Electronic Supplementary Information

Single-atom Fe-N_4 site for hydrogenation of nitrobenzene : theoretical and experimental study

Yan Liu [a], Wenzhuang Zhang [a], Yamin Zheng [a], Konglin Wu [b], Panpan Dong [a], Rong He [c], Ning Lu [a] and Junjie Mao*[a]

[a]Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Province Key Laboratory of Optoelectric Materials Science and Technology and Anhui Laboratory of Molecule-Based Materials, Anhui Normal University, Wuhu, 241002, China

[b]School of Chemistry and Chemical Engineering, Anhui University of Technology, Maanshan 243002, China

[c]State Key Laboratory of Environment-friendly Energy Materials, Southwest University of Science and Technology, Mianyang, 621010, China

1. Experimental Section

1.1 Chemicals. All the chemicals were used without further purification. The iron nitrate nonahydrate ($Fe(NO_3)_3 \cdot 9H_2O$, >99%), sodium carbonate (Na_2CO_3, 99.0%), sodium hydroxide (NaOH, 99.0%), potassium persulfate ($K_2S_2O_8$, ≥99.5%), ethyl acetate ($C_4H_8O_2$, ≥99.5%), and ethanol (C_2H_6O, 99.0%) were purchased from Sinopharm Chemical Reagent Co. Ltd. (Shanghai, China). The styrene (C_8H_8, 99.0%), methacrylic acid ($C_4H_6O_2$, 98%), nitrobenzene ($C_6H_5NO_2$, 99%), and hydrazine hydrate ($N_2H_4 \cdot H_2O$, 80wt%) were all purchased from Aladdin Chemistry Co. Ltd. (Shanghai, China). The m-aminophenol (C_6H_7NO, 98%) and n-dodecane ($C_{12}H_{26}$, 99%) were provided from Alfa Aesar Chemical Co. Ltd. (China). The formaldehyde (HCHO, 37.0-40.0%) was purchased from Xilong Chemicals Co. Ltd. (China). Ultrapure Millipore water (18.2 MΩ) was used in all experiments.

1.2 Synthesis of polystyrene nanospheres (PS). The synthetic procedure of the PS was adopted from the previous literature with slight modification. In a typical synthesis, 7.68 mL of styrene and 0.35 mL of methacrylic acid were dissolved in 80 mL of deionized water in sequence in a 200-mL three-necked flask, followed by drumming bubble of N_2 for 15 min and keeping at 70 ºC for 30 min under magnetic stirring. After that, 5 mL of aqueous solution containing 24 mg of NaOH and 24 mg Na_2CO_3 was added into the solution. Then, 5 mL of aqueous solution containing 30 mg of $K_2S_2O_8$ was quickly injected into the mixture to start the polymerization. The reaction was maintained at 70 ºC for 24 h under magnetic stirring. After cooled down naturally, the latex was washed by ethanol and water for several times, and then freeze dried for further use.

1.3 Synthesis of Fe SAs/NHCSs. In a typical synthesis, 500 mg of PS was uniformly dissolved in 20 mL of deionized water in 50 mL round-bottom flask under vigorous stirring. The solution was then sonicated for 30 min to form a homogeneous solution. Then, 10.0 mL of aqueous solution containing 100 mg of m-aminophenol and 6 mg of $Fe(NO_3)_3 \cdot 9H_2O$ was added into the round-bottom flask, followed by injecting 0.15 mL of HCHO. After that, the mixture was heated at 85 ºC for 6 h. The PS@Fe(III)–APFR product was collected by centrifugation and washed by deionized water and ethanol for three times. The PS@Fe(III)–APFR was dried at 70 ºC overnight and grinded into powder. In the pyrolysis step, the powder was heated at 600 ºC with a

heating rate of 2 ºC min^{-1} and maintained at 600 ºC for 2 h at Ar atmosphere, followed by raising the temperature to 800 ºC with a heating rate of 5 ºC min^{-1} and calcined at 800 ºC for 3 h.

1.4 Synthesis of NHCSs. The synthetic procedure of the NHCSs was similar with that of Fe SAs/NHCSs except for the addition of $Fe(NO_3)_3 \cdot 9H_2O$ precursor.

1.5 Synthesis of Fe nanoparticles (Fe NPs/NHCSs). In a typical synthesis, 60 mg of $Fe(NO_3)_3 \cdot 9H_2O$ and 200 mg of NHCSs were uniformly grinded. The mixture was then heated at 600 ºC with a rate of 2 ºC min^{-1} and maintained at 600 ºC for 2 h at Ar atmosphere, followed by raising the temperature to 800 ºC with a heating rate of 5 ºC min^{-1} and calcined at 800 ºC for 3 h.

1.6 Characterization. Powder X-ray diffraction patterns were measured with a Bruker D8 with Cu Kα radiation (λ = 1.5406 Å). Transmission electron microscopy and high-resolution Transmission electron microscopy images were recorded by a Hitachi H-800 operated at 100 kV and a JEOL-2100F operated at 200 kV, respectively. The aberration-corrected HAADF-STEM images were performed using a Titan 80-300 scanning/transmission electron microscope operated at 300 kV, equipped with a probe spherical aberration corrector. The in-situ environmental microscopic study was carried out on a Titan ETEM microscope (FEI) operated at 300 kV equipped with an image Cs-corrector. Inductively coupled plasma optical emission spectroscopy (ICP-OES) was measured by Thermo Fisher IRIS Intrepid II. The X-ray photoelectron spectroscopy (XPS) was measured by a PHI Quantera SXM system under $3.1*10^{-8}$ Pa using Al^{+} radiation at room temperature.

