Supplementary Information

Chitosan-modified nickel ferrite nanocomposite for ciprofloxacin adsorption: experimental and density functional theory study

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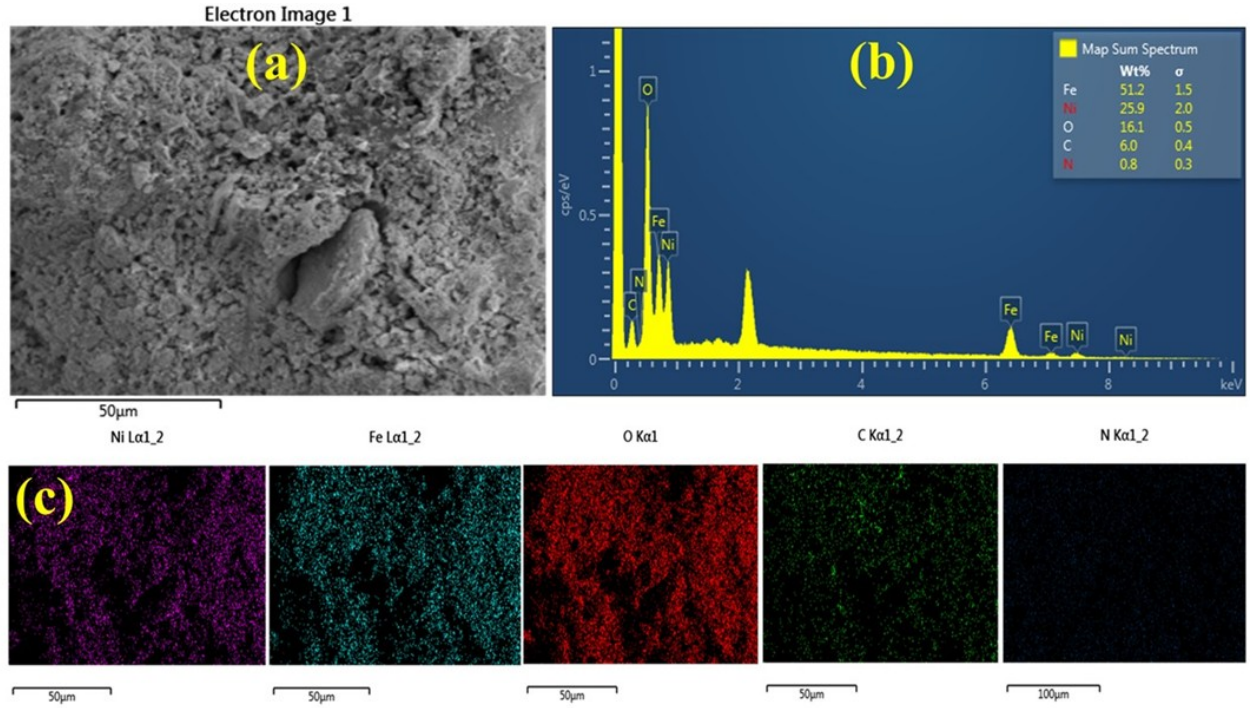
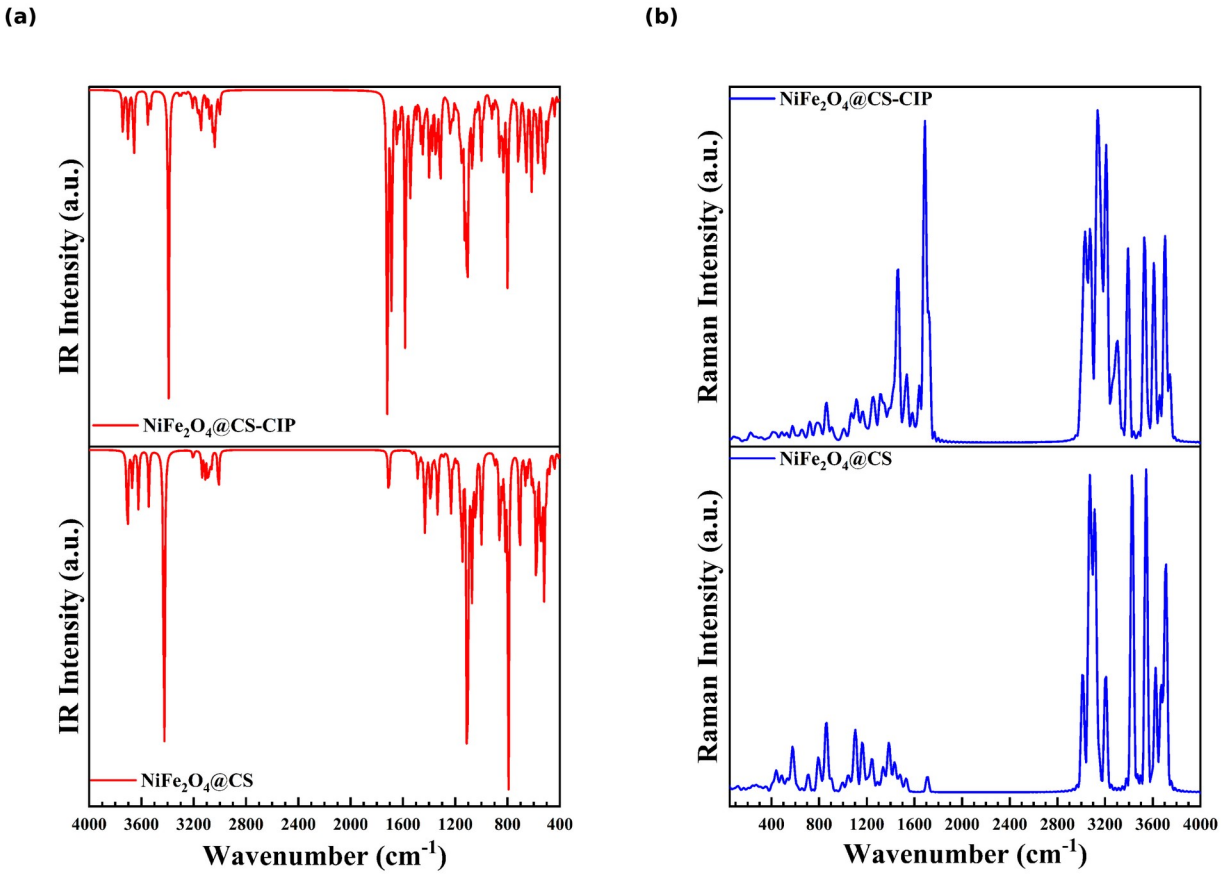
Supplementary Figure S1



