AIMS Materials Science, 11(5): 991–1012.
DOI: 10.3934/matersci.2024047
Received: 11 July 2024
Revised: 26 August 2024
Accepted: 03 September 2024
Published: 25 October 2024

https://www.aimspress.com/journal/Materials

Research article

Citrate coated iron oxide nanoparticles: Synthesis, characterization, and performance in protein adsorption

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Supplementary

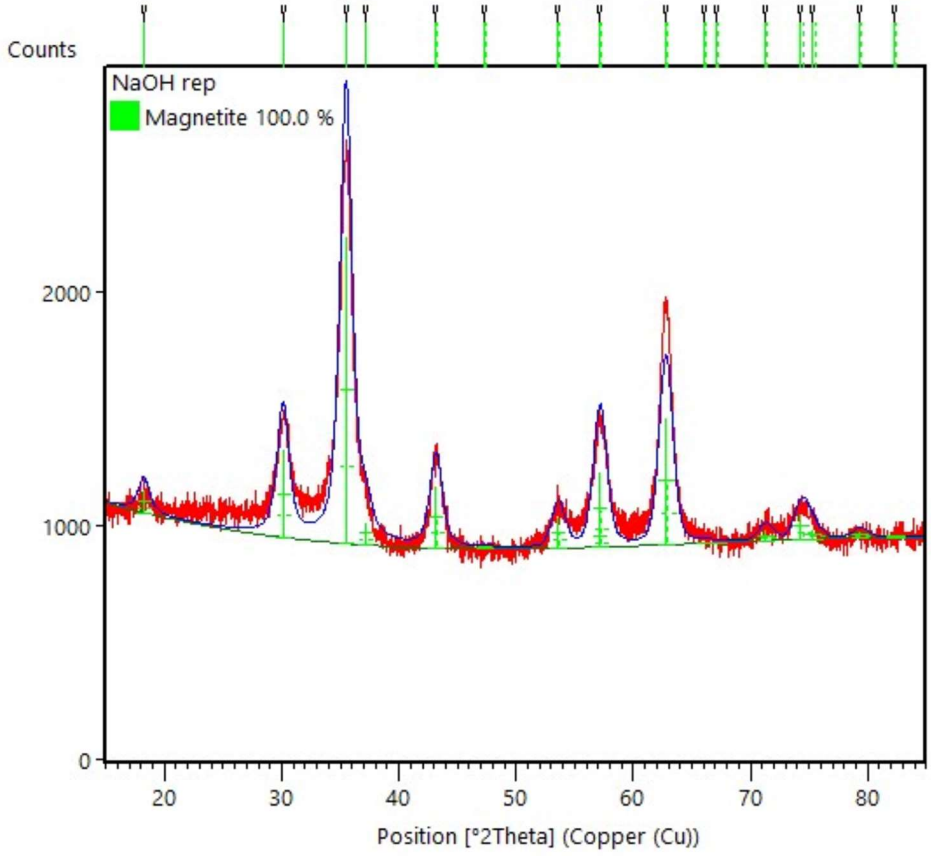

Figure S1. Curve obtained from Rietveld refinement for IONPs.

Table S1. Agreement indices from IONPs's Rietveld refinement.

Parameter	Value
R expected	3.05178%
R profile	3.86551%
Weighted r profile	4.82372%
D-statistics	1.69837
Goodness of fit	1.33069