1.7 XAFS measurement and data analysis. The X-ray absorption find structure data (Co K-edge) were collected at 1W1B station in Beijing Synchrotron Radiation Facility (BSRF). The storage rings of BSRF were operated at 2.5 GeV with a maximum current of 250 mA. The data were collected at room temperature in transmission mode using N_2-filled ionization chamber. All samples were pelletized as disks of 13 mm diameter using graphite powder as a binder. The acquired EXAFS data were processed according to the standard procedures using the ATHENA module implemented in the IFEFFIT software packages. The k^3-weighted EXAFS spectra were obtained by subtracting the post-edge background from the overall absorption and then normalizing with respect to the edge-jump step. Subsequently, k^3-weighted

χ(k) data of Co K-edge were Fourier transformed to real (R) space using a hanning windows (dk = 1.0 $Å^{-1}$) to separate the EXAFS contributions from different coordination shells. To obtain the quantitative structural parameters around central atoms, least-squares curve parameter fitting was performed using the ARTEMIS module of IFEFFIT software packages. The following EXAFS equation was used:

$$\chi(k)=\sum_j \frac{N_j S_o^2 F_j(k)}{k R_j^2}\exp[-2k^2\sigma_j^2]\exp[\frac{-2R_j}{\lambda(k)}]\sin[2kR_j+\phi_j(k)]$$

S_0^2 is the amplitude reduction factor, $F_j(k)$ is the effective curved-wave backscattering amplitude, N_j is the number of neighbors in the j^{th} atomic shell, R_j is the distance between the X-ray absorbing central atom and the atoms in the j^{th} atomic shell (backscatterer), λ is the mean free path in Å, $\phi_j(k)$ is the phase shift (including the phase shift for each shell and the total central atom phase shift), σ_j is the Debye-Waller parameter of the j^{th} atomic shell (variation of distances around the average R_j). The functions $F_j(k)$, λ and $\phi_j(k)$ were calculated with the ab initio code FEFF8.2.

1.8 Catalytic test. In the catalytic hydrogenation of nitro-aromatic compounds, 1 mmol of nitro-aromatic, 2 mL of ethanol, and 10 mg of Fe SAs/NHCSs were added in a 15-mL glass vial under ultrasonic treatment. After the injection of 2 mL of $N_2H_4{\cdot}H_2O$, the vial was sealed and maintained at 40 °C for 6 h under magnetic stirring. The product of the reaction was analyzed by gas chromatography-mass spectrometer (GC-MS) through using n-dodecane as internal standard. In the stability test, the Fe SAs/NHCSs was seperated by centifugation after each cycle. The collected catalyst was then washed by ethanol and water and dried for the next cycle.

1.9 Computational Methods. The Vienna ab initio simulation package (VASP)[1] code was utilized to implement spin-polarized density functional theory (DFT) calculations with the Perdew-Burke-Ernzerhof (PBE) functional of the generalized gradient approximation[2] and the projector augmented wave (PAW)[3] method. A plane-wave basis set with 400 eV cutoff was performed and a 3×3×1 K point mesh was employed for Brillouin zone integration[4]. The vacuum thickness was set to 15 Å to avoid adjacent interaction between layers. The 6×6 graphene supercells was adopted in this works. All structures were optimized until the force and energy on each atom less than 0.02 eV/Å and 10^{-5} eV. The PBE+U approach[5] was carried out to correctly describe the strong Coulomb interactions of Fe d-orbitals with 4 eV U-correction.

Grimme's energy correction method (DFT-D2)[6] was employed to describe the long-range van der Waals interactions. The minimum energy paths were conducted using climbing nudged elastic band (CI-NEB)[7] method. All the transitions states were further confirmed by frequency analysis.

2. Supplementary Figures

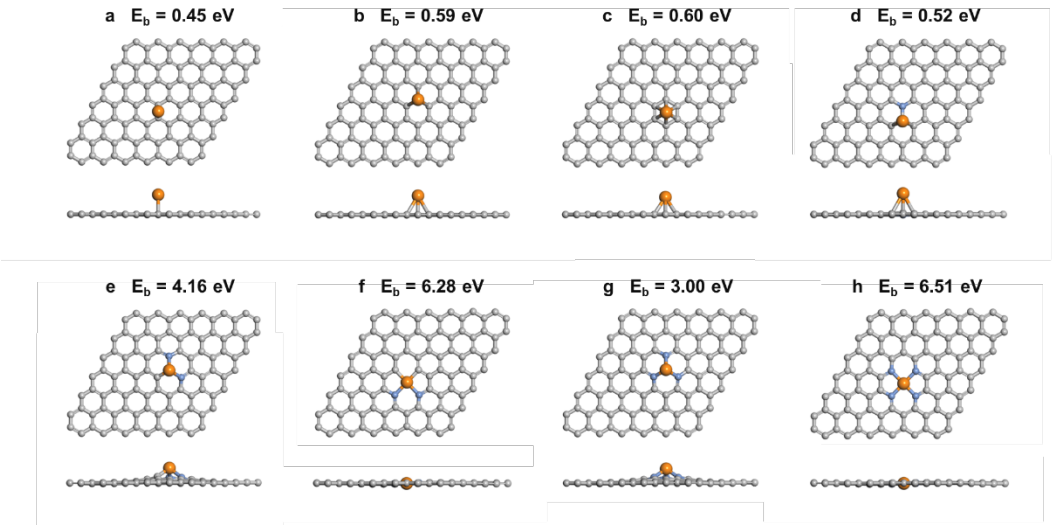


Figure S1. Optimized geometries and the binding energies of adsorbing Fe atom at the different sites of the graphene, (a) bridge site, (b) top site, (c) hole site, (d)N-doping graphene, (e) FeN_2C_1 site, (f) FeN_2C_2 site, (g) FeN_3 site, (h) FeN_4 site, C, N and Fe atoms are represented by grey, blue and orange balls, respectively.