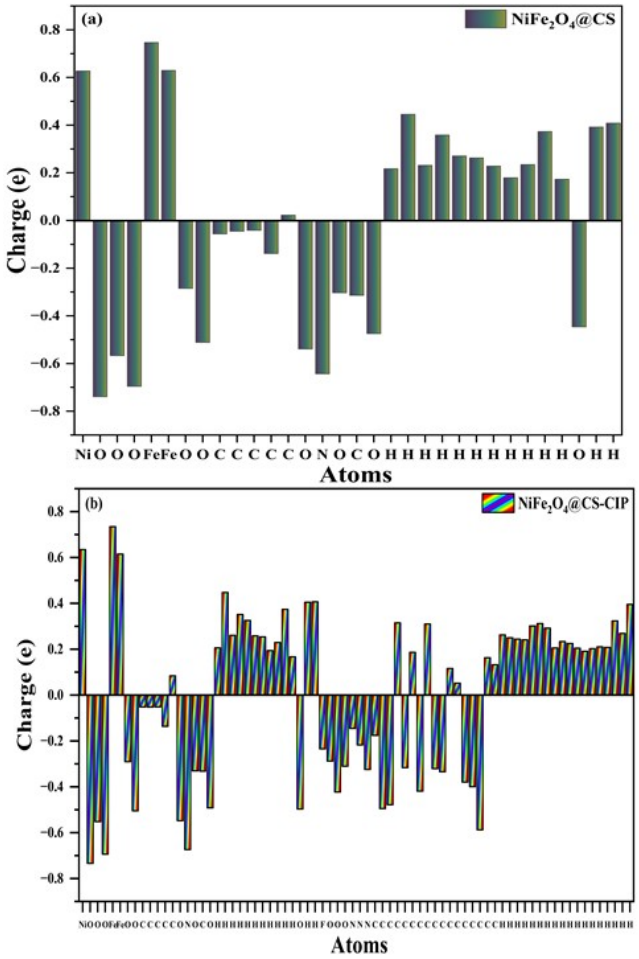
Supplementary Figure S1. (a) SEM image of the analysed region, (b) EDS spectrum with semi-quantitative elemental composition, and (c) elemental maps of Ni, Fe, O, C and N for $NiFe_2O_4$@CS.