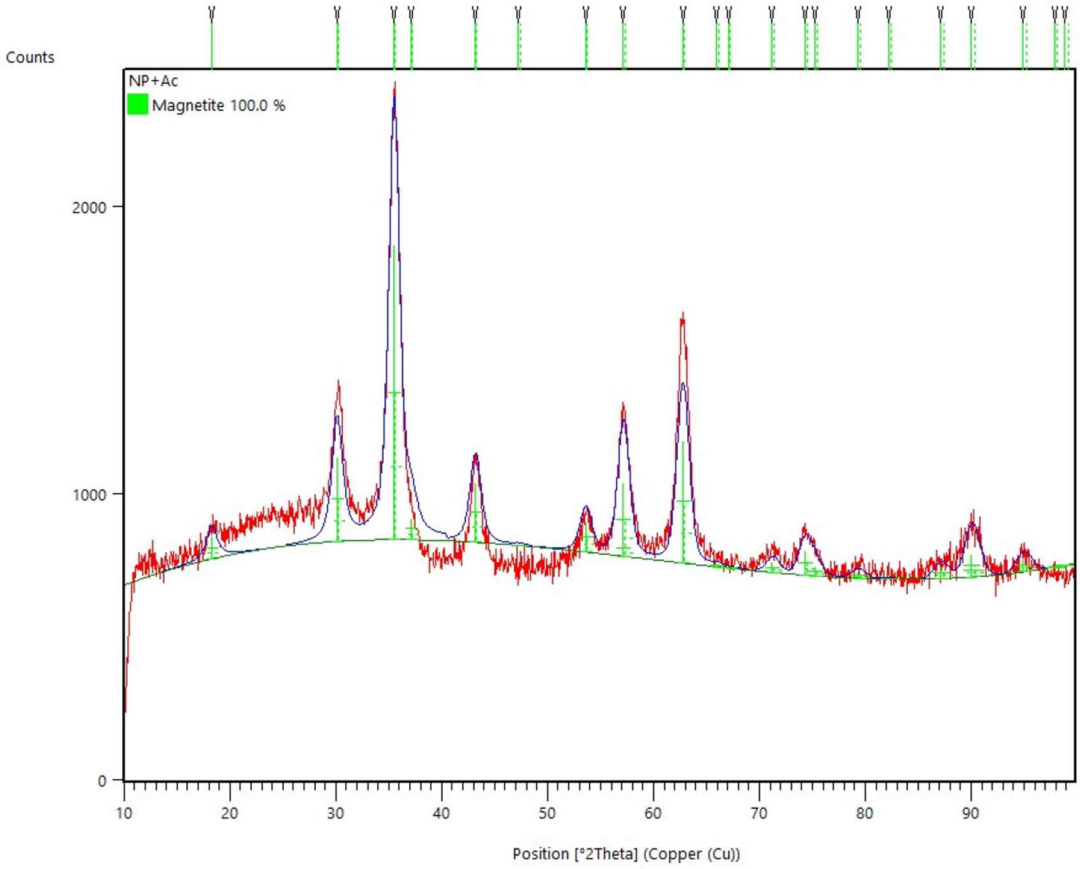

Figure S2. Curve obtained from Rietveld refinement for IONPs@CA.

Table S2. Agreement indices from IONPs@CA's Rietveld refinement.

Parameter	Value
R expected	4.53826%
R profile	5.14652%
Weighted r profile	5.93235%
D-statistics	1.70527
Goodness of fit	1.42954

Table S3. Molecular docking properties of magnetite, citrate and lysozyme (A: Polypeptide A chain; ASN: Asparagine; GLN: Glutamine; TRP: Tryptophan; LYS: Lysine; GLY: Glycine; SER: Serine; ILE: Isoleucine; VAL: Valine; the numbers represent the position of the amino acid in the A-chain-H represents binding of the corresponding amino acid by hydrogen, UNL1:H binding of magnetite by hydrogen, UNL1:O binding of magnetite by oxygen).

Candidates	Bond position	Distance (Å)	Type	Number
IONPs	A:ASN59:HN-UNL1:O	2.34	Conventional	4
	A:GLN57:O-UNL1:O	3.29		
	A:ASN59:HN-UNL1:O	2.10		
	A:TRP63:H31-UNL1:O	1.76		
	A:ILE58:HA-UNL1:FE	2.28	Carbon	2
	A:TRP63:HD1-UNL1:O	2.46		
	A:ASN59:HB2-UNL1:FE	2.01	Bump	1
	A:TRP63:HD1-UNL1:O	3.12	Pi-donor	1
	A:GLN57:O-UNL1:FE	2.67	Metal-Acceptor	1
	A:ASN59:HN-UNL1:FE	2.11	Metal-Donor	2
	A:TRP63:HE1-UNL1:FE	2.45		
Citrate-11	A:TRP63:HHW-UNL1:O	3.46	Van der Waals	4
	A:LYS97:HD1-UNL1:O	4.28		
	A:GLY104:HN-UNL1:O	2.38		
	A:SER100:N-UNL1:O	4.18		
	A:ILE98:O-UNL1:H	1.91	Hydrogen bond	2
	A:ASN103:HT1-UNL1:O	1.94		
	A:ASN103:HT1-UNL1:O	2.10	Carbon hydrogen bond	1
Citrate-19	A:TRP63:HE1-UNL1:0	3.21	Van der Waals	3
	A:LYS97:HD1-UNL1:O	3.18		
	A:SER100:0-UNL1:O	4.25		
	A:VAL99:HA-UNL1:O	3.56	Hydrogen bond	5
	A:GLY104:N-UNL1:O	1.98		
	A:ASN103:HT1-UNL1:O	2.39		
	A:ILE98:O-UNL1:H	2.18		
	A:ILE98:AH-UNL1:O	4.21		
Citrate-49	A:TRP63:HH2-UNL1:O	2.01	Van der Waals	2
	A:SER100:O-UNL1:H	2.45		
	A:LYS97:O-UNL1:O	2.99	Hydrogen bond	5
	A:VAL99:O-UNL1:O	3.21		
	A:GLY104:HN-UNL1:O	2.10		
	A:ASN103:HT1-UNL1:O	1.76		
	A:ILE98:O-UNL1:H	1.99		

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