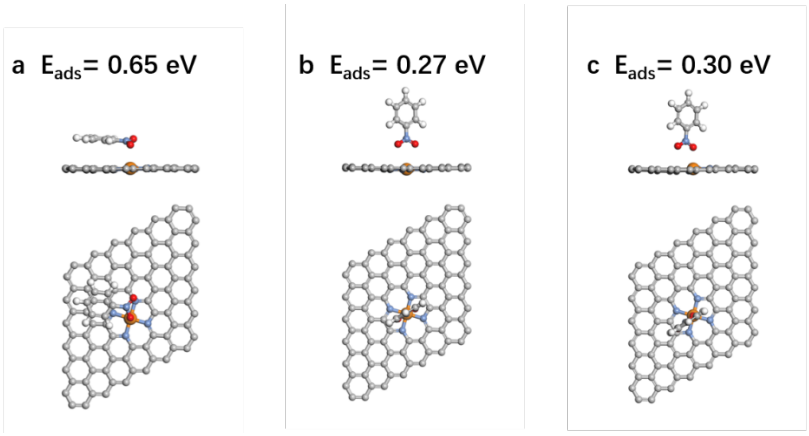
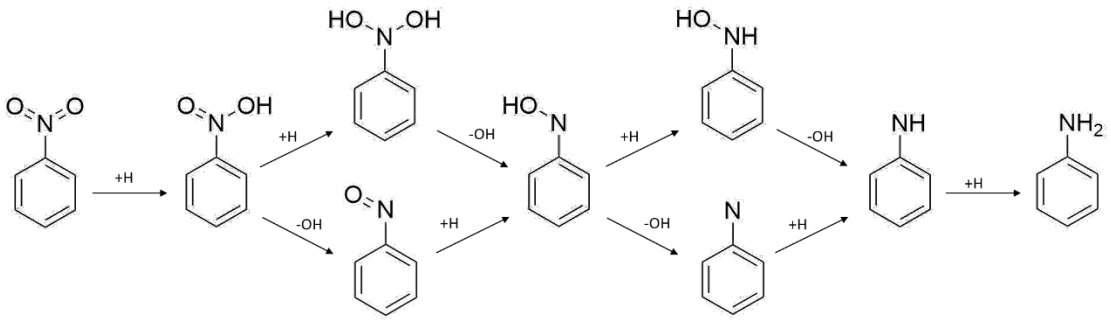


Figure S2. The optimized geometries and the adsorption energies of $C_6H_5NO_2$ on the Fe SAs surface. C, N, O, H and Fe atoms are represented by grey, blue, red, white, and orange balls, respectively.



Scheme S1. The possible reaction pathways for the hydrogenation of nitrobenzene into aniline on the Fe SAs surface.

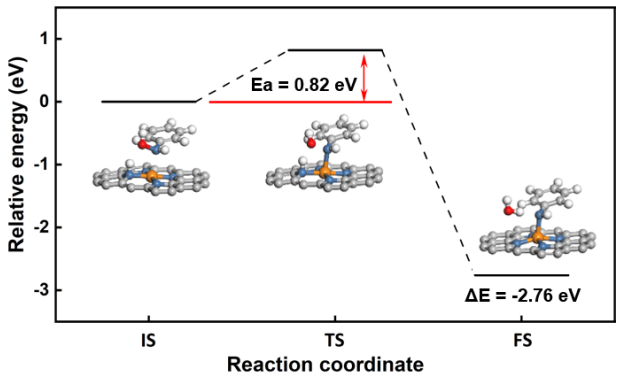


Figure S3. Energy profiles of possible pathway for the N-O bond cleavage of PhNHOH by forming a five-membered ring transition state.

