ultrapure

water. Then 10ml ammonium hydroxide and 3ml tetraethyl ortho silicate were added in a reaction flask and the solution was mechanically stirred at 80°C for an hour. After complete reaction, the particles were washed with ultrapure water and ethanol and dried in an oven at 60 ^{o}C.

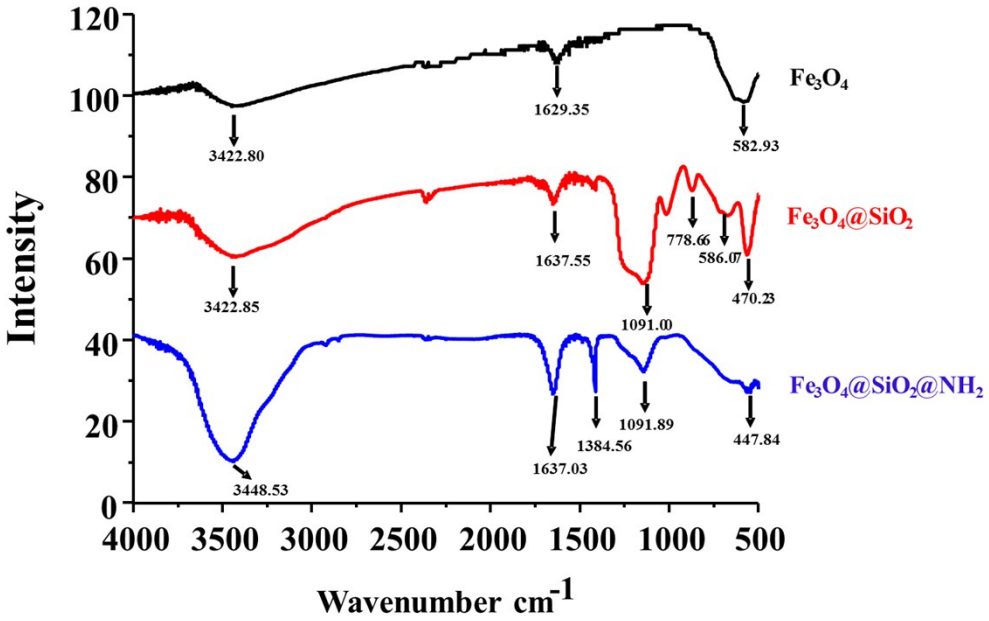
Amine Functionalization of Silica Coated Nanoparticles (Fe_3O_4@SiO_2-NH_2)

Amine fabrication on silica-coated iron oxide (Fe_3O_4) NPs was carried out by taking 0.5g of silica-coated iron oxide nanoparticle (Fe_3O_4@SiO_2), in 50ml dry chloroform and degassed with N_2 for 10min, followed by adding 0.2ml of (AEAPTMS) and refluxing the reaction at 70°C for 12 hours. The obtained (Fe3O4@SiO2@NH2) nanoparticles were separated and washed with (4:1) ethanol and deionized water mixture over three times and dried in an oven at 60°C.

Characterization

FT-IR study of synthesized magnetic nanoparticles

FT-IR widely used as a primary tool to explore the functional groups present in synthesized products. The FT-IR spectra are given in Fig. S1 are of bare iron oxide Fe_3O_4, silica capped iron oxide Fe_3O_4@SiO_2 and amine-functionalized silica capped iron oxide $Fe_3O_4SiO_2$@NH_2 nanoparticles. The peak positioned at 582.93 $cm^{-1}$is a distinguishing peak of Fe-O antisymmetric vibration from the magnetite phase. The clear band at 1091.0 $cm^{-1}$is assigned to Si-O-Si band from the silanol group beside these two shoulder peaks at 778.8 and 470.2 cm^{-1} corresponds to Si-O-H and Si-O bonds vibration, respectively. Which indicated the successful fabrication of silica layer on the magnetic nanoparticles. while in amine-functionalized nanoparticles a characteristic peak appeared at 1384.56 cm^{-1} is due to the C-N vibration furthermore the band in the range of 3300 to 3500 cm^{-1} has been broadened which could be due to overlapping of N-H and O-H bond vibrations this gives a clear view of successfully -NH_2 functionalization on silica caped iron oxide nanoparticles.



SEM study of synthesized magnetic nanoparticles

The morphological study of Fe_3O_4 were studied by the SEM, the results are shown in Fig. S2. It is clear from from the SEM images that most of the Fe_3O_4 possess spherical shape and uniform in nature.

