

## Supporting Information

### **Facilitating the acidic oxygen reduction of Fe-N-C catalysts by fluorine-doping**

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## Methods.

**Preparation of the F-FeNC and FeNC catalysts.** 65 mg of  $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$  and 2.2 g of  $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  were dissolved in 250 mL methanol with 5 min sonication (solution I). 2.5 g of 2-methylimidazole and 260 mg of PFTA surfactants were dissolved in 250 methonal (Solution II). Solution I was added into solution II rapidly in a flask. After 24 h reaction with vigorous stirring at 60 °C, as-prepared product was collected by a centrifugation process and washed with methanol three times, and dried in a vacuum at 80 °C. The precursors were heated with a heating ramp of 35 °C  $\text{min}^{-1}$  to 1000 °C for 1 h under an Ar environment, and then cooled to room temperature. The samples prepared by 169:1, 85:1 and 68:1 were denoted as F-FeNC-1, F-FeNC-2, and F-FeNC-3, respectively. For comparison, the FeNC sample was also prepared with the same method but without using PFTA surfactant. The F-NC reference was prepared by adding the same PFTA with F-FeNC-2 but without Fe source.

**Physical characterization.** Powder X-ray diffraction (PXRD) was carried out to characterize the crystalline phases of precursors and catalysts on a Rigaku SmartLab diffractometer with Cu  $K\alpha$  X-rays ( $\lambda = 1.5406 \text{ \AA}$ ) and a scanning speed of 0.4°  $\text{min}^{-1}$ . The elemental quantifications of catalysts were determined by X-ray photoelectron spectroscopy (XPS), which were conducted on Axis Ultra DLD imaging XPS using hybrid mode (700 x 300  $\mu\text{m}$ ) with 80 pass energy for survey spectra, as well as 20 pass energy for high-resolution spectra of elements. Inductively coupled plasma atomic emission spectroscopy (ICP-AES) was employed to measure the Fe loading (VISTA MPX, Varian Inc.). The preparation of the sample for ICP measurement was as

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followed: Sample (2 mg) in a quartz boat was heated in atmosphere at 800 °C for 1 h to remove carbon support. The concentrated nitric acid (3 mL) was used to dissolve iron oxide in the quartz boat to obtain iron extract. The above extract then was transferred to a 50 mL volumetric flask and made up to volume with ultrapure water. The porous structure was analysed using N<sub>2</sub> adsorption-desorption experiments carried out at 77 K on a Quantachrome SI-MP Instrument. Non-local density functional theory (NLDFT) model was used to determine the pore size distributions. Before measurements, samples were degassed at 120 °C for 24 h under vacuum. Transmission electron microscopy (TEM) and high-resolution TEM (HR-TEM), together with element mapping images were acquired on Tecnai G2 F30 S-Twin (FEI, Netherlands) working at 200 kV. High-angle annular dark-field scanning TEM (HAADF-STEM) and aberration-corrected (AC-HAADF-STEM) images were collected using Theims Z field emission electron microscope (FEI, Netherlands) working at 200 kV. The Raman spectra of pellet samples were measured with a Bruker RFS 100/S Raman spectrometer excited by a 532 nm laser. The Raman spectra of three random spots were collected for each sample. X-ray absorption spectroscopy (XAS) experiments were carried out at the 1W1B station of the Beijing Synchrotron Radiation Facility (BSRF) that was operated at 2.5 GeV with a maximum current of 250 mA. Data reduction, analysis and EXAFS fitting were performed using the ATHENA module implemented in the IFEFFIT software packages according to the standard procedures.

**<sup>57</sup>Fe Mössbauer Spectroscopy.** Mössbauer spectra were obtained by using a <sup>57</sup>Co/Rh source in transmission mode at room temperature. Both samples (80–100 mg) are

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prepared in a sample holder (diameter: 15 mm) covered by tesa tape, and the measurements were carried out in a velocity range of  $\pm 6.8 \text{ mm s}^{-1}$  at room temperature. Calibration of the velocity axis was done with respect to  $\alpha\text{-Fe}$ . While the initially obtained spectrum covered the range of 1024 channels, due to the low iron content in the samples and low signal to noise ratio, all original spectra and the calibration file were converted to 512 channels, to improve the count statistics. Thus after folding and calibration, 256 data points cover the overall velocity range. The “Recoil” program was used to fit the data.

**Electrochemical measurements.** Electrochemical measurements were performed using a standard three-electrode system controlled by a CHI 760E electrochemical station (CH Instruments, Inc., Shanghai). A graphite rod and an Ag/AgCl (4 M KCl) electrode were used as a counter electrode and reference electrode, respectively. A rotating disk electrode (RDE) with a glassy carbon disk (5.0 mm diameter) and a rotating ring-disk electrode (RRDE) electrode with a Pt ring (6.25 mm inner diameter and 7.92 mm outer diameter) and a glassy carbon disk (5.61 mm diameter) served as the substrate for the working electrodes. Before use, RDE/RRDE electrodes were polished using aqueous alumina suspensions (3.0 to 0.05  $\mu\text{m}$ ). The catalytic ink was prepared by blending 2.5 mg catalyst with 500  $\mu\text{L}$  of a mixture solution containing 490  $\mu\text{L}$  of ethanol and 10  $\mu\text{L}$  Nafion solution (5 wt%) followed by ultrasonication. A certain volume of ink was pipetted on the disk electrode to yield a uniform film with a catalytic loading of  $0.6 \text{ mg cm}^{-2}$ . Cyclic voltammetry (CV) measurements were carried out in  $\text{O}_2$ -saturated electrolyte solution at  $50 \text{ mV s}^{-1}$  to activate the catalysts until the CV

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profile was stable. ORR polarization curves were recorded with a sweep speed of 5 mV s<sup>-1</sup> at a rotating rate of 900 rounds per minute (rpm). Four-electron selectivity by RRDE technique was determined by measuring the ring current at 1.3 V and calculating the H<sub>2</sub>O<sub>2</sub> yield. Catalyst durability was tested by potential cycling from 0.6 to 1.0 V in O<sub>2</sub>-purged 0.5 M H<sub>2</sub>SO<sub>4</sub> at a scan rate of 50 mV s<sup>-1</sup>. A commercial Pt/C catalyst (20 wt% Pt on carbon; Fuel Cell Store) was served as a reference catalyst with a Pt loading of 0.1 mg cm<sup>-2</sup> in O<sub>2</sub>-saturated 0.1 M HClO<sub>4</sub> solution.

The yield of hydrogen peroxide and the number of electron transfers were calculated by the following equations:

$$H_2O_2(\%) = 200 \times \frac{\frac{i_r}{N}}{i_d + \frac{i_r}{N}}$$

$$n = 4 \times \frac{i_d}{i_d + \frac{i_r}{N}}$$

Where  $i_r$  is the ring current,  $i_d$  is the disk current, and  $N = 0.37$  is the Pt ring current collection efficiency.

**Preparation of the Membrane Electrode Assemblies (MEA).** A catalyst ink suspension was prepared by dispersing 80 mg Pt/C Elyst Pt20 0390 (Umicore AG& Co. KG.) in 800 μl H<sub>2</sub>O, 800 μl Nafion™ (PFSA 5 wt%) and 1600 μl isopropanol for the anode side. The cathode ink suspension was prepared by dispersing 80 mg of F-FeNC-2 catalyst in 276 μl H<sub>2</sub>O, 987 μl Nafion™ (PFSA 5 wt%) and 1974 μl isopropanol. All catalyst inks were dispersed in an ultrasonic bath for 1 h, followed by spray coating on a gas diffusion layer (GDL, Freudenberg SE H23C9) with an area of 4.84 cm<sup>2</sup>. The obtained loadings were 0.21 mg<sub>Pt</sub> cm<sup>-2</sup> for the anode gas diffusion

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electrode (GDE) and  $2 \text{ mg}_{\text{catalyst}} \text{ cm}^{-2}$  for the cathode GDE. By hot pressing the anode and cathode GDE with a Nafion N212 membrane (Quintech GmbH) at  $125^{\circ}\text{C}$  and 4 bar for 2 minutes the MEA was fabricated.

For the preparation of the Pt/C reference catalyst on the cathode side, 10 mg Pt/C Elyst Pt50 0550 (Umicore AG& Co. KG.) and 90 mg Ketjenblack 300 were dispersed in  $345 \mu\text{l}$  water,  $1234 \mu\text{l}$  Nafion<sup>TM</sup> (PFSA 5 wt%) and  $2468 \mu\text{l}$  isopropanol. The catalyst ink suspension was dispersed in an ultrasonic bath for 1.5 h followed by spray coating and hot pressing analog to the other catalysts with the exception of a catalyst loading of  $0.1 \text{ mg}_{\text{Pt}} \text{ cm}^{-2}$  and a pressure of 18 bar, respectively.

**Fuel Cell Testing:** Fuel Cell measurements were carried out in a 850e fuel cell test station (Scribner Associates Inc., North Carolina) at  $81^{\circ}\text{C}$  with 96 % humidification and 1 bar gauge back pressure. The gas flows for  $\text{H}_2$  and Air were set at 200 sccm. The measurement protocol consisted of started with recording the open-circuit voltage for 180 s, followed by a polarization curve measured stepwise starting at a current of 0 A and increasing the current with a stepwidth of 0.03 A every 10 s until the cutoff condition of 0.2 V was reached. The stability was measured by applying a constant potential of 500 mV for 24 h. In the case of the Pt/C reference a breakin procedure was carried out by cycling 80 times between 600 mV and 300 mV with a holding time of 1 min for each potential before starting the measurement protocol.

### **Computational details.**

*Models:* The two-dimensional models of graphene hexagonal supercell, consisting of 73 atoms, is separated by a vacuum region of  $15 \text{ \AA}$  along the direction normal to the

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sheet plane to avoid artificial interactions between graphene layers. A series of models of five-coordinated FeN<sub>(2+2)</sub> site dispersed on F N co-doped graphene and corresponding intermediates (\*OOH, \*OH, and \*O) was built in Fig-S1.

*Calculated details.* All the density functional theory (DFT) calculations were constructed and implemented in the Vienna ab initio simulation package (VASP).<sup>1, 2</sup> Using the electron exchange and correlation energy was treated within the generalized gradient approximation in the Perdew–Burke–Ernzerhof functional (GGA-PBE),<sup>3</sup> the calculation were done with a plane-wave basis set defined by a kinetic energy cutoff of 450 eV. The geometry optimization and energy calculation were finished when the electronic self-consistent iteration and force were reach 10<sup>-5</sup> eV and 0.02 eV Å<sup>-1</sup>, respectively.

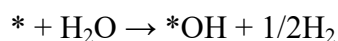
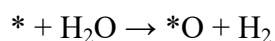
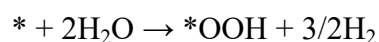
*The Adsorption Energy.* The adsorption energy ( $\Delta E_{\text{ads}}$ ) of the key ORR intermediates, including \*OOH, \*O, and \*OH, was calculated relative to H<sub>2</sub>O and H<sub>2</sub> under conditions of T = 298.15 K, pH = 0, and U = 0 V (vs. SHE) according to following equations:

$$\Delta E_{*OOH} = E_{*OOH} + 3/2 E_{H_2} - E^* - 2 E_{H_2O}$$

$$\Delta E_{*O} = E_{*O} + E_{H_2} - E^* - E_{H_2O}$$

$$\Delta E_{*OH} = E_{*OH} + 1/2 E_{H_2} - E^* - E_{H_2O}$$

Where \* represents the adsorption sites associated with FeN<sub>4</sub> doped graphene. The above  $\Delta G_{\text{ads}}$  is defined as the reaction free energies of the following reactions.