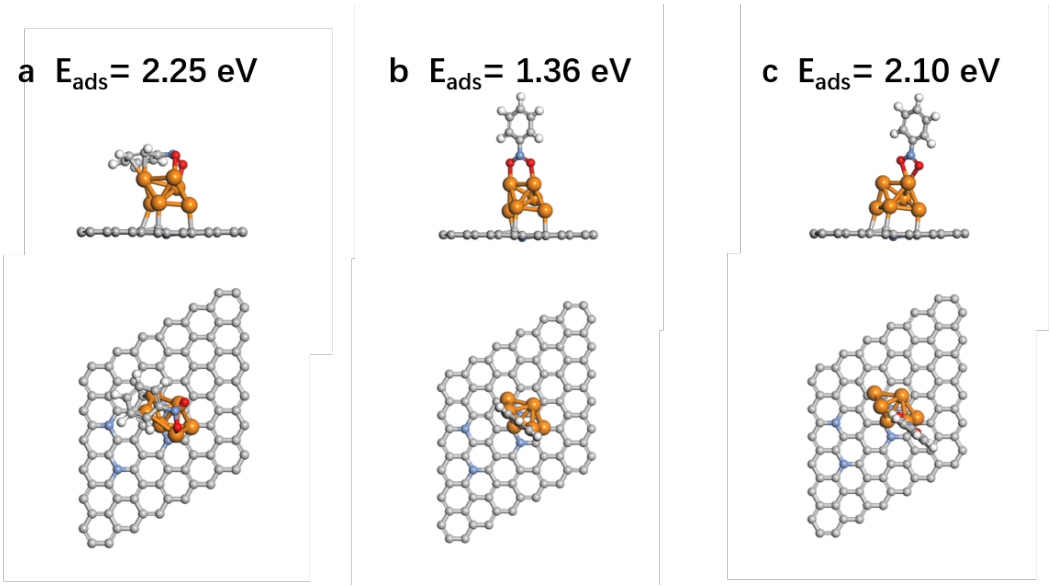


Figure S4. The optimized geometries and the adsorption energies of $C_6H_5NO_2$ on the Fe NPs surface. C, N, O, H and Fe atoms are represented by grey, blue, red, white, and orange balls, respectively

Table S1. Calculated activation barriers (Ea, in eV) and reaction energies (ΔE, in eV) of the elementary steps involved in nitrobenzene reduction to aniline on the Fe SAs.

Reactions	Ea	ΔE
$C_6H_5NO_2^* + H^* \rightarrow C_6H_5NOOH^*$	0.60	-0.70
$C_6H_5NOOH^* + H^* \rightarrow C_6H_5N(OH)_2^*$	0	-1.61
$C_6H_5NOOH^* \rightarrow C_6H_5NO^* + OH^*$	0.67	-0.58
$C_6H_5N(OH)_2^* \rightarrow C_6H_5NOH^* + OH^*$	0.89	-0.23
$C_6H_5NO^* + H^* \rightarrow C_6H_5NOH^*$	0.02	-1.27
$C_6H_5NOH^* + H^* \rightarrow C_6H_5NHOH^*$	0.02	-2.21
$C_6H_5NOH^* \rightarrow C_6H_5N^* + OH^*$	1.61	0.66
$C_6H_5NHOH^* \rightarrow C_6H_5NH^* + OH^*$	0.87	-0.15
$C_6H_5N^* + H^* \rightarrow C_6H_5NH^*$	0.10	-2.48
$C_6H_5NH^* + H^* \rightarrow C_6H_5NH_2^*$	0	-2.57

Table S2. Calculated activation barriers (Ea, in eV) and reaction energies (ΔE, in eV) of the elementary steps involved in nitrobenzene reduction to aniline on Fe NPs.

Reactions	Ea	ΔE
$C_6H_5NO_2^* + H^* \rightarrow C_6H_5NOOH^*$	0.72	0.07
$C_6H_5NOOH^* + H^* \rightarrow C_6H_5N(OH)_2^*$	2.99	1.18
$C_6H_5NOOH^* \rightarrow C_6H_5NO^* + OH^*$	0	-2.79
$C_6H_5N(OH)_2^* \rightarrow C_6H_5NOH^* + OH^*$	0	-3.53
$C_6H_5NO^* + H^* \rightarrow C_6H_5NOH^*$	1.09	0.13
$C_6H_5NOH^* + H^* \rightarrow C_6H_5NHOH^*$	1.77	0.66
$C_6H_5NOH^* \rightarrow C_6H_5N^* + OH^*$	0	-2.76
$C_6H_5NHOH^* \rightarrow C_6H_5NH^* + OH^*$	0.16	-3.93
$C_6H_5N^* + H^* \rightarrow C_6H_5NH^*$	1.60	-0.29
$C_6H_5NH^* + H^* \rightarrow C_6H_5NH_2^*$	2.03	0.68

Table S3. Calculated the adsorption energies of the adsorbate involved in the hydrogenation of nitrobenzene into aniline on the Fe SAs and Fe NPs surface.

Adsorbate	E_{ads}(Fe SAs, eV)	E_{ads}(Fe NPs, eV)
$C_6H_5NO_2$	0.65	2.25
C_6H_5NOOH	0.64	2.02
$C_6H_5N(OH)_2$	0.77	0.92
C_6H_5NO	0.68	1.70
C_6H_5NOH	0.64	2.29
C_6H_5NHOH	0.74	0.88
C_6H_5N	1.24	3.36
C_6H_5NH	1.10	2.87
$C_6H_5NH_2$	0.79	0.93

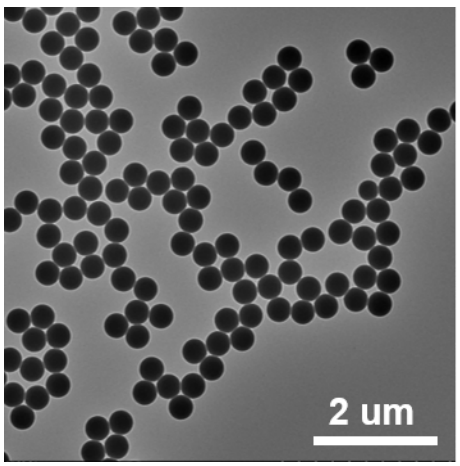


Figure S5. TEM image of the PS.