XRD study of synthesized magnetic nanoparticles

The phase purity and crystalline nature of synthesized iron oxide, silica capped iron oxide, ammine functionalized iron oxide, were analyzed by x-ray diffraction technique and then compared to one another. In Fig. S3 (a) of iron oxide Fe_3O_4 and silica capped iron oxide $Fe_3O_4SiO_2$ different prominent diffraction planes at 220, 311, 400, 511, and 440 have been observed which when compared with standard JCPDS file no. 19-0629 revealed the face-centered cubic structure of bare iron oxide nanoparticles while these planes have been observed

in all XRD spectra in Fig. S3 (b) of iron oxide silica capped iron oxide, ammine functionalized iron oxide. But there is a successive decrease in the peak intensities and slightly shifting in diffraction planes have been observed that can be attributed to the successive layer formation and polymerization on the surface of the bare iron oxide. On comparison of all XRD spectra, it displays a clear vision of proper polymerization on the surface of the core material.

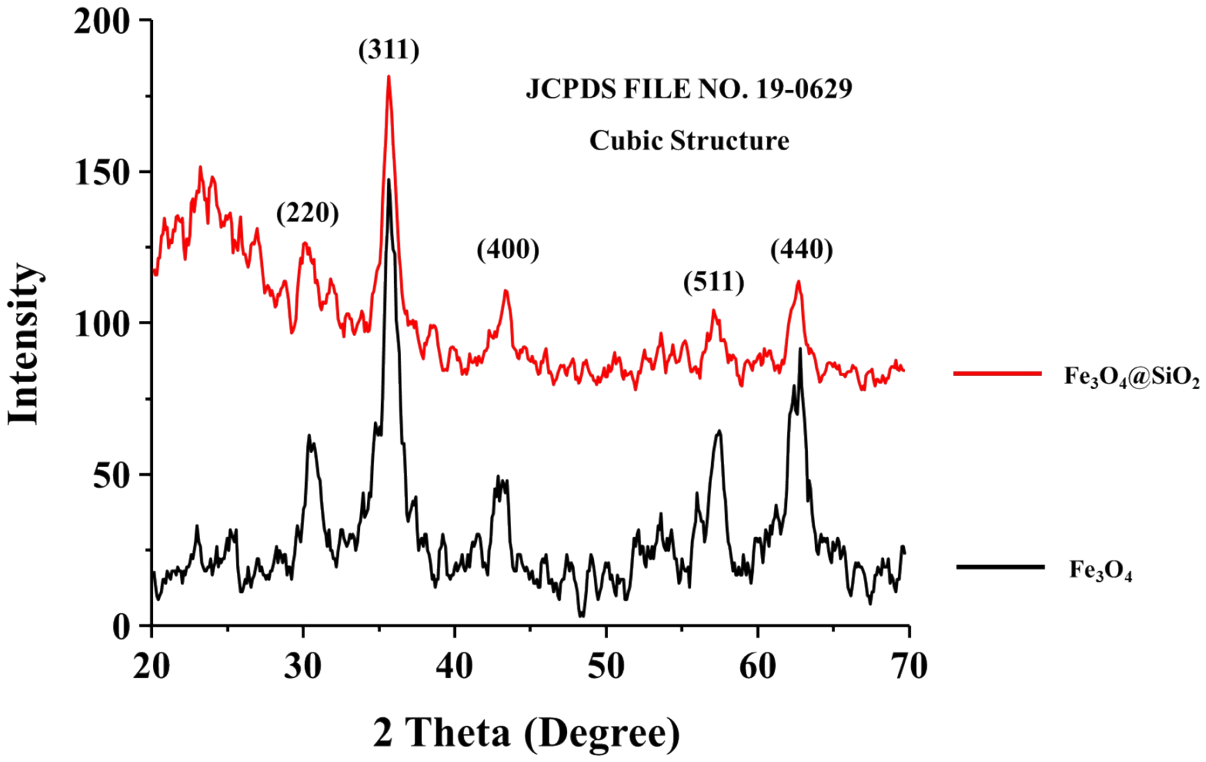


Table. S1 Illustrates Langmuir and Freundlich isotherm constants for the adsorption of Cr-(VI) ions.

Langmuir				**Freundlich**		
q_0 (mgg^{-1})	**b(Lmg^{-1})**	**RL**	**R^2**	**n**	**1/n**	**KfR^2**
169.49	0.662	0.056-0.232	0.999	0.33	3.02	6.910.939

Table. S2 Different kinetic parameters of Pseudo first and Pseudo second order for the adsorption of Cr-(VI) ions.

Pseudo first order			**Pseudo second order**		
K_1(min^{-1})	**qe(mg/g)**	**R^2**	**K_2 (mg^{-1} min^{-1})**	**qe(mg/g)**	**R^2**
0.613	0.333	0.901	0.032	3.650.983	

Table. S3 Thermodynamic Parameters of Cr-(VI) Adsorption at different Temperatures.

T(K)	**ΔG^0(kJ/mol)**	**ΔH^0 (kJ/mol)**	**ΔS^0 (kJ/mol k)**	**R^2**
303	-6.152	-41.55	0.118	0.979
313	-4.12625			
323	-3.09543			
333	-1.96065			
343	-0.92045			
353	-0.11741			