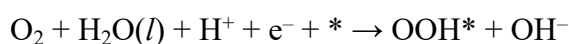
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*The Gibbs free energy variation.* The change in Gibbs free energy ( $\Delta G$ ) of each adsorbed intermediate is calculated based on the computational hydrogen electrode method developed by Nørskov et al.<sup>3</sup> At standard condition (T = 298.15 K, pH = 0, and U = 0 V (vs. standard hydrogen electrode, SHE)), the free energy G is defined as the following equation:

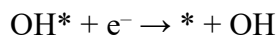
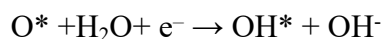
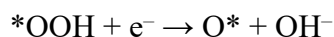
$$\Delta G = \Delta E + \Delta E_{ZPE} - T\Delta S + \Delta G_{pH} + \Delta G_U$$

Where  $\Delta E$  is the energy change obtained from DFT calculation,  $\Delta E_{ZPE}$  is the difference between the adsorbed state and gas, which was calculated by summing vibrational frequency for all model based on the equation:  $E_{ZPE} = 1/2 \sum h\nu_i$  (T is the temperature (298.15 K) in the above reaction system, and  $\Delta S$  represents the difference on the entropies between the adsorbed state and gas phase. The entropies of free molecules were obtained from NIST database (<https://janaf.nist.gov/>).  $\Delta G_{pH} = -kT \ln[H^+] = \text{pH} \cdot kT \cdot \ln 10 = -0.0591 \text{pH}$  is used to correct the free energy of  $H^+ + e^-$  referenced by a SHE at various pH values.  $\Delta G_U = -neU$ , where U is the applied electrode potential and n is the number of electrons transferred. Therefore, the equilibrium potential  $U^0$  for ORR at pH = 13 was determined to be 0.462 V (vs. SHE).

The free energy of  $O_2(g)$  was derived as  $G_{O_2(g)} = 2G_{H_2O(l)} - 2G_{H_2} + 4.92 \text{ eV}$ , and the free energy of  $OH^-$  was calculated by  $G_{OH^-} = G_{H_2O(l)} - G_{H^+}$ , which the energy of  $H^+$  is approximately equal to the energy of  $1/2H_2$ . The overall reaction of  $O_2$  reduction to  $OH^-$  in a alkaline environment is:  $O_2 + H_2O + 4e^- \rightarrow 4OH^-$ , which is divide into the four fundamental reactions as following:







OOH\*, O\* and OH\* present the OOH, O and OH moieties on the adsorption site.

*Theoretical ORR Overpotential.* The theoretical ORR overpotential ( $\eta_{\text{SHE}}$ , vs. SHE)

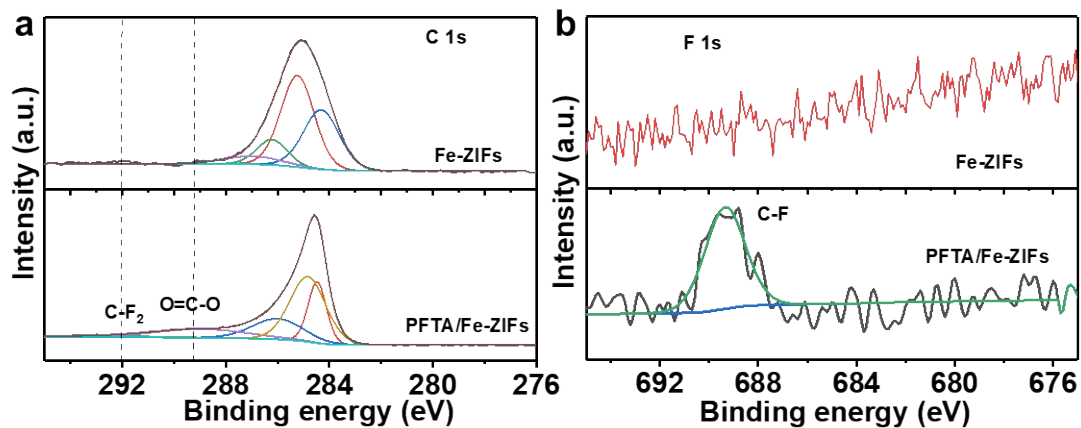
associated with different active sites was calculated according to following equation

$\eta_{\text{SHE}} = 0.462 \text{ V} + \Delta G_{\text{max}}$ , where 0.462 V is defined as the equilibrium potential of the

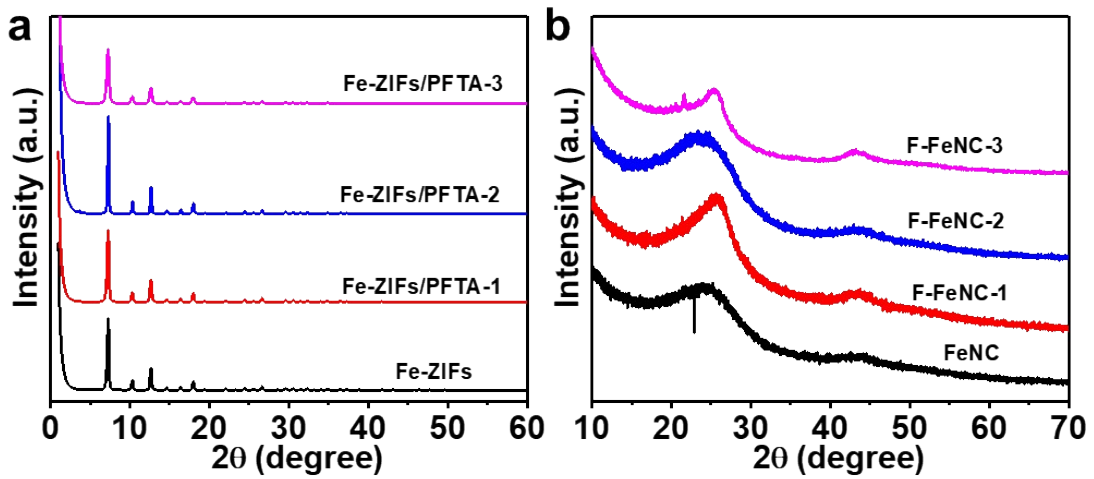
overall 4-electron ORR at the standard state, and  $\Delta G_{\text{max}}$  represents the most positive

free energy variation associated with the proton-electron-transfer steps.

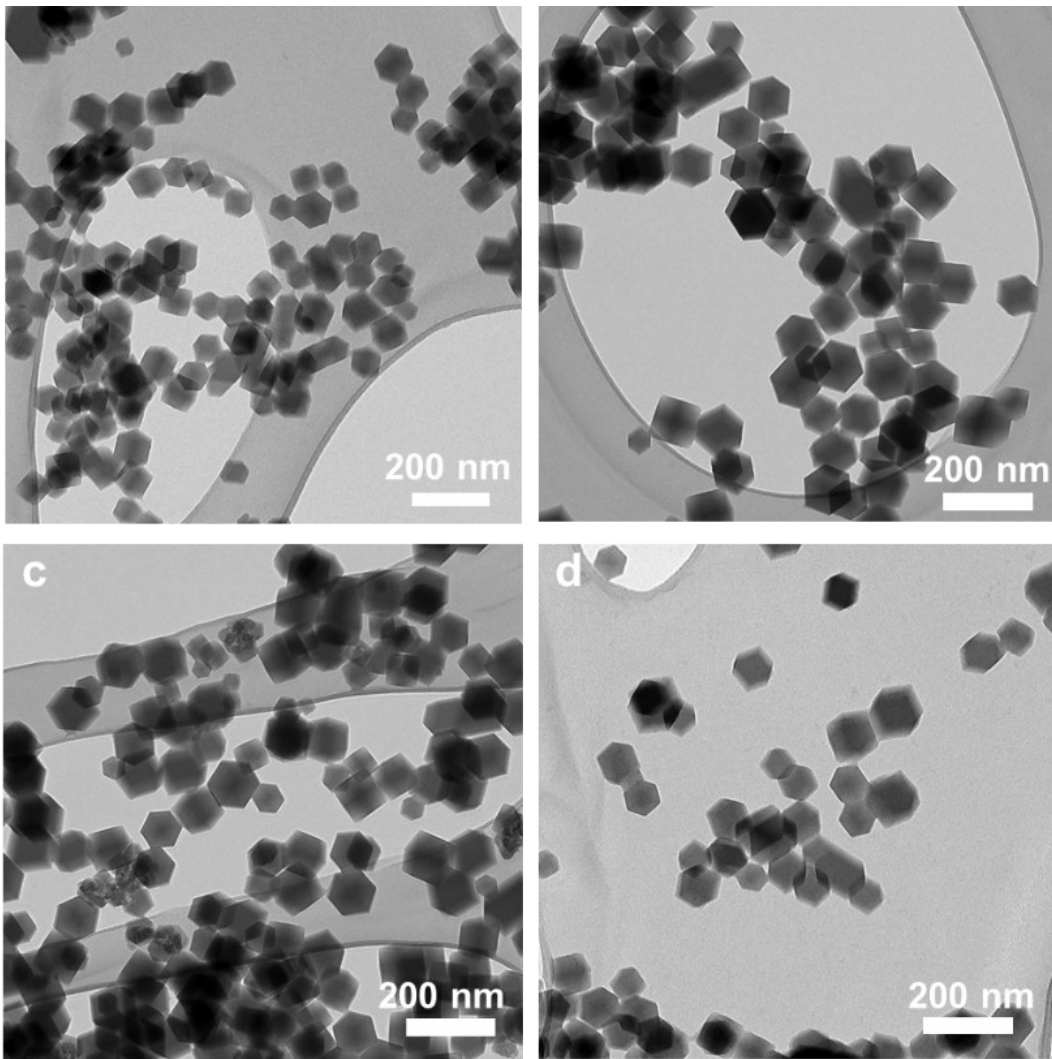
### Supplementary Figures and Tables



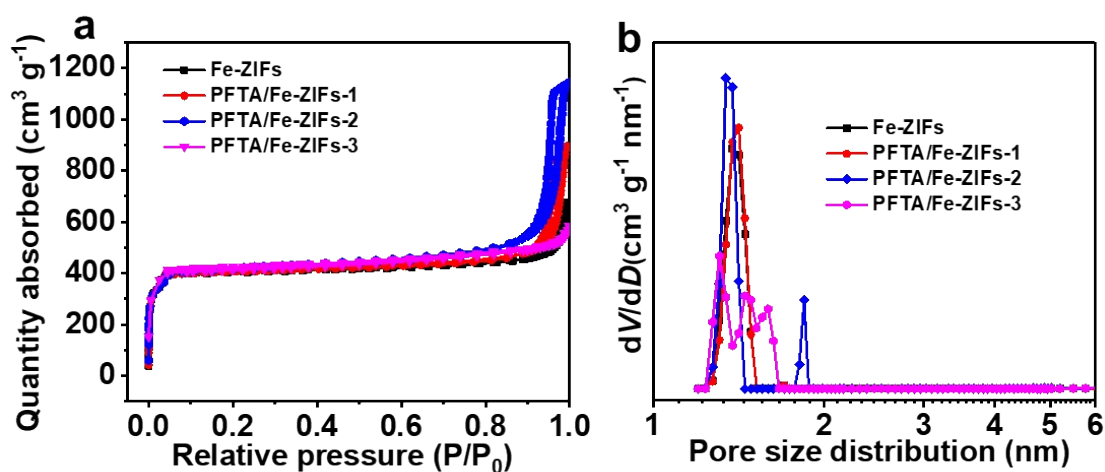
**Fig. S1.** High-resolution XPS of (a) C 1s, (b) F 1s of Fe-ZIFs and PFTA/Fe-ZIFs precursors.