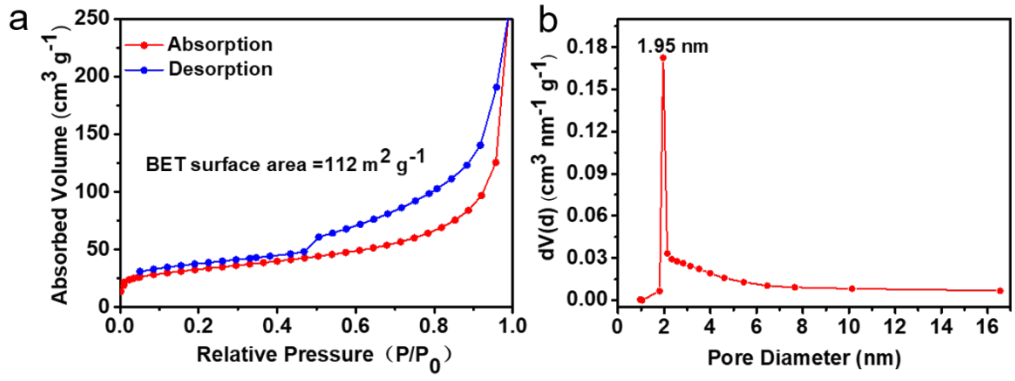


Figure S6. (a) Nitrogen isotherm adsorption/desorption of Fe SAs/NHCSs. (b) BJH pore size distribution of Fe SAs/NHCSs.

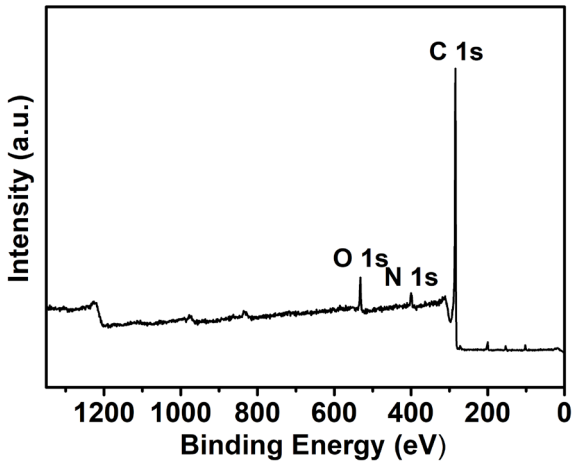


Figure S7. XPS spectra of Fe SAs/NHCSs.

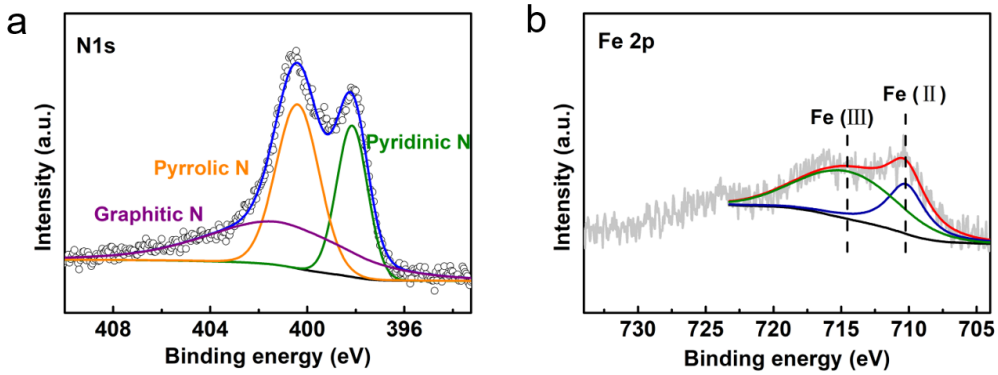


Figure S8. XPS survey spectra of Fe SAs/NHCSs. (a) N 1s spectra. (b) Fe 2p spectra.

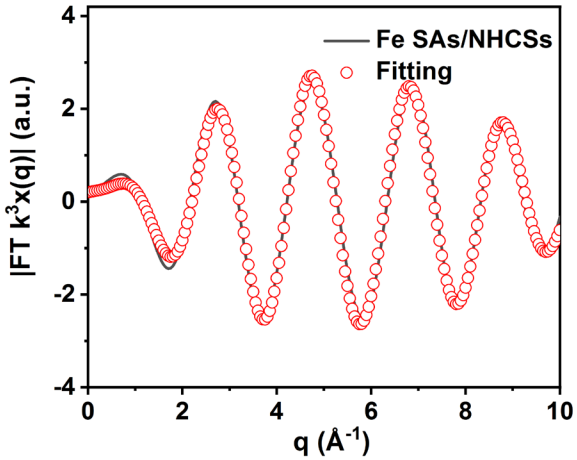


Figure S9. The EXAFS fitting curves of Fe SAs/NHCSs at q space.

Table S4. Structural parameters extracted from the Fe K-edge EXAFS fitting. (S_0^2=0.713)

Sample	Scattering pair	CN	R(Å)	$\sigma^2(10^{-3}Å^2)$	ΔE_0(eV)	R factor
Fe SAs/NHCSs	Fe-N	4.35	2.02	8.4	3.6	0.02
Fe foil	Fe-Fe1	8*	2.46	6.2	4.4	0.008
	Fe-Fe2	6*	2.84	7.8		

S_0^2 is the amplitude reduction factor; CN is the coordination number; R is interatomic distance (the bond length between central atoms and surrounding coordination atoms); σ^2 is Debye-Waller factor (a measure of thermal and static disorder in absorber-scatterer distances); ΔE_0 is edge-energy shift (the difference between the zero kinetic energy value of the sample and that of the theoretical model). R factor is used to value the goodness of the fitting.