Supplementary Figure S2



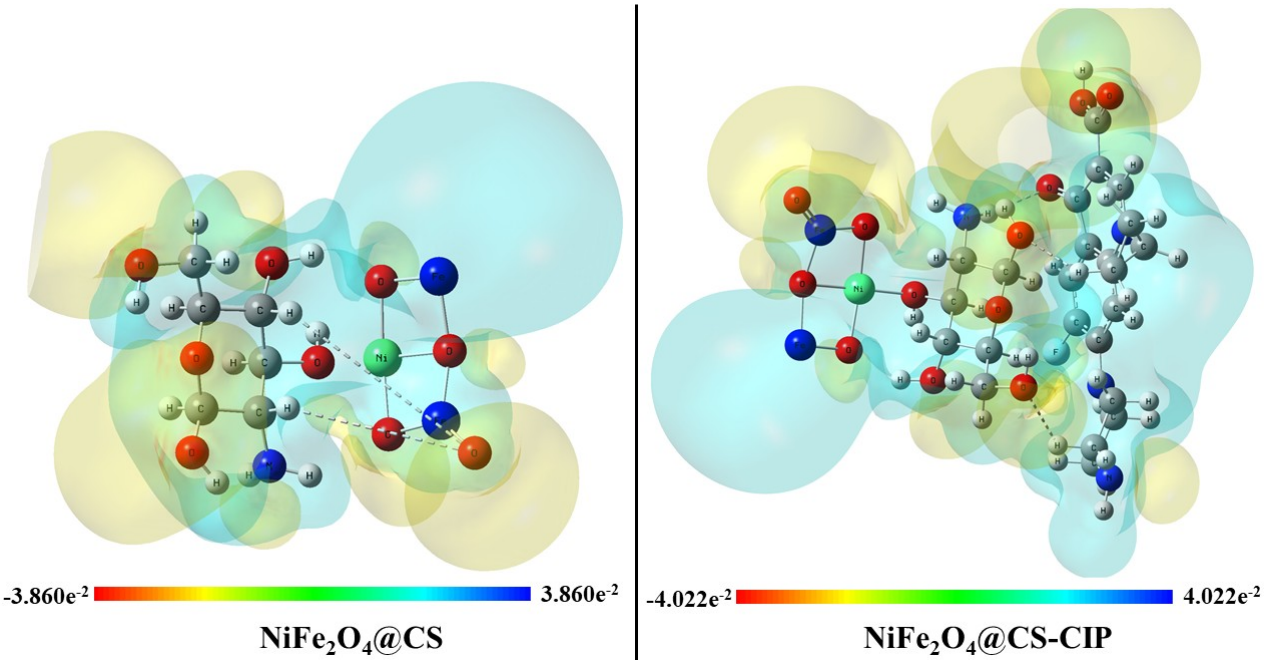
Supplementary Figure S2. Simulated (a) infrared and (b) Raman spectra of the finite-cluster model systems.

