Selective removal and recovery of Ni(II) using a sulfonic-based magnetic rattle-type ion-imprinted polymer: Adsorption performance and mechanisms

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Gaussian calculation

1. Selective Adsorption

Cartesian coordinates at the pbe1pbe/def2SVP level.

AMPS-Ni(II)
pbe1pbe/def2SVP scrf=(smd,solvent=water) empiricaldispersion=gd3bj
1 1

C	0.47892900	0.62729700	0.16106400
C	1.07656400	1.89293000	-0.44716600
C	2.42286500	2.22608800	0.18690700
C	0.11403300	3.06766100	-0.30216600
C	-2.00707800	0.80243500	-0.33181600
C	-2.48314200	1.00136000	1.03977100
C	-2.15519400	0.27110400	2.11249700
O	-2.63106800	1.12323800	-1.30957600
N	-0.71848300	0.12958900	-0.56550800
S	1.61415200	-0.79048600	0.13963200

O	2.55915000	-0.73241800	1.24513100
O	2.13251800	-0.93177800	-1.21921200
O	0.56907400	-1.91678900	0.46219000
Ni	-1.00152400	-1.76576600	-0.38702900
H	0.23117300	0.76617200	1.22265800
H	1.23393600	1.68723300	-1.52049100
H	2.78607900	3.17773700	-0.22668000
H	3.18792300	1.46440900	-0.01671500
H	2.33018700	2.34365100	1.27795300
H	0.59413200	3.97814900	-0.68886300
H	-0.81626100	2.93430700	-0.87082100
H	-0.14109300	3.24051300	0.75506700
H	-3.25026400	1.77771700	1.10342500
H	-2.64094800	0.46827800	3.07192200
H	-1.43664800	-0.55355500	2.09074400
H	-0.55184400	0.22620500	-1.57975000

AMPS-Co(II)

pbe1pbe/def2SVP scrf=(smd,solvent=water) empiricaldispersion=gd3bj

1 2

C	0.58873900	0.56662000	0.14723700
C	1.48278200	1.64086600	-0.46775300
C	2.80994400	1.74763500	0.27277600
C	0.76047400	2.98433200	-0.48676300
C	-1.82825700	1.19457300	-0.11240500
C	-2.20459700	1.15258200	1.30879100
C	-1.92580600	0.16802500	2.17133500
O	-2.45793500	1.81438500	-0.93564700
N	-0.69594200	0.41205900	-0.56953300
S	1.38312700	-1.07412300	0.17089500
O	2.22957800	-1.18927600	1.35730800
O	2.01708300	-1.28624000	-1.13454300
O	0.14536700	-1.98872000	0.34125100
Co	-1.37254300	-1.51332000	-0.64817400
H	0.38994500	0.78452300	1.20606300
H	1.68031400	1.32885200	-1.50864800
H	3.40904400	2.55704700	-0.16878800
H	3.40161100	0.82415500	0.21330400
H	2.64870100	1.98560800	1.33627300
H	1.44366900	3.76140800	-0.85932300
H	-0.11872200	2.98328700	-1.14621500

H	0.43634000	3.27448500	0.52568700
H	-2.84499500	1.99026100	1.59763600
H	-2.32146800	0.20295500	3.18980600
H	-1.32870300	-0.70965500	1.90289300
H	-0.56793400	0.64927000	-1.56185000

AMPS-Cu(II)

pbe1pbe/def2SVP scrf=(smd,solvent=water) empiricaldispersion=gd3bj

1 2

C	0.67799400	0.53653600	0.14748200
C	1.70411000	1.47681300	-0.48666700
C	3.09294500	1.31871700	0.12014900
C	1.22415600	2.91962900	-0.36453600
C	-1.64541200	1.45310000	-0.14372200
C	-2.03748700	1.47686900	1.27477100
C	-1.88219100	0.47146100	2.14297800
O	-2.20358800	2.12441500	-0.98179400
N	-0.60735400	0.55635700	-0.56822900
S	1.25230000	-1.19400400	0.19719800
O	2.12430900	-1.37524800	1.35722100
O	1.80562600	-1.51516100	-1.12413100
O	-0.06743400	-1.95907100	0.43727700
Cu	-1.55702500	-1.37519000	-0.59701200
H	0.51513000	0.79276400	1.20370300
H	1.75832700	1.20515600	-1.55562300
H	3.76684100	2.06351900	-0.32757800
H	3.52293700	0.32620400	-0.06981300
H	3.07560100	1.48753900	1.20816700
H	1.97855700	3.59623400	-0.79189900
H	0.28251900	3.10384300	-0.90069200
H	1.08157300	3.19499900	0.69271200
H	-2.57847200	2.38532500	1.55277200
H	-2.27718900	0.55418600	3.15910300
H	-1.37929000	-0.46542400	1.88298700
H	-0.45414900	0.72748300	-1.56936900