* This value was fixed during EXAFS fitting, based on the known structure.

Error bounds that characterize the structural parameters obtained by EXAFS spectroscopy were estimated as N ± 20 %; R ± 1 %; σ^2 ± 25 %; ΔE_0 ± 10 %.

Fe SAs/NHCSs (FT range: 2.0-12.0 $Å^{-1}$; fitting range: 1.2-2.2 Å).

Fe foil (FT range: 2.0-12.0 $Å^{-1}$; fitting range: 1.4-3 Å).

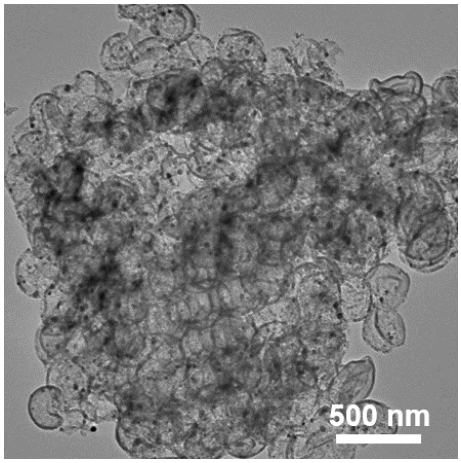


Figure S10. TEM image of Fe NPs/NHCSs.

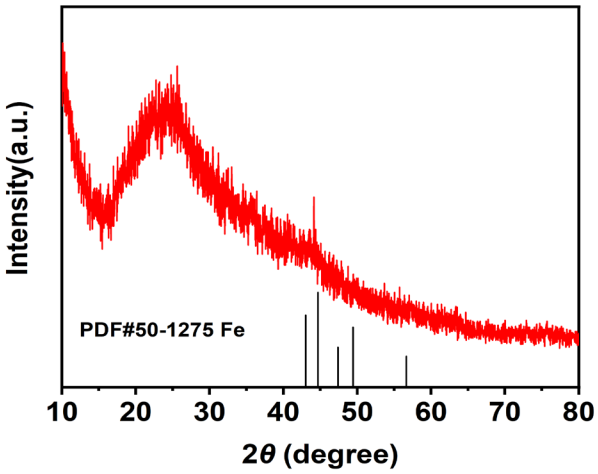


Figure S11. XRD pattern of Fe NPs/NHCSs.

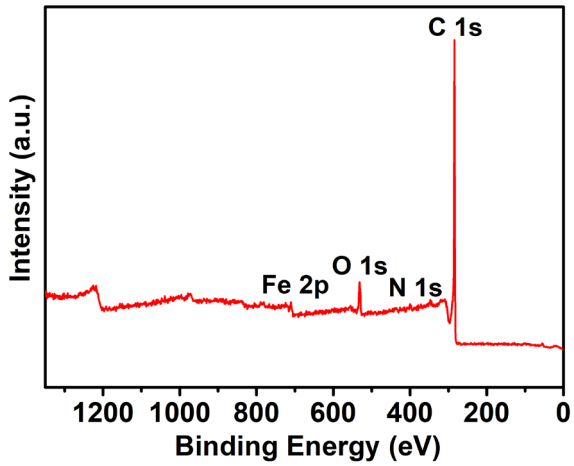


Figure S12. XPS spectra of Fe NPs/NHCSs.

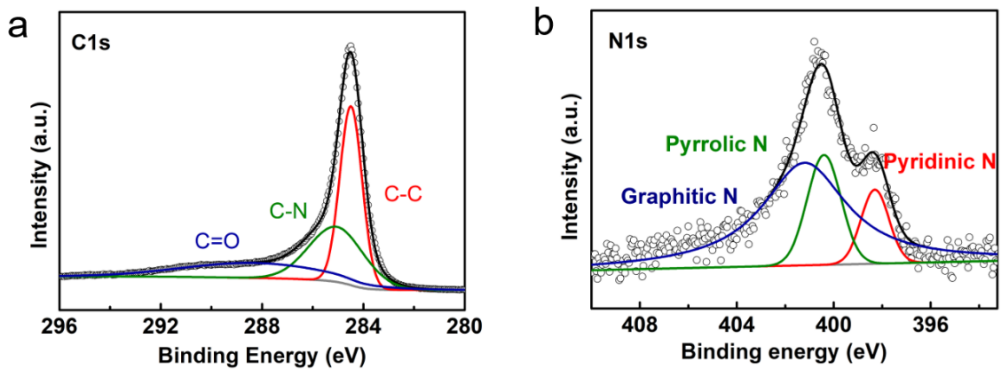


Figure S13. XPS survey spectra of Fe NPs/NHCSs. (a) C 1s spectra. (b) N 1s spectra.