Supplementary Figure S3



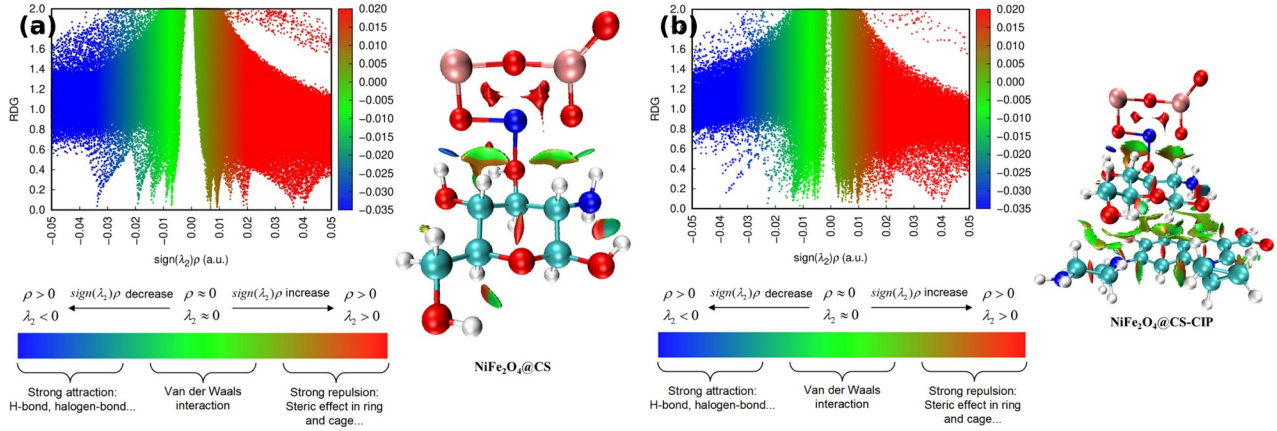
Supplementary Figure S3. Mulliken charge-distribution plots for the finite-cluster model systems.