AMPS-Pb(II)

pbe1pbe/def2SVP scrf=(smd,solvent=water) empiricaldispersion=gd3bj

1 1

C	1.71448700	0.09646100	0.09252500
C	2.97075400	0.13070000	-0.78733100
C	4.07973600	-0.78124300	-0.27832300

C	3.47004600	1.56847700	-0.90082300
C	0.43643000	2.24266400	-0.06177900
C	0.47855300	2.58641200	1.37361300
C	0.19863200	1.76474100	2.39150000
O	0.15936100	3.07802000	-0.90095400
N	0.64233700	0.90696200	-0.47131600
S	1.10016200	-1.60974800	0.33790800
O	1.93637500	-2.26458900	1.34685200
O	1.03064600	-2.23644900	-0.99142100
O	-0.31606800	-1.40136900	0.90322800
Pb	-1.88676000	-0.17135400	-0.21619200
H	1.94992400	0.44157500	1.10877800
H	2.66050100	-0.21820700	-1.78834600
H	4.97091500	-0.65245900	-0.90983200
H	3.80005900	-1.84238100	-0.30641700
H	4.35860700	-0.52642200	0.75643200
H	4.39155400	1.59239300	-1.50075600
H	2.74564000	2.23421400	-1.39133100
H	3.70288900	1.98268800	0.09343300
H	0.65739700	3.65135100	1.54614200
H	0.16804500	2.14817000	3.41495200
H	-0.02794000	0.70269400	2.25568700
H	0.66342400	0.89045700	-1.49627600

AMPS-Zn(II)

1 1

pbe1pbe/def2SVP scrf=(smd,solvent=water) empiricaldispersion=gd3bj

C	0.81950800	0.41670000	0.13607800
C	2.02700300	1.13355700	-0.47829700
C	3.32609600	0.81237900	0.24939600
C	1.78261000	2.63933600	-0.50356700
C	-1.26364700	1.77310900	-0.15216400
C	-1.62064600	1.88092100	1.27687300
C	-1.68544200	0.85727500	2.13457900
O	-1.74623000	2.51908200	-0.98304500
N	-0.41760700	0.72704100	-0.56703300
S	1.04997400	-1.40044900	0.14940400
O	1.86131500	-1.73376600	1.32789600
O	1.60623800	-1.78447700	-1.15792200
O	-0.36455700	-1.94976000	0.32800600
Zn	-1.94683200	-1.11657300	-0.49920000

H	0.71483000	0.67880900	1.19795600
H	2.10890800	0.77232500	-1.51861200
H	4.14922000	1.38294400	-0.20535400
H	3.58583500	-0.25289800	0.19654700
H	3.26295500	1.09793300	1.31168000
H	2.67529800	3.15086600	-0.89258500
H	0.93944500	2.92191900	-1.14978600
H	1.58615200	3.02585000	0.50971900
H	-1.95211900	2.88213300	1.56578100
H	-2.04936300	1.01243800	3.15401200
H	-1.39830500	-0.16422500	1.86360600
H	-0.26125100	0.81870800	-1.57505900

AMPS$^-$

pbe1pbe/def2SVP scrf=(smd,solvent=water) empiricaldispersion=gd3bj

-1 1

C	-0.34197200	0.35719700	-0.46274000
C	-1.15174200	1.64072600	-0.23625700
C	-2.39332900	1.71168000	-1.11575500
C	-1.47881000	1.92250700	1.22478000
C	2.07858000	0.10635800	-0.68562200
C	3.39336900	0.09097300	0.00675000
C	3.66821900	0.61100600	1.20553600
O	2.01344000	-0.15696300	-1.88719500
N	0.99428300	0.44026000	0.05081900
S	-1.04375700	-1.19282700	0.22255500
O	-2.47739600	-1.24887200	-0.16082600
O	-0.23129100	-2.26503500	-0.40876200
O	-0.83105200	-1.10989600	1.69445800
H	-0.26543200	0.15859100	-1.54064000
H	-0.46350400	2.43197800	-0.58259100
H	-2.84087700	2.71565300	-1.05638700
H	-2.14636100	1.51299600	-2.17062900
H	-3.14756100	0.97830200	-0.80143500
H	-1.94457200	2.91542900	1.31931600
H	-0.57785600	1.91894400	1.85785700
H	-2.17844100	1.17692300	1.62979900
H	4.18188600	-0.37251300	-0.59366700
H	4.68164900	0.56334200	1.61372300
H	2.91656600	1.10935200	1.82653700
H	1.08914600	0.49785700	1.05994600