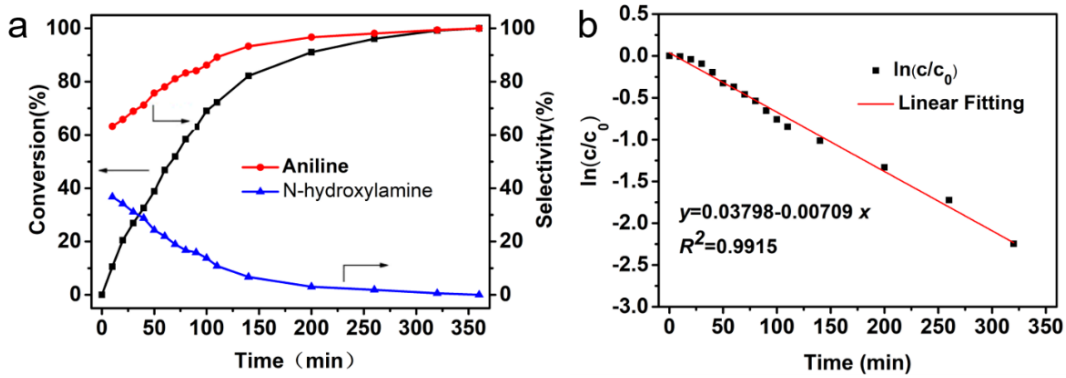


Figure S14. (a) Kinetic analysis and (b) linear fitting results hydrogenation of nitrobenzene.

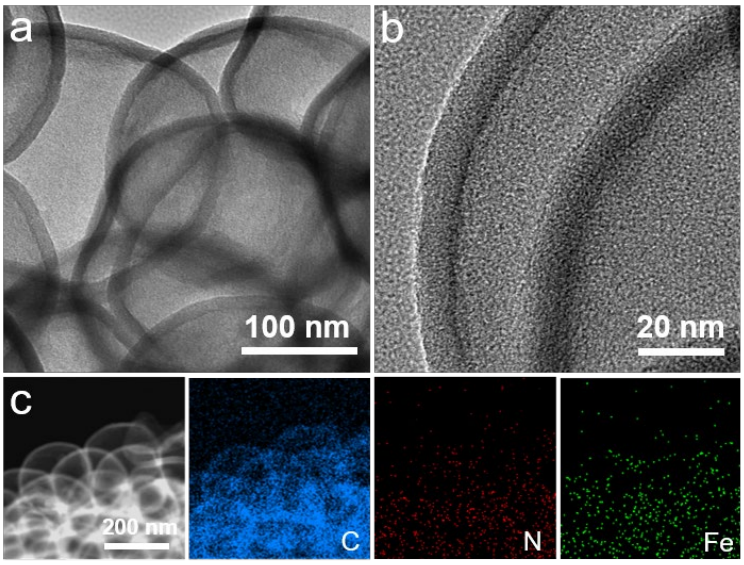


Figure S15. The characterization of Fe SAs/NHCSs after five reaction hydrogenation cycles for (a) TEM image. (b) HRTEM image. (c) EDX element mapping.

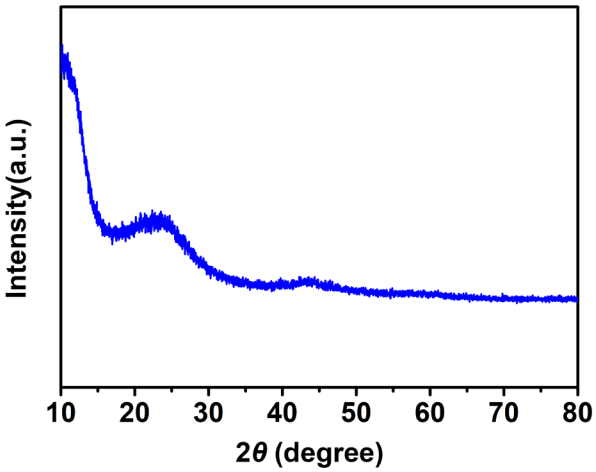


Figure S16. XRD pattern of Fe SAs/NHCSs after five reaction hydrogenation cycles.

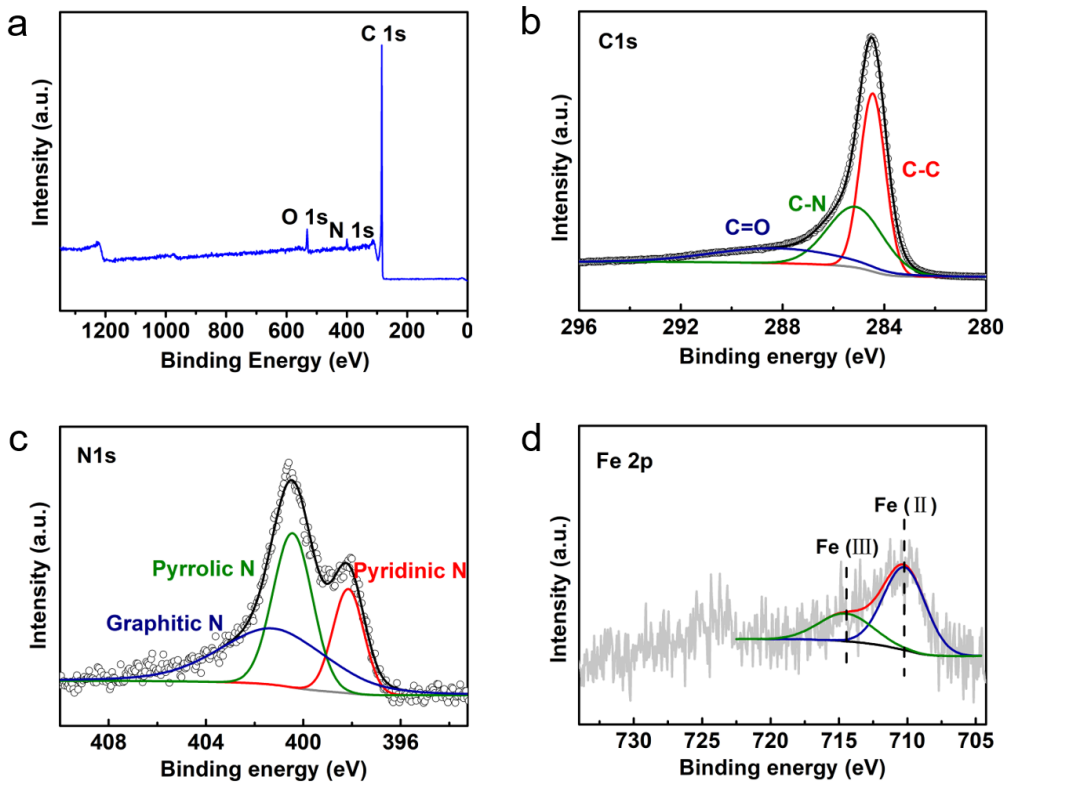
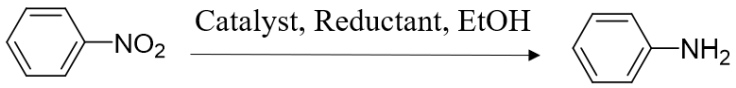