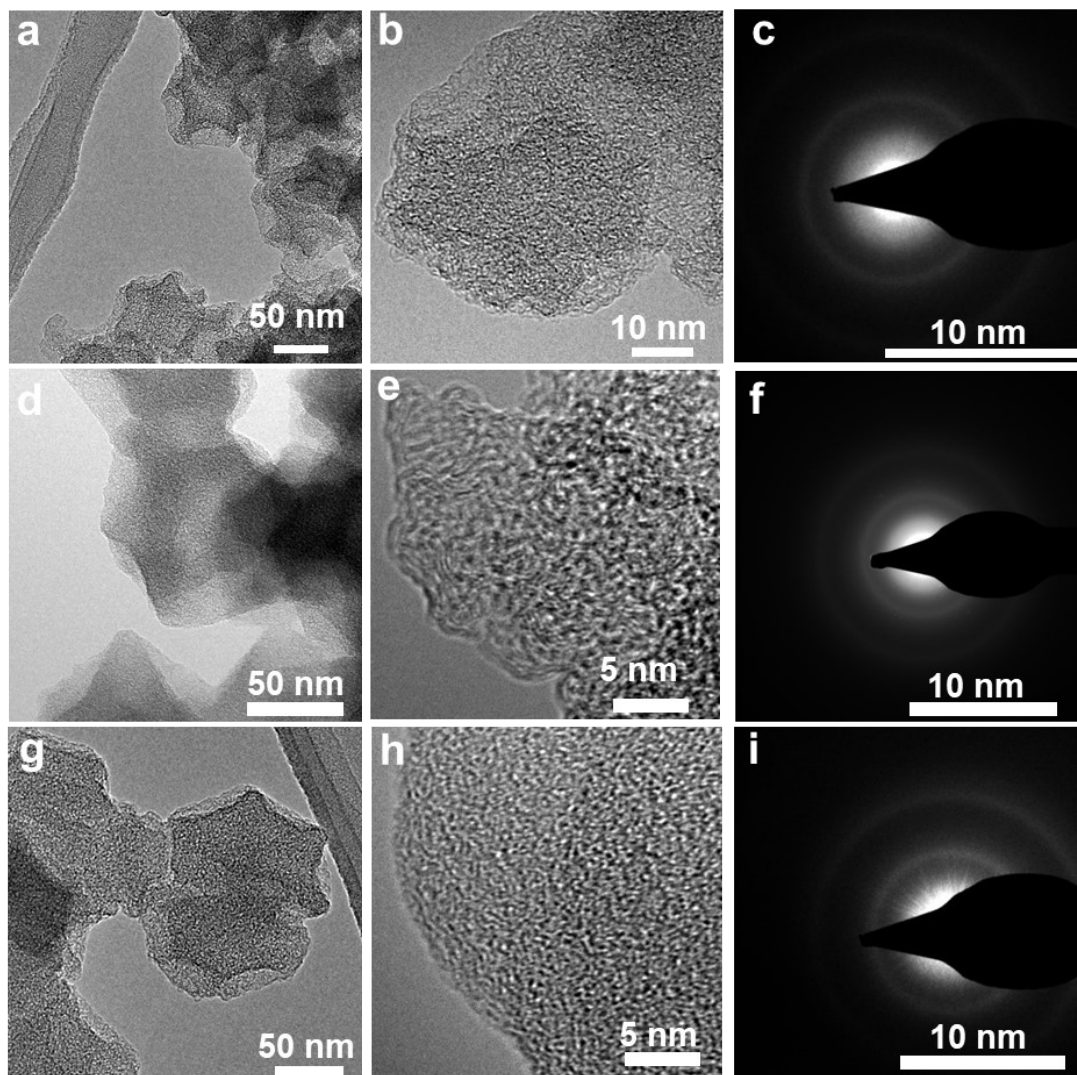
**Fig. S2.** XRD patterns of (a) Fe-ZIFs, PFTA/Fe-ZIFs-1, PFTA/Fe-ZIFs-2 and PFTA/Fe-ZIFs-3 precursors and (b) FeNC, F-FeNC-1, F-FeNC-2 and F-FeNC-3.



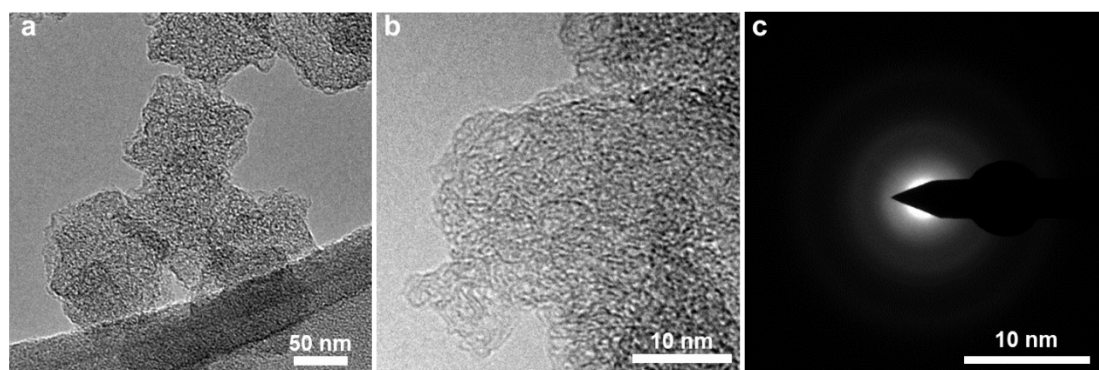
**Fig. S3.** TEM images of Fe-ZIFs, PFTA/Fe-ZIFs-1, PFTA/Fe-ZIFs-2 and PFTA/Fe-ZIFs-3 precursors.



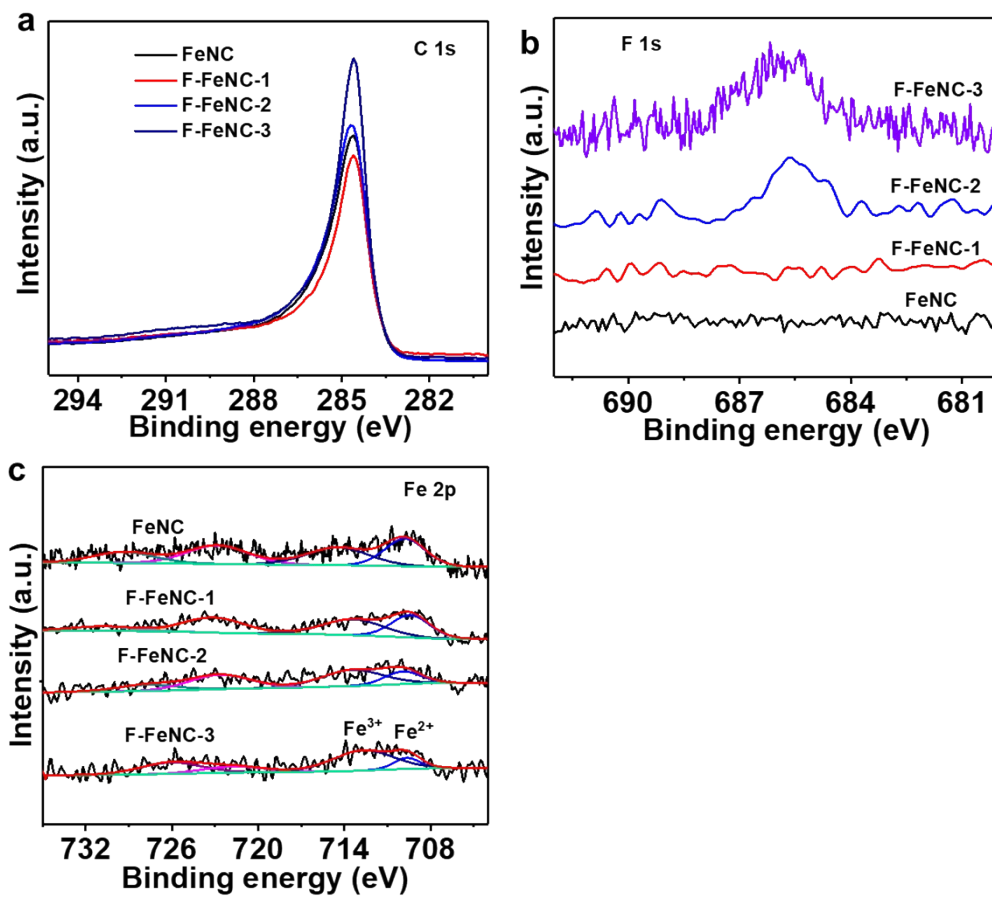
**Fig. S4.** (a)  $N_2$  adsorption/desorption isotherms of Fe-ZIFs, PFTA/Fe-ZIFs-1, PFTA/Fe-ZIFs-2, and PFTA/Fe-ZIFs-3 and the corresponding pore size distributions processed from NLDFT approach (b). All the PFTA/Fe-ZIFs showed a slightly larger Brunauer-Emmett-Teller (BET) surface areas of  $\sim 1680 m^2 g^{-1}$  than that of Fe-ZIFs ( $1444 m^2 g^{-1}$ ). The larger BET surface area is caused by the involved PFTA surfactants into micropores of ZIFs and the new micropores. The emergence of new larger micropores is very likely caused by the formation of defects in ZIF-8 due to the coordination of PFTA and metals.