2. Adsorption mechanism

Cartesian coordinates at the pbe1pbe/def2TZVP level, scrf=(smd,solvent=water), em=gd3bj

AMPS$^-$

-1 1

C	-0.31016900	0.29164000	-0.45240900
C	-0.97124700	1.66693500	-0.28388500
C	-2.17088200	1.86003000	-1.19800300
C	-1.30683500	2.03746600	1.15206300
C	2.10496100	-0.07596300	-0.63945600
C	3.41250300	-0.04993000	0.05609800
C	3.70504800	0.67851900	1.12606500
O	2.04955700	-0.39958200	-1.83007200
N	1.02527700	0.27393700	0.07712600
S	-1.17514300	-1.14464200	0.24992800
O	-2.56719700	-1.05420100	-0.18056600
O	-0.47963900	-2.29936400	-0.31666900
O	-1.01456500	-1.05222700	1.70071200
H	-0.23885200	0.06663900	-1.51723800
H	-0.19113900	2.35511800	-0.63010000
H	-2.46409700	2.91282300	-1.19828700
H	-1.93538800	1.57559900	-2.22695800
H	-3.02714300	1.27072100	-0.86926400
H	-1.61953200	3.08359600	1.19428200
H	-0.45139900	1.92154900	1.82218800
H	-2.12508800	1.42681000	1.53916400
H	4.17175500	-0.65444300	-0.42932800
H	4.70323700	0.66286400	1.54881500
H	2.98193500	1.32571300	1.61217000
H	1.13551800	0.44052800	1.06575000

AMPS-Ni(II) (**Fig. S6 (a)**)

1 1

C	-0.47983700	0.59366300	-0.38000400
C	-0.68358000	2.10115200	-0.55525900
C	-1.57898100	2.30788300	-1.76939300
C	-1.24475900	2.81106400	0.66661800
C	-1.99989300	-1.29996100	-0.48305100
C	-3.23721400	-1.92590900	0.02261300

C	-4.00384000	-1.47370200	1.00734300
O	-1.35491800	-1.82893200	-1.38318200
N	-1.61159400	-0.12652900	0.08103500
S	0.89972900	0.22372700	0.73261700
O	2.15206000	0.84443500	0.14191600
O	0.60747900	0.56458200	2.08145800
O	1.28280100	-1.22857200	0.50563100
Ni	2.80596000	-0.78110100	-0.42321500
H	-0.14446200	0.15461900	-1.32316300
H	0.30233400	2.51662200	-0.78615300
H	-1.68225500	3.37618400	-1.96819200
H	-1.16187600	1.83008600	-2.65848200
H	-2.57771800	1.90044300	-1.59435500
H	-1.35572800	3.87215000	0.43595400
H	-0.59734600	2.72575400	1.53986900
H	-2.23650700	2.43450500	0.93291400
H	-3.48714600	-2.84379800	-0.49833400
H	-4.89356200	-2.01805200	1.30269900
H	-3.79569100	-0.56359200	1.56052500
H	-2.18218800	0.29472900	0.79785200

AMPS-Ni(II) (**Fig. S6 (a)**)

1 1

C	0.48564400	0.62780300	0.15800800
C	1.07195100	1.88542500	-0.47223400
C	2.40814300	2.24422000	0.16320500
C	0.10423700	3.05375000	-0.33663700
C	-2.01497600	0.77958900	-0.31081300
C	-2.46427700	1.00407600	1.05916600
C	-2.13447600	0.27578000	2.12167800
O	-2.66524500	1.06034400	-1.28202200
N	-0.71936100	0.12853900	-0.56600900
S	1.59897900	-0.79005400	0.15484900
O	2.52399900	-0.72374800	1.24740700
O	2.13290500	-0.93685500	-1.17197100
O	0.57549900	-1.89145300	0.46919600
Ni	-0.97580300	-1.75446700	-0.40535000
H	0.22732800	0.78993300	1.20472200
H	1.22986900	1.67156000	-1.53514200
H	2.75329200	3.18940500	-0.25924000
H	3.18064700	1.49764400	-0.02326300

H	2.30491200	2.37416100	1.24365800
H	0.57278000	3.95149200	-0.74376200
H	-0.82671900	2.90489800	-0.88504600
H	-0.13387200	3.24157700	0.71357700
H	-3.20755200	1.79048000	1.12906300
H	-2.59799100	0.48198300	3.07940600
H	-1.43940100	-0.55594700	2.09062700
H	-0.56368600	0.23883200	-1.57542300