Supplementary Figure S4



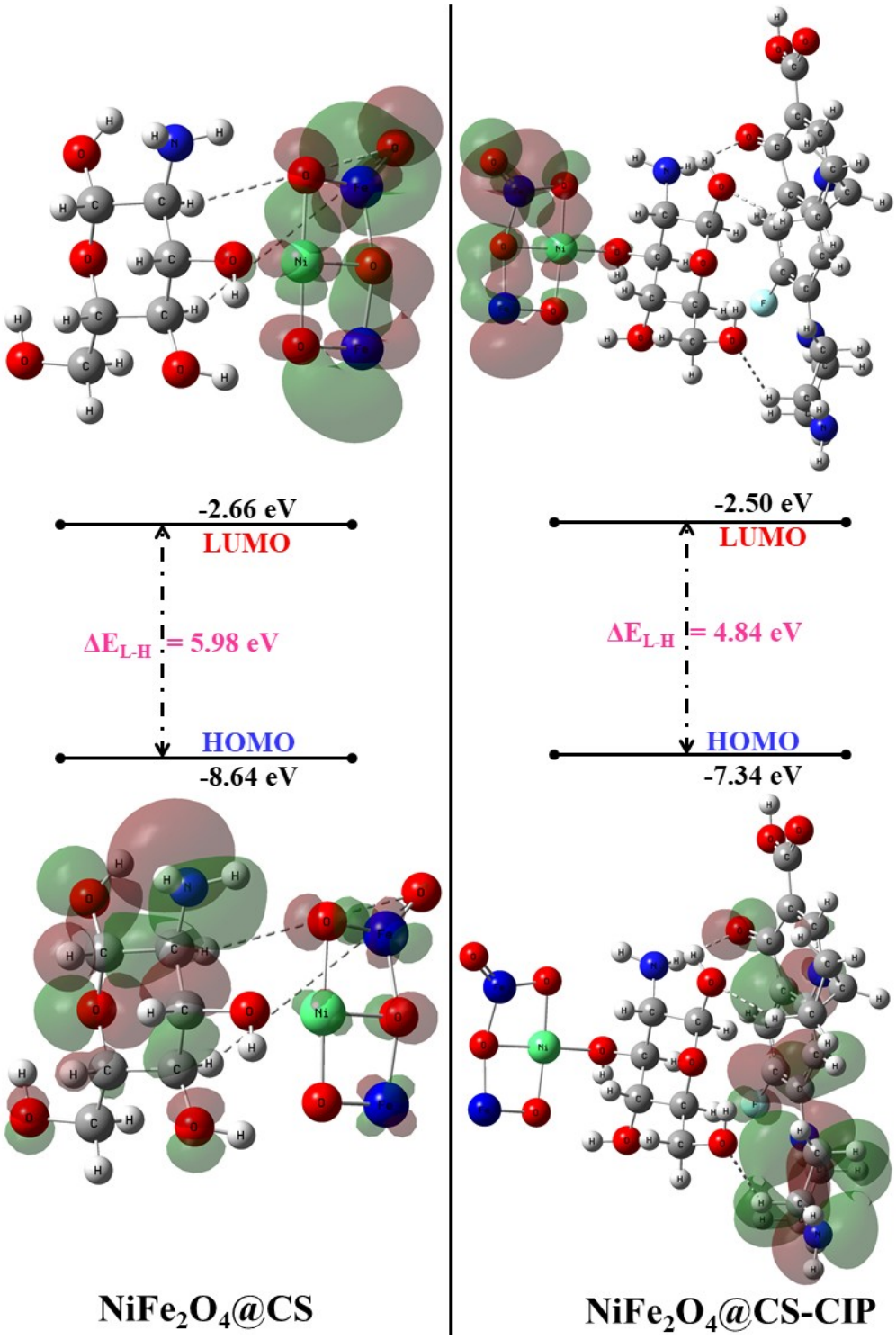
Supplementary Figure S4. Electrostatic-potential maps of the $NiFe_2O_4$@CS and $NiFe_2O_4$@CS–CIP finite-cluster models.

Supplementary Figure S5



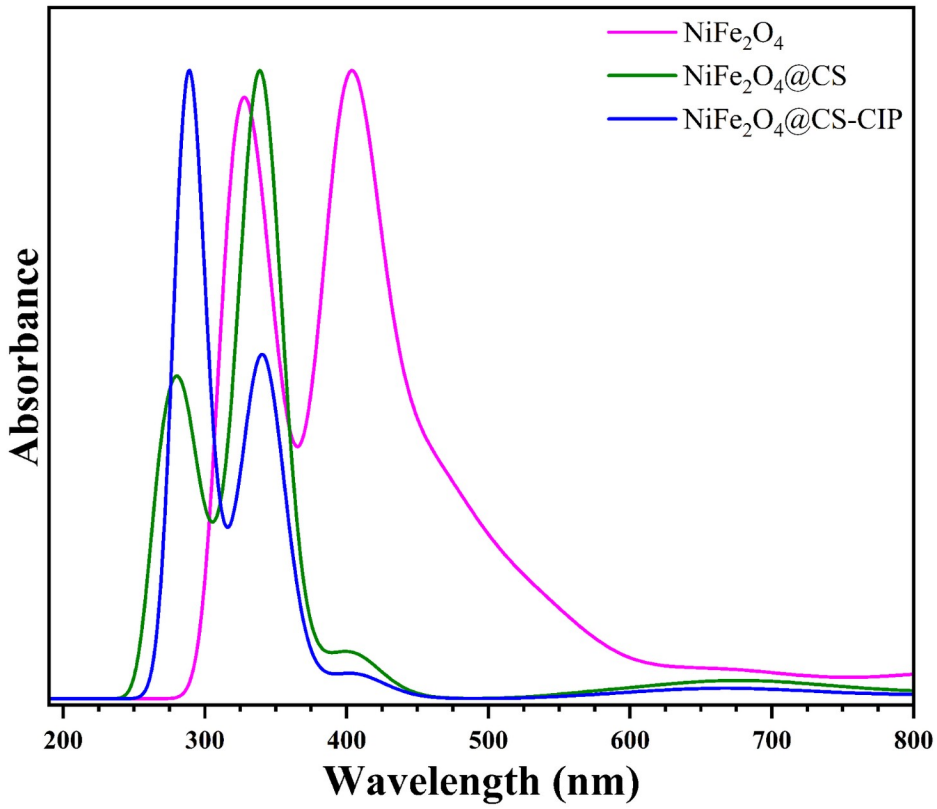
Supplementary Figure S5. Noncovalent-interaction analyses for (a) $NiFe_2O_4$@CS and (b) $NiFe_2O_4$@CS–CIP finite-cluster models.