Figure S17. The XPS survey spectra of Fe SAs/NHCSs after stability test. (a) XPS spectra. (b) C 1s spectra. (c) N 1s spectra. (d) Fe 2p spectra.

Table S5. Control experiment of nitrobenzene hydrogenation[a]



Entry	Catalyst	Reductant	Temperature / °C	Time / h	Conversion[b] /%	Selectivity[c] /%
1	Fe SAs/NHCSs	$N_2H_4•H_2O$	40	6	99	99
2	None	$N_2H_4•H_2O$	40	6	0.5	99
3	NHCSs	$N_2H_4•H_2O$	40	6	10	99
4	Fe NPs/NHCSs	$N_2H_4•H_2O$	40	6	26	80

[a] Standard reaction condition: nitrobenzene (1 mmol), EtOH (2.0 mL) and reductant (2.0 mL, 80 wt%). Fe SAs/NHCSs (10 mg). Fe NPs/NHCSs (10 mg). NHCSs (10 mg).

[b] Conversion is determined by GC with n-dodecane as internal standard.

[c] Selectivity is determined by GC-MS.

Table S6. Comparison of the performance of nitrobenzene hydrogenation in literatures.

Catalyst	Hydrogen source	T/ °C	Time / h	Conv/%	Ref.
Fe SAs/NHCSs	$N_2H_4•H_2O$	40	6	99	This work
Co–L_1/C	H_2 (50 bar)	110	4	>99	*Nat. Chem.* **2013**[S8]
Rh_3Ni_1	H_2	R. T.	5	99	*ACS Catal.* **2013**[S9]
Fe NPs	$NaBH_4$	R. T.	2-3	95	*Chem. Commun.* **2012**[S10]
Fe_3O_4	$N_2H_4•H_2O$	80	1.5	99	*Chem. Asian J.* **2011**[S11]
$PtNi_3$	H_2 (1 atm)	R. T.	3	100	*Angew. Chem. Int. Ed.* **2012**[S12]
Pt–Ni nanodendrites	H_2 (1 atm)	R. T.	1	100	*Chem. Commun.* **2013**[S13]
Pt_1/α-MoC	H_2 (2 MPa)	35	1.5	100	*Nat. Nanotechnol.* **2019**[S14]
Au/Sn–TiO_2-123	H_2 (1.3 MPa)	100	1.5	>99.5	*Nat. Commun.* **2018**[S15]
Co SAs/NC	H_2 (3 MPa)	110	4	99.7	*ACS Appl. Mater. Interfaces.* **2020**[S16]
Co@mesoNC	H_2 (3 MPa)	110	3	73	*J. Catal*. **2018**[S17]
Pd@SiO_2	H_2 (1 atm)	45	1	83.3	*J. Phys. Chem. C* **2013**[S18]
Ru@C_{60}	H_2 (30 bar)	80	4	100	*ACS Catal.* **2016**[S19]
Pt/CeO_2-R-600	H_2 (1 MPa)	R. T.	2	100	*ACS Catal.* **2020**[S20]
Fe_3O_4@CS_AgNi	$NaBH_4$	R. T.	1	77	*ACS Omega* **2019**[S21]
Fe_3O_4	$N_2H_4•H_2O$	90	3	99	*Sci. Rep.* **2017**[S22]

R. T.: room temperature. **L_1:** 1,10-phenanthroline. **R:** rod.

3. References

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Optimized geometries

The optimized geometries of each state reported in the manuscript are given in coordinates (with atomic positions in Å) below. The coordinates are in the VASP POSCAR format.

For FeN_4 catalyst

Structure-I

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7.3866954629999997 12.8008386819000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 18.0000000000000000

C N Fe H O

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C N Fe H O

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Structure-Ⅱ

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C N Fe H O

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C N Fe H O

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Structure-III

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C N Fe H O

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Direct

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C N Fe H O

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C N Fe H O

72 5 1 7 1

Direct

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C N Fe H O

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C N Fe H O

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C N Fe H O

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C N Fe H

72 5 1 7

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C N Fe H

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For Fe nanoparticles catalyst

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C N Fe H O

74 5 6 6 2

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C N Fe H O

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