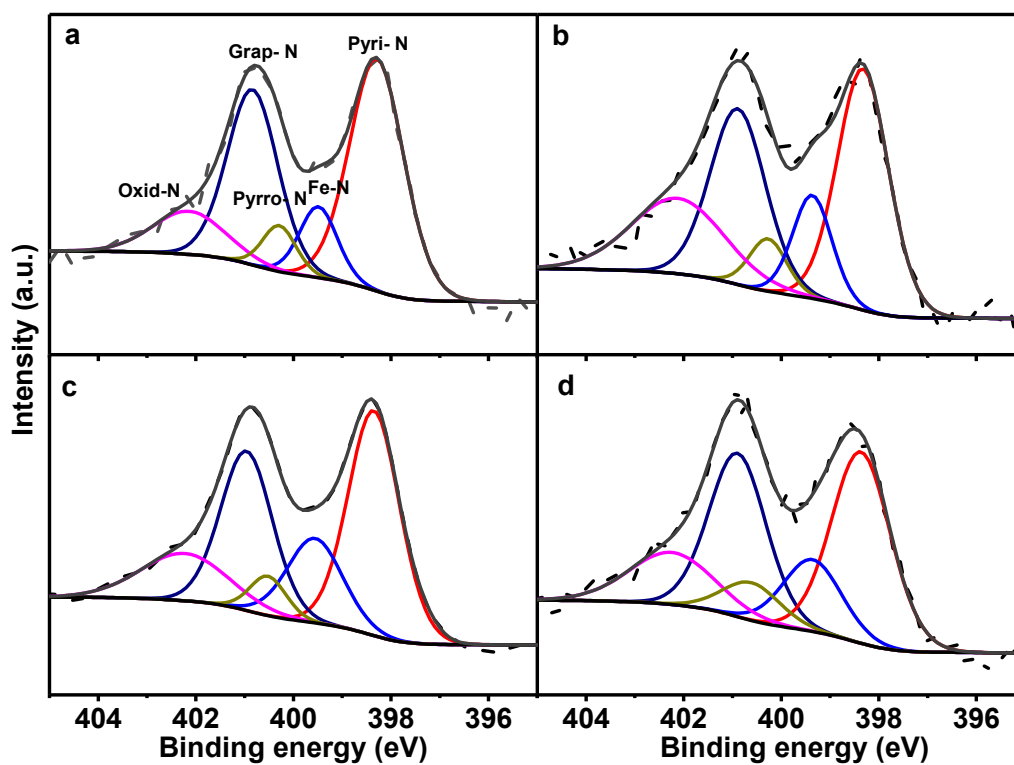
**Fig. S5.** (a, d, g) TEM (b, e, h) HRTEM and (c, f, i) SAED images of F-FeNC-1 (a-c), F-FeNC-2 (d-f) and F-FeNC-3 (g-i).



**Fig. S6.** (a) TEM (b) HRTEM and (c) SAED images of the control FeNC.



**Fig. S7.** High-resolution XPS spectra of (a) C 1s, (b) F 1s and (c) Fe 2p of FeNC, F-FeNC-1, F-FeNC-2 and F-FeNC-3.



**Fig. S8.** High-resolution XPS spectra of N 1s for (a) FeNC, (b) F-FeNC-1, (c) F-FeNC-2 and (d) F-FeNC-3.

**Table S1.** The contents of Fe<sup>2+</sup> and Fe<sup>3+</sup> species in FeNC, F-FeNC-1, F-FeNC-2 and F-FeNC-3 based on Fe 2p<sub>3/2</sub> XPS spectra.

Catalyst	Fe <sup>2+</sup> (%)	Fe <sup>3+</sup> (%)
Binding energy (Fe 2p <sub>3/2</sub> )	710 (eV)	713 (eV)
FeNC	28	27
F-FeNC-1	28	32
F-FeNC-2	17	36
F-FeNC-3	11	48

**Table S2.** Fitting results for N 1s spectra of the FeNC, F-FeNC-1, F-FeNC-2 and F-FeNC-3.

Catalyst	Pyridinic N (%)	Pyrrolic N	Graphitic N (%)	FeN <sub>x</sub> (%)	NO <sub>x</sub> (%)
Binding energy	398.4 (eV)	400.3 (eV)	401.2 (eV)	399.4 (eV)	402.1 (eV)
FeNC	43.7	5.4	30.9	9.2	10.8
F-FeNC-1	35.2	5.6	27.8	11.5	19.9
F-FeNC-2	38.9	4.7	27.3	15.4	13.6
F-FeNC-3	35.8	6.9	30.0	13.3	14.0

**Table S3.** Elemental compositions of the FeNC, F-FeNC-1, F-FeNC-2 and F-FeNC-3 according to XPS measurements, contents of Fe in samples measured by ICP-AES.

Catalyst	C (at%)	N(at%)	O(at%)	F (at%)	Zn(at%)	Fe (wt%)
FeNC	89.9	4.8	4.8	/	0.2	1.49
F-FeNC-1	88.5	5.5	4.5	0.1	0.2	1.49
F-FeNC-2	89.0	5.8	4.5	0.1	0.1	1.68
F-FeNC-3	90.6	3.3	5.4	0.2	0.1	1.43

**Table S4.** Raman calculation<sup>a</sup> results of FeNC, F-FeNC-1, F-FeNC-2 and F-FeNC-3

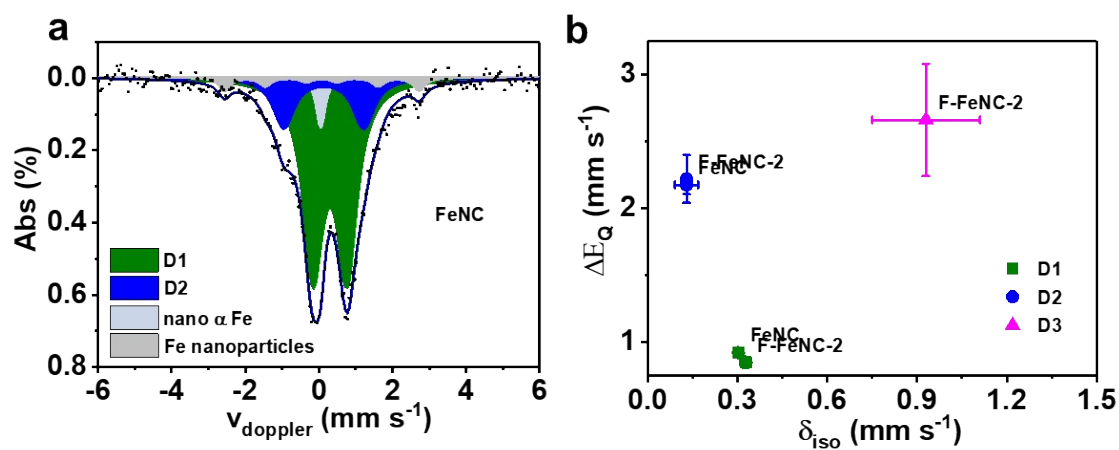
Catalyst	I <sub>D</sub> /I <sub>G</sub>	L <sub>a</sub> (nm)
FeNC	1.17 (0.11)	16.55 (1.52)
F-FeNC-1	1.30 (0.09)	14.88 (1.02)
F-FeNC-2	1.37 (0.07)	14.03 (0.71)
F-FeNC-3	1.46 (0.18)	13.33 (1.73)

a: Tuinstra Koenig Relation to calculate the crystallite size by using Raman Spectroscopy.<sup>4, 5</sup>

$$L_a(\text{nm}) = (2.4 \times 10^{-10}) \lambda_{\text{laser}}^4 \left(\frac{I_D}{I_G}\right)^{-1}$$

**Table S5.** Porosities of FeNC, F-FeNC-1, F-FeNC-2 and F-FeNC-3.

Catalyst	Pore Volume ( $\text{cm}^3 \text{g}^{-1}$ )	$S_{\text{Micropore}}$ ( $\text{m}^2 \text{g}^{-1}$ )	External Surface area ( $\text{m}^2 \text{g}^{-1}$ )	BET Surface area ( $\text{m}^2 \text{g}^{-1}$ )
FeNC	1.3	362	447	809
F-FeNC-1	1.12	601	420	1022
F-FeNC-2	0.8	665	421	1085
F-FeNC-3	0.92	561	460	1021



**Fig. S9.** (a) Mössbauer spectrum of FeNC and (b) Comparison of Mössbauer parameters of FeNC and F-FeNC-2 catalysts.



**Table S6.**  $^{57}\text{Fe}$  Mössbauer parameters derived from the fittings. Isomer shift (IS), quadrupole splitting (QS), line width (LW) of each component.

Sites		FeNC	F-FeNC	Assignment
S1	$\delta_{\text{iso}}$ (mm s $^{-1}$ )	$0.05 \pm 0.04$	$-0.00 \pm 0.05$	Nano $\alpha$ -Fe
	fwhm (mm s $^{-1}$ )	0.29*	0.28*	
D1	$\delta_{\text{iso}}$ (mm s $^{-1}$ )	$0.30 \pm 0.01$	$0.33 \pm 0.02$	Fe <sup>II</sup> N <sub>4</sub> , low spin
	$\Delta E_Q$ (mm s $^{-1}$ )	$0.92 \pm 0.02$	$0.85 \pm 0.04$	Fe <sup>III</sup> N <sub>4</sub> , high spin
	fwhm (mm s $^{-1}$ )	0.66*	0.65*	Fe or Fe oxide clusters
D2	$\delta_{\text{iso}}$ (mm s $^{-1}$ )	$0.13 \pm 0.04$	0.13*	Fe <sup>III</sup> N <sub>4</sub> , low spin
	$\Delta E_Q$ (mm s $^{-1}$ )	$2.18 \pm 0.07$	$2.22 \pm 0.18$	
	fwhm (mm s $^{-1}$ )	0.7*	0.7*	
D3	$\delta_{\text{iso}}$ (mm s $^{-1}$ )		$0.93 \pm 0.18$	L <sub>x</sub> -Fe <sup>II</sup> N <sub>4</sub> , high spin (x = 1, 2)
	$\Delta E_Q$ (mm s $^{-1}$ )		$2.66 \pm 0.42$	
	fwhm (mm s $^{-1}$ )		0.7*	
Sext1	$\delta_{\text{iso}}$ (mm s $^{-1}$ )	$0.08 \pm 0.08$		Iron nano particles
	H (T)	$16.4 \pm 0.7$		
	fwhm (mm s $^{-1}$ )	0.38*		

\* indicates a fixed value; error bar (95% confidence interval) were given behind  $\pm$   
The color codes are the same as those used in Figure 4e.

**Table S7.** . Structural parameters of the reference materials FeO, Fe<sub>2</sub>O<sub>3</sub> and Fe foil and the catalysts FeNC, and F-FeNC-2 extracted from the EXAFS fitting ( $S_0^2=0.85$ ).

	Path	CN <sup>a</sup>	$\Delta E(\text{eV})^b$	R( $\text{\AA}$ ) <sup>c</sup>	$\sigma^2(\text{\AA}^2)^d$	R-factor <sup>e</sup>
Fe foil	Fe-Fe	8	4.9 (1.1)	2.46 (0.01)	0.0045	0.0053
	Fe-Fe1	6		2.84 (0.01)		
FeO	Fe-O	6	-1.83 (2.13)	2.12 (0.02)	0.014	0.009
	Fe-Fe	12	-2.61 (1.10)	3.06 (0.01)	0.011	
Fe <sub>2</sub> O <sub>3</sub>	Fe-O	6	7.51 (3.22)	1.96 (0.02)	0.011	0.018
	Fe-Fe	6	0.96 (2.31)	2.98 (0.02)	0.0089	
FeNC	Fe-N	4.5 (0.5)	-9.0 (5.60)	2.02 (0.07)	0.0087	0.0077
	Fe-Fe	1.2 (0.3)	-2.0 (2.4)	2.54 (0.02)	0.0020	
F-FeNC-2 <sup>f</sup>	Fe-N	5.4 (0.4)	1.30 (1.6)	2.00 (0.02)	0.0102	0.0187
F-FeNC-2 <sup>g</sup>	Fe-N	3.9 (0.9)	1.3 (2.2)	2.04 (0.04)	0.0056	0.0056
	Fe-O	1.1 (0.7)		1.89 (0.04)	0.0021	

<sup>a</sup>CN: coordination numbers; <sup>b</sup> $\Delta E_0$ : the inner potential correction. <sup>c</sup>R: bond distance; <sup>d</sup> $\sigma^2$ : Debye-Waller factors; <sup>e</sup>R factor: goodness of fit.  $S_0^2$  was set to 0.66, according to the experimental EXAFS fit of Fe foil reference by fixing CN as the known crystallographic value;  $\delta$ : percentage. f: Fe-N, g: Fe-N and Fe-O scattering paths, respectively.