Supplementary Figure S6



Supplementary Figure S6. Frontier molecular orbital maps of $NiFe_2O_4$@CS and $NiFe_2O_4$@CS–CIP finite-cluster models.

Supplementary Figure S7



Supplementary Figure S7. Simulated UV–visible absorption spectra of $NiFe_2O_4$, $NiFe_2O_4$@CS and $NiFe_2O_4$@CS–CIP finite-cluster models.

Supplementary Table S1

Supplementary Table S1. Kinetic parameters for CIP adsorption by $NiFe_2O_4$@CS.

Adsorption model	Parameter	Value
Elovich	α (mg g^{-1} min^{-1})	11.88
Elovich	β (g mg^{-1})	0.43
Elovich	R^2	0.825
PFO	q_e,cal (mg g^{-1})	16.25
PFO	k_1 (min^{-1})	0.07
PFO	R^2	0.951
PSO	q_e,cal (mg g^{-1})	17.59
PSO	q_e,exp (mg g^{-1})	16.82
PSO	k_2 (g mg^{-1} min^{-1})	0.005
PSO	R^2	0.994

Supplementary Table S2

Supplementary Table S2. Electronic parameters calculated for the finite-cluster model systems.

Structure	RMSD	Total energy (eV)	Eads (eV)	EHOMO (eV)	ELUMO (eV)	EFL (eV)	Φ (eV)	ΔEL–H (eV)
CS	7.97×10^{-4}	−18122.7817	–	−8.62	2.05	−3.28	3.28	10.67
$NiFe_2O_4$	10.14×10^{-4}	−19483.3509	–	−8.66	−2.91	−5.78	5.78	5.95
CIP	3.49×10^{-4}	−31237.6688	–	−5.95	−1.45	−3.70	3.78	4.50
$NiFe_2O_4$@CS	13.62×10^{-4}	−37633.7344	–	−8.64	−2.66	−5.65	5.65	5.98
$NiFe_2O_4$@CS–CIP	20.58×10^{-4}	−68872.0128	−0.6069	−7.34	−2.50	−4.92	4.92	4.84

RMSD values indicate numerical convergence of the optimized finite-cluster structures. Eads is reported only for the $NiFe_2O_4$@CS–CIP adduct and is interpreted as a model-level electronic interaction energy.

Supplementary Table S3

Supplementary Table S3. Global chemical-reactivity descriptors for the finite-cluster model systems.

Structure	IP (eV)	EA (eV)	η (eV)	S (eV^{-1})	μ (eV)	χ (eV)	ω (eV)
CS	8.62	−2.05	5.335	0.187	−3.285	3.285	1.011
$NiFe_2O_4$	8.66	2.91	2.975	0.336	−5.785	5.785	5.624
CIP	5.95	1.45	2.25	0.444	−3.700	3.700	3.042
$NiFe_2O_4$@CS	8.64	2.66	2.99	0.334	−5.650	5.650	5.338
$NiFe_2O_4$@CS –CIP	7.34	2.50	2.42	0.413	−4.920	4.920	5.001

The descriptors compare the selected finite-cluster structures and should not be interpreted as direct experimental bulk or thermodynamic quantities.