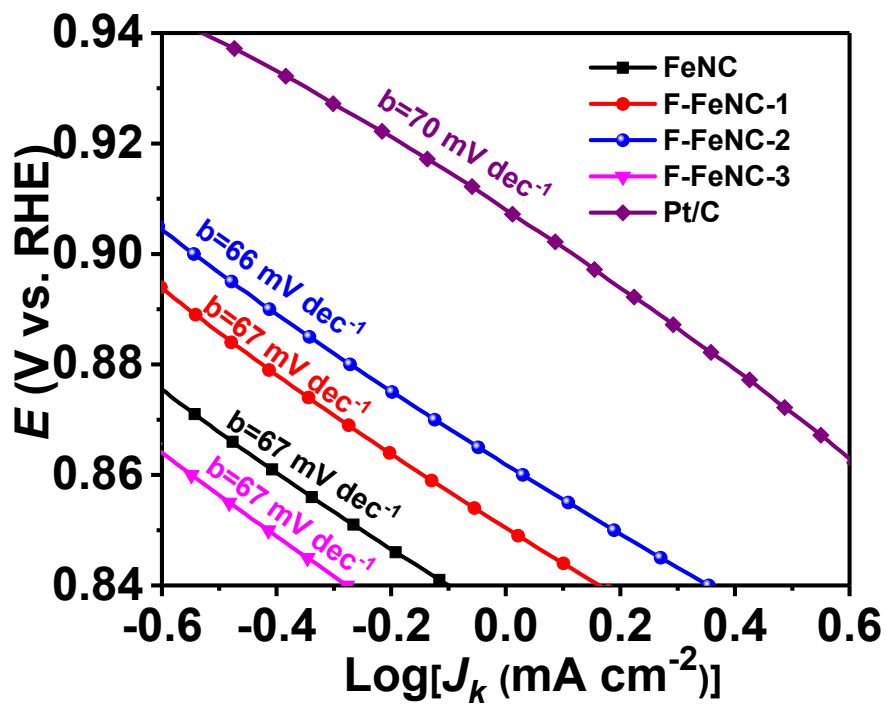


Fig. S10. Tafel slopes of FeNC, F-FeNC-1, F-FeNC-2 and Pt/C.

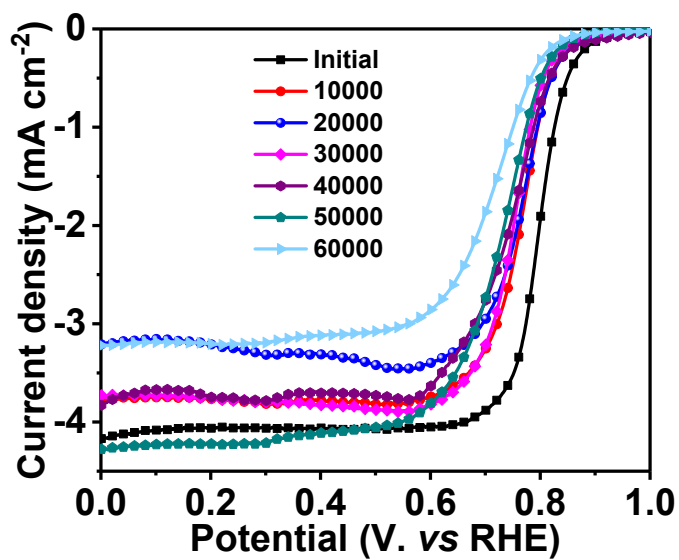
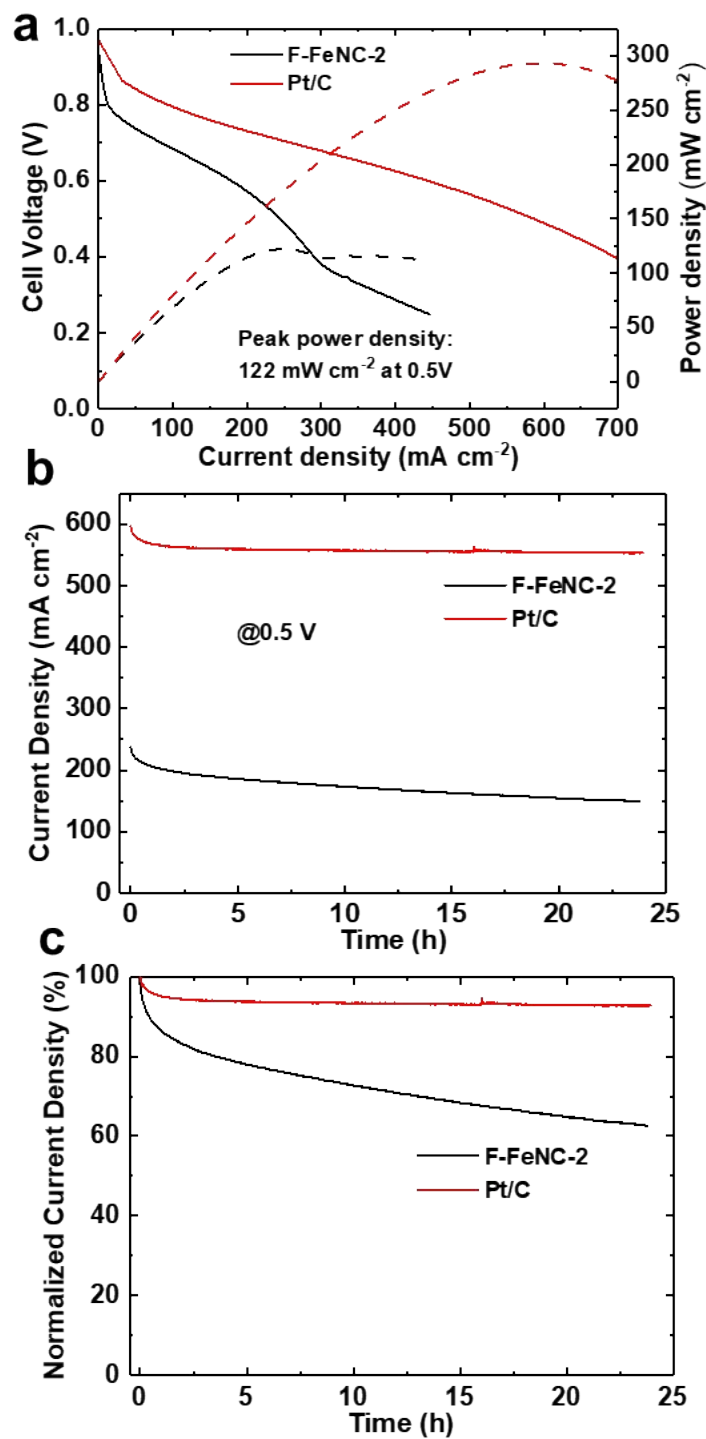


Fig. S11. Steady-state ORR polarization plots before and after potential cycling stability tests (0.6-1.0 V) for FeNC sample measured in 0.5M  $\text{H}_2\text{SO}_4$ .

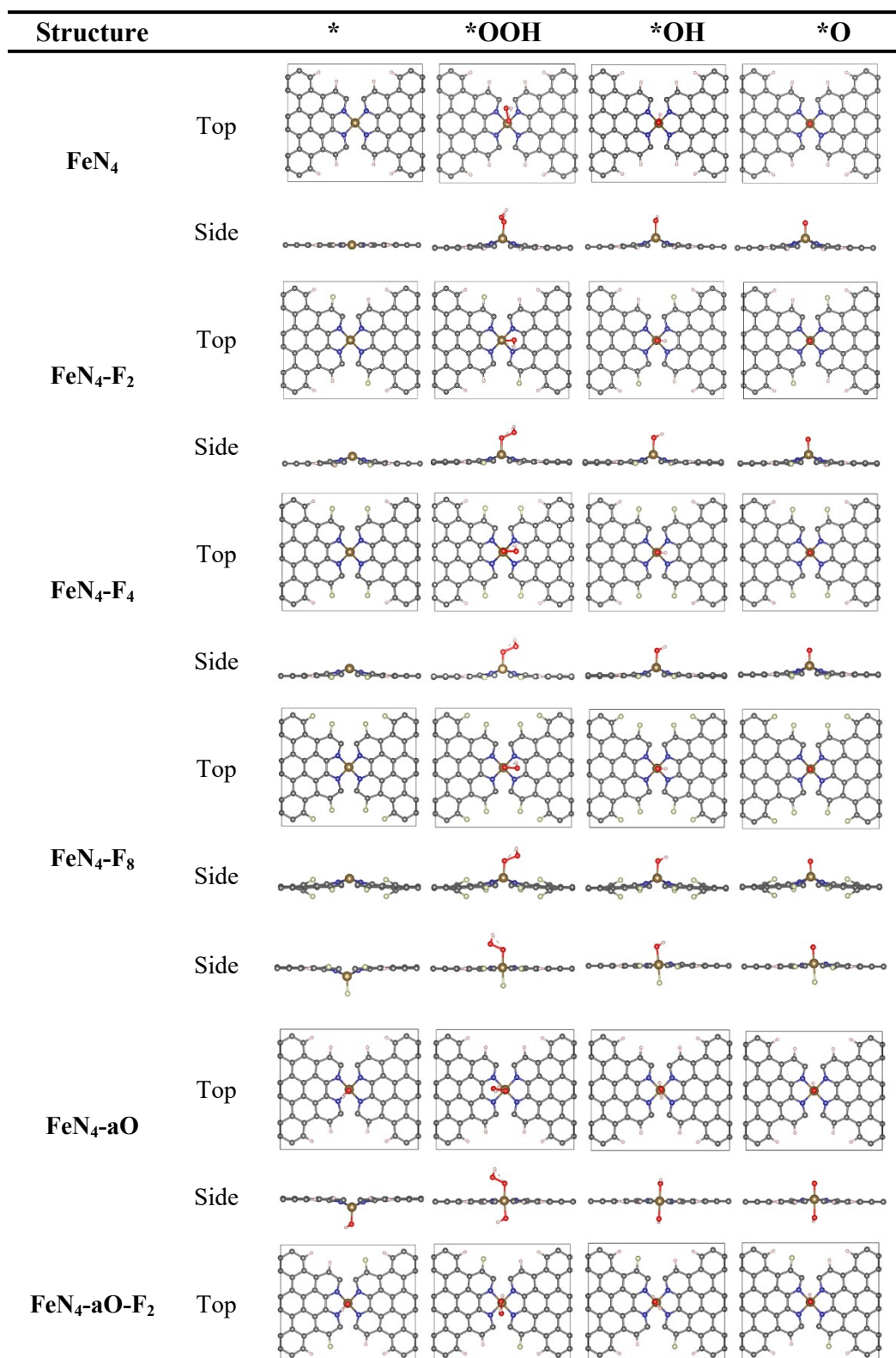
**Table S8.** Comparison of ORR performance for present Fe-N-C catalysts in acidic solution, and the platinum reference catalyst.

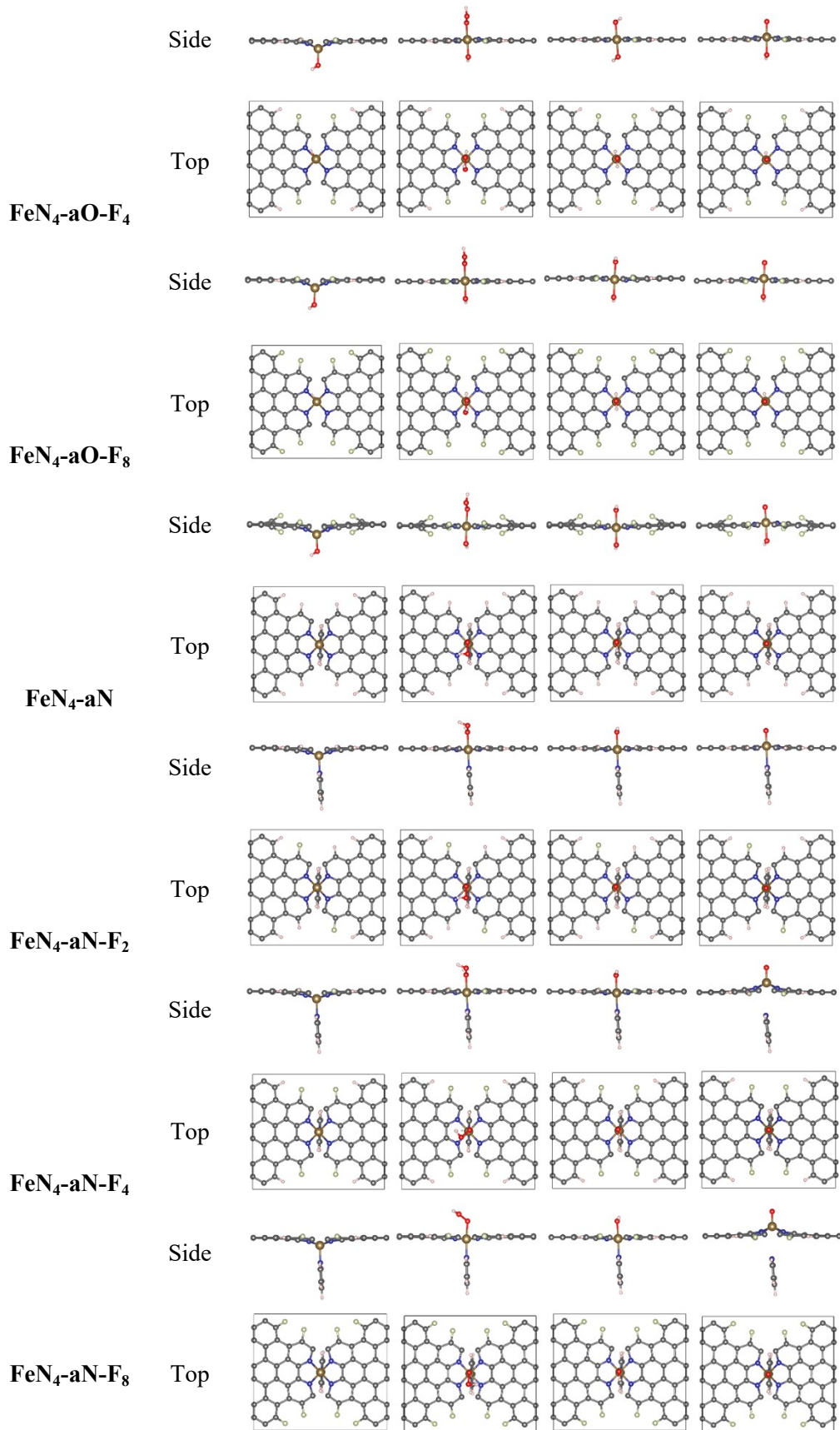
<b>Catalysts</b>	<b><math>E_{onset}</math> (V)</b>	<b><math>E_{1/2}</math> (V)</b>	<b><math>J_{k-0.85 V}</math> (mA m<sup>-2</sup>)</b>	<b>Tafel slope (mV dec<sup>-1</sup>)</b>	<b>Electrolyte</b>
FeNC	0.93	0.80	0.55	67	
F-FeNC-1	0.94	0.815	1.06	67	0.5M H <sub>2</sub> SO <sub>4</sub>
F-FeNC-2	0.96	0.83	1.63	66	
F-FeNC-3	0.90	0.79	0.40	67	
Pt/C	0.97	0.85	5.80	70	0.1 M HClO <sub>4</sub>

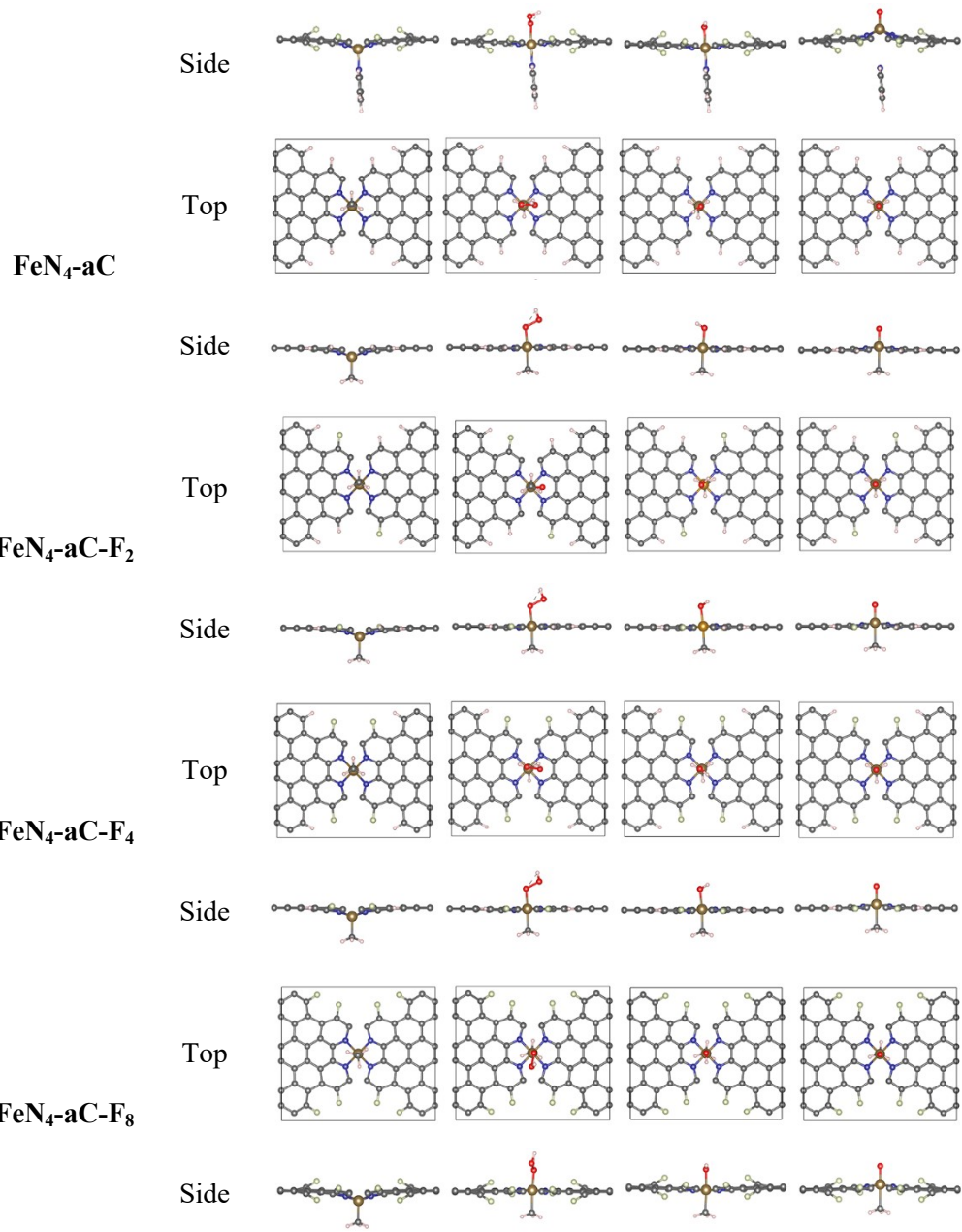


**Fig. S12.** Fuel cell performance (a) polarization curve and chronoamperometric potential holding with b) absolute current densities and c) normalized current densities as a function of time for F-FeNC-2 catalyst ( $2 \text{ mg}_{\text{catalyst}} \text{ cm}^{-2}$ ) and Pt/C reference catalyst ( $0.1 \text{ mg}_{\text{Pt}} \text{ cm}^{-2}$ ) on cathode; Anode:  $0.21 \text{ mg}_{\text{Pt}} \text{ cm}^{-2}$ ; measured under  $\text{H}_2$ -air  $0.2 \text{ L min}^{-1}$ ; cell  $81 \text{ }^\circ\text{C}$ , 96% humidification and 1 bar gauge back pressure, Membrane N212;  $4.84 \text{ cm}^{-2}$  serpentine flow field. All shown values were not  $iR$  corrected.

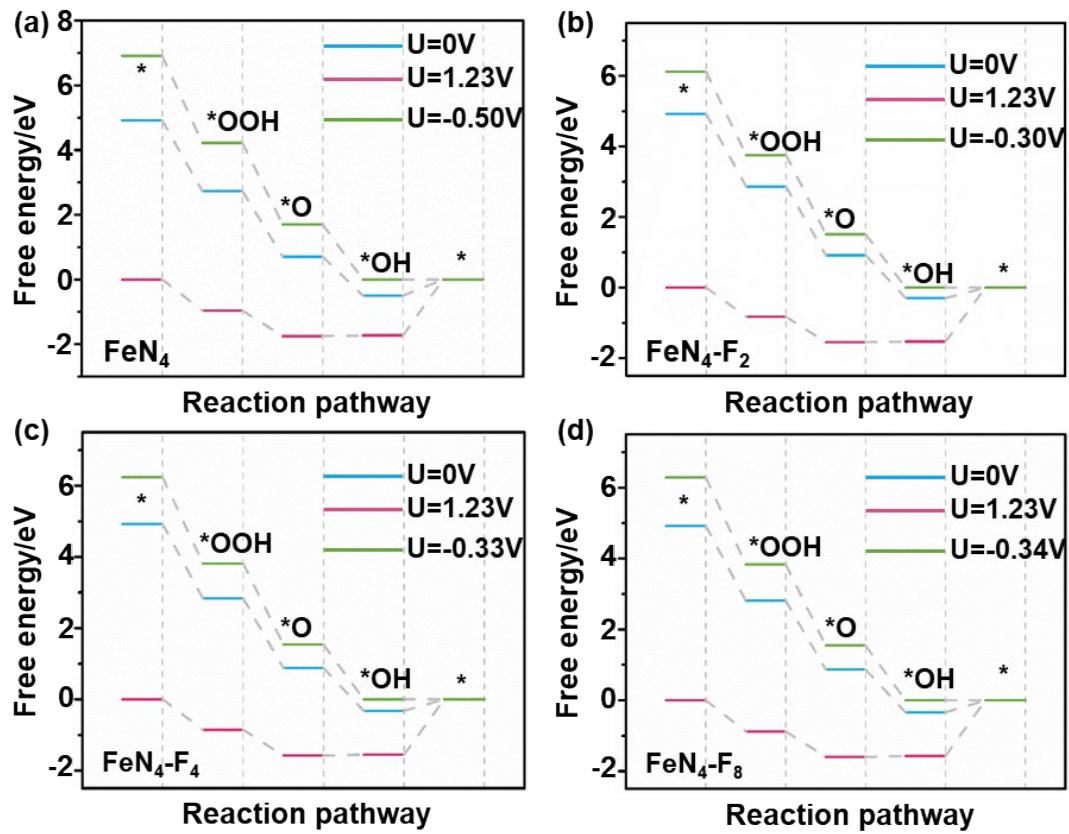
**Table S9.** Top and side views of a series of configurations with adsorbed species (\*OOH, \*OH, and \*O) after optimization, where white, grey, blue, green, light blue and gold balls represent the H, C, N, O, F and Fe atoms, respectively.











**Fig. S13.** The calculated free energy profiles of (a)  $\text{FeN}_4$ , (b)  $\text{FeN}_4\text{-F}_2$ , (c)  $\text{FeN}_4\text{-F}_4$ , and (d)  $\text{FeN}_4\text{-F}_8$ .

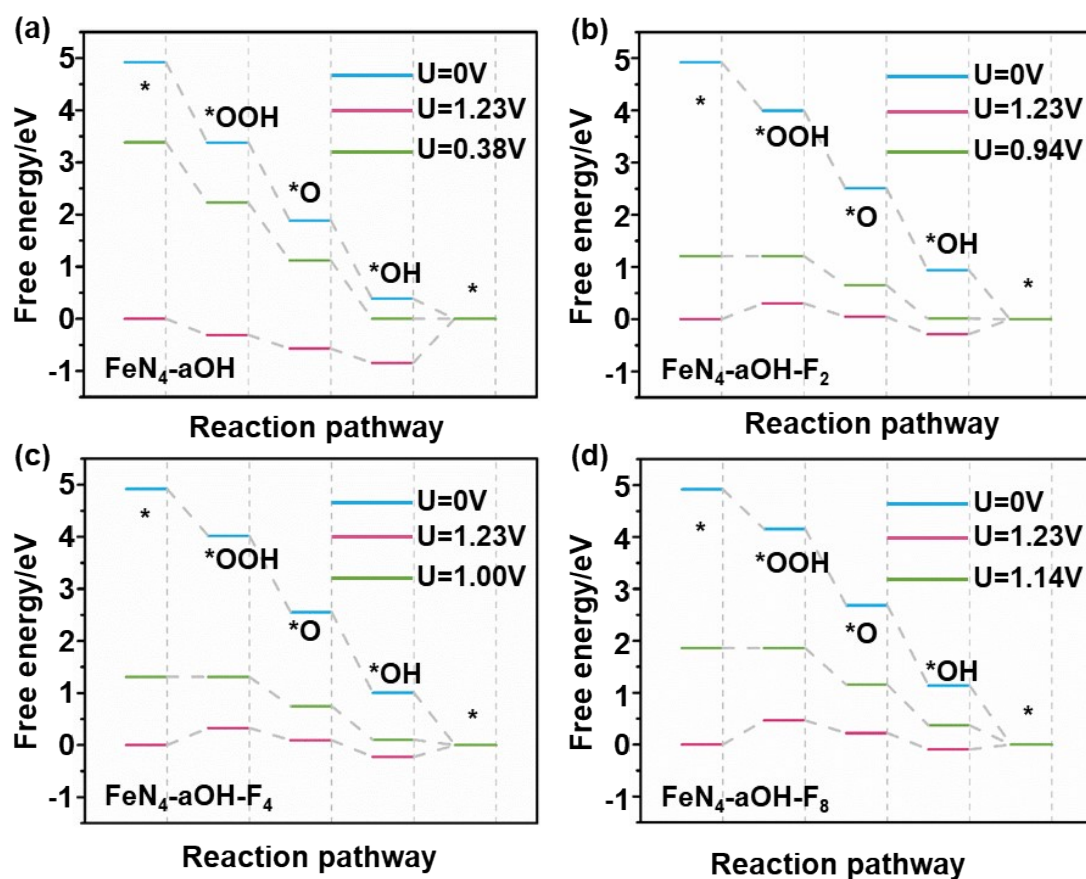


Fig. S14. The calculated free energy profiles of (a) FeN<sub>4</sub>-aOH, (b) FeN<sub>4</sub>-aOH-F<sub>2</sub>, (c) FeN<sub>4</sub>-aOH-F<sub>4</sub>, and (d) FeN<sub>4</sub>-aOH-F<sub>8</sub>.

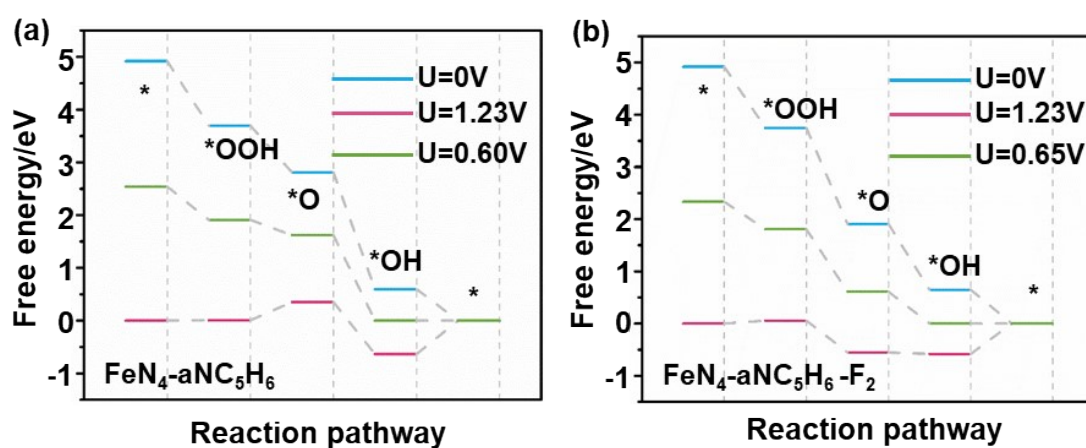
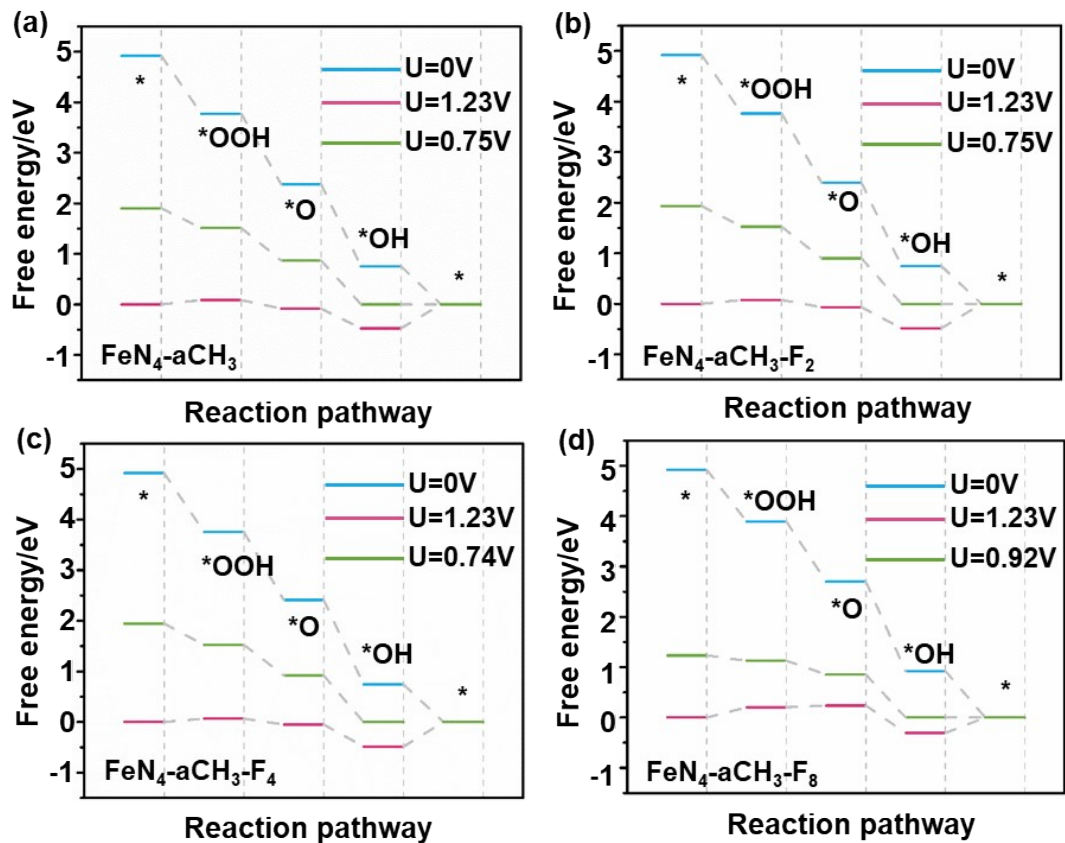


Fig. S15. The calculated free energy profiles of (a) FeN<sub>4</sub>-aNC<sub>5</sub>H<sub>6</sub>, (b) FeN<sub>4</sub>-aNC<sub>5</sub>H<sub>6</sub>-F<sub>2</sub>.



**Fig. S16.** The calculated free energy profiles of (a) FeN<sub>4</sub>-aCH<sub>3</sub>, (b) FeN<sub>4</sub>-aCH<sub>3</sub>-F<sub>2</sub>, (c) FeN<sub>4</sub>-aCH<sub>3</sub>-F<sub>4</sub>, and (d) FeN<sub>4</sub>-aCH<sub>3</sub>-F<sub>8</sub>.

**Table S10.** Atomistic coordinates for the FeN<sub>4</sub> structure.

1.0000000000000000			
14.7677999999999994	0.0000000000000000	0.0000000000000000	
0.0000000000000000	12.8094000000000001	0.0000000000000000	
0.0000000000000000	0.0000000000000000	29.9093000000000018	
H	C	N	Fe
8	50	4	1
Selective dynamics			
Direct			
0.3614874578597485	0.8532053488384181	0.6051812851464250	
0.6388356991611837	0.8532039146451907	0.6058762803205475	
0.2298454073044595	0.9306184531222649	0.6047905926518189	
0.7704922422937351	0.9306152174470235	0.6070500269676334	
0.3616387040893543	0.1465932203182481	0.6051414282187144	
0.6386215547529267	0.1465905245688319	0.6050062479622381	
0.2298766553726449	0.0690198882399831	0.6049095813913862	
0.7704434582252498	0.0689844967875420	0.6044894396065044	
0.0001599091573991	0.1114303676083475	0.6050446892472292	
0.0862582896340197	0.2776107343261685	0.6049808244206175	
0.0001564337164034	0.2226172347127238	0.6050164718773866	
0.0848882854278437	0.0567467643693434	0.6049832633764232	
0.1665017985717884	0.1121787970097745	0.6049400021181084	
0.2610556995319090	0.2756489791740910	0.6049136442444192	
0.1727233739474124	0.2209722490075989	0.6050291608276233	
0.4341602905935225	0.2951274432813351	0.6050139184560667	
0.3546350318365658	0.2313021921353831	0.6049587981774024	
0.5661596186711239	0.2951252899680061	0.6049947829461439	
0.7392564063904842	0.2756101789463767	0.6048174706723015	
0.6456955809490746	0.2312940896735662	0.6048696699054676	
0.8338110888217463	0.1121403928360533	0.6048066652407884	
0.9140410030802104	0.2775746495530267	0.6049532873576440	
0.8275967884978921	0.2209266164538524	0.6049311770434989	
0.9154445205529278	0.0567281931785166	0.6051044428773958	
0.0001253593278136	0.4440198678984696	0.6046580724580917	
0.0844255128106154	0.6111817899596156	0.6047237663486619	
0.0001137766608310	0.5556453090538146	0.6046515380737552	
0.0844513068732001	0.3885361965474190	0.6047225806174346	
0.1682127236083405	0.4442155826140550	0.6046091032327044	
0.2522529225690148	0.6130181646243985	0.6046917852231569	
0.1682032284051634	0.5555574304932198	0.6045966667114183	
0.2522783287751530	0.3867567954647844	0.6046818944772392	
0.3323387864017823	0.4442552754919724	0.6047046957820796	
0.3323402221431745	0.5555614682415615	0.6047353517674448	

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0.6679486723933249	0.4442429273394112	0.6047575274520880
0.7480447331365321	0.6129971704678948	0.6049301804701831
0.6679638100124494	0.5555540357020592	0.6048459108078063
0.7480162875812532	0.3867304188149617	0.6047071822809279
0.8320639134487785	0.4441791857567613	0.6046516843905855
0.9158269532396822	0.6111919580309063	0.6047906900653965
0.8320681507263746	0.5555448393077973	0.6047122508211260
0.9158190030549558	0.3884967290101174	0.6047313052744111
0.0001414486778941	0.7770914113163885	0.6051653250647802
0.0848605652172131	0.9429580836896694	0.6049439940454713
0.0001413547680416	0.8883123248259231	0.6050992408019411
0.0862212426166362	0.7220904093822708	0.6050221874453613
0.1726738096260182	0.7786991251758292	0.6050218120285779
0.1664595396330475	0.8874848854633360	0.6048801244218266
0.2610111169672252	0.7241041550897190	0.6049401961404616
0.3545418171770718	0.7684967306531827	0.6050626009213069
0.4341154482156677	0.7047261756306132	0.6051964958324865
0.5661933346672974	0.7047152433106793	0.6053521175333537
0.6457745235520019	0.7684937154441481	0.6055663675447307
0.7392852605218350	0.7240734058967515	0.6054477093004660
0.8276142440044186	0.7787064531839119	0.6056360478565774
0.9154438715065645	0.9429543296788175	0.6054113822472139
0.8338579316344974	0.8874945497989242	0.6060579498211445
0.9140374206516770	0.7221067512185623	0.6051802235979243
0.4166270092860338	0.6011928516282827	0.6051188420335248
0.4166397432236849	0.3986559329790193	0.6049851156977247
0.5836730560550483	0.6011857263194818	0.6051871491860286
0.5836552184830067	0.3986521780568591	0.6050186030623873
0.5001460539070495	0.4999251802367436	0.6052931781084172

**Table S11.** Atomistic coordinates for the FeN<sub>4</sub>-F<sub>2</sub> structure.

1.0000000000000000					
14.7677999999999994	0.0000000000000000	0.0000000000000000			
0.0000000000000000	12.8094000000000001	0.0000000000000000			
0.0000000000000000	0.0000000000000000	29.9093000000000018			
H	C	N	F	Fe	
6	50	4	2	1	
Selective dynamics					
Direct					
0.6349402448838481	0.8502847448611900	0.5989095264902222			
0.2296848353031179	0.9314702424817400	0.6033308642990177			
0.7704383974497112	0.9309369113177262	0.6035311215921447			
0.3667033702859406	0.1495414156240814	0.5986647930516189			
0.2304421377198460	0.0684303566089822	0.6036964868152735			
0.7710410883517922	0.0681912620013572	0.6032795988642917			
0.0006087445945074	0.1115076437482289	0.6030316334243575			
0.0872567250375219	0.2776467666490529	0.6027654022807398			
0.0005871844690342	0.2231207893880894	0.6027442562583590			
0.0855265672096492	0.0572309738659365	0.6031693455660790			
0.1672412864991309	0.1119419189872244	0.6032428946952646			
0.2629564606775110	0.2758197509737290	0.6039418609364716			
0.1741841055537474	0.2213129966668285	0.6029927185740943			
0.4370054873743865	0.2977688845696910	0.6083285765722497			
0.3581287566551765	0.2333802064910168	0.6032569614080343			
0.5618160970371474	0.2980784337195355	0.6084505281890820			
0.7384203744372789	0.2757509725805352	0.6039103017227818			
0.6424769188546782	0.2359448352100131	0.6034784458086782			
0.8339950811870580	0.1116118406740395	0.6030596098238810			
0.9139007348070037	0.2775176251353101	0.6027653850193688			
0.8269447443092570	0.2209712338246559	0.6028895902175390			
0.9157355165980270	0.0571675742002598	0.6031750310049058			
0.0005571798956800	0.4438297216353660	0.6028585422028760			
0.0853642750751779	0.6108917195992556	0.6030704521216652			
0.0004965719705169	0.5556900505023112	0.6029094283719614			
0.0854825565168722	0.3888482893288996	0.6029157259824721			
0.1695213102334936	0.4440467594982876	0.6038981317044754			
0.2538910379177062	0.6127207756845336	0.6057071154443057			
0.1694898792125864	0.5557778825807368	0.6039883430333506			
0.2538959146439585	0.3870183647011093	0.6054519063827167			
0.3339429619421094	0.4444225047749912	0.6102265316950326			
0.3339808610729053	0.5554015638030533	0.6103924150707405			
0.6669520976255876	0.4444766457397512	0.6103405928839709			
0.7472339418942677	0.6125765329587168	0.6057271778878300			

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0.6670946788482729	0.5554080230769483	0.6105090541319682
0.7469781782936928	0.3870495977107042	0.6054641488863084
0.8315209634367997	0.4438035504625532	0.6039049394270126
0.9155966391241094	0.6106829122618072	0.6030431337135848
0.8315608625393571	0.5554987678578863	0.6039830881496352
0.9156365794394691	0.3886622697612452	0.6029696780091415
0.0004034846669271	0.7764643126582994	0.6029625557596773
0.0850294080672322	0.9424734472047415	0.6032405749181377
0.0002192908550563	0.8881153206131353	0.6031873859257810
0.0870130561932165	0.7220267413630255	0.6029794221198382
0.1738438617046238	0.7787208119817896	0.6031656370222422
0.1667475462762349	0.8880725060129787	0.6032222377445431
0.2623189712453030	0.7240741823237908	0.6042691115360544
0.3581309889485179	0.7641937331126738	0.6038757613839962
0.4388140601134555	0.7020831887243103	0.6088398038409858
0.5644069939634904	0.7023239249735125	0.6087586973339392
0.6433217241212418	0.7664604391767724	0.6035960531355430
0.7383640596769777	0.7237265024863947	0.6042395530182515
0.8269739427095357	0.7781480439291055	0.6031399341093020
0.9153270865612687	0.9423783916889775	0.6032196520133138
0.8336987581614630	0.8875403921674657	0.6032402512080312
0.9138446785568822	0.7218833449015751	0.6029707812114351
0.4179941666020979	0.5995925343047649	0.6148428148753790
0.4180939271652688	0.4004401186539385	0.6145948955382600
0.5830205892726484	0.5996002532811153	0.6150005549466483
0.5828796926924491	0.4004881404664545	0.6146687724279470
0.3690427994394850	0.8693649437510026	0.5982658730024323
0.6312039970594980	0.1308622702054278	0.5979036714058887
0.5004575669692096	0.4999311445013881	0.6303326678088684

**Table S12.** Atomistic coordinates for the FeN<sub>4</sub>-F<sub>4</sub> structure.

1.0000000000000000				
14.7677999999999994		0.0000000000000000		0.0000000000000000
0.0000000000000000		12.8094000000000001		0.0000000000000000
0.0000000000000000		0.0000000000000000		29.9093000000000018
H	C	N	F	Fe
4	50	4	4	1
Selective dynamics				
Direct				
0.2297480894302532		0.9317694043515259		0.6028526280994453
0.7711475547590853		0.9318164223083123		0.6025067646722098
0.2297522297936182		0.0678358413384546		0.6027218614626667
0.7710894250728288		0.0678712891169620		0.6026258515321268
0.0004491750668724		0.1115992930631308		0.6028786769289791
0.0875098473633378		0.2771993470869730		0.6028626644834203
0.0004697726543409		0.2230674625116235		0.6027500040782168
0.0852052008335161		0.0575247989435946		0.6028695801631077
0.1667963736616583		0.1112898310841114		0.6027021801087842
0.2634775693201184		0.2753219074107202		0.6040215085804742
0.1741680148001680		0.2211545444541818		0.6027866512097845
0.4410116909124847		0.2973046617638775		0.6086178375303991
0.3592869105867181		0.2354136451165437		0.6035252167754194
0.5598307117494655		0.2973404129149598		0.6084718894206783
0.7373576808693847		0.2752745224078023		0.6038632241838887
0.6414836338199779		0.2353618508228104		0.6034037637052301
0.8340696523465987		0.1112753856674333		0.6026756614239249
0.9134118929873856		0.2772475353667002		0.6028534530691976
0.8267023480150444		0.2211469520782512		0.6027642457507895
0.9157037509542898		0.0575662020123660		0.6028877771046314
0.0004772173406910		0.4437412253054426		0.6031442850964601
0.0855729811891427		0.6105148292889201		0.6032734412547702
0.0004575824091572		0.5558702437628850		0.6031657074252492
0.0855758789392717		0.3890846431180752		0.6032824547995866
0.1697848168895370		0.4435263194230618		0.6045374971387528
0.2543971198662395		0.6128219514002873		0.6061065655236062
0.1697971949509833		0.5561452844144608		0.6044961170473235
0.2543989843875593		0.3869003314104647		0.6061693835861046
0.3342597812093435		0.4440311937501224		0.6113814292306381
0.3342465730933749		0.5557094809275968		0.6113526555331854
0.6666470391731693		0.4440604399128946		0.6109506076248422
0.7465127963638588		0.6128889343008599		0.6058509440961277
0.6666429238219468		0.5557048970915904		0.6109493830847416



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0.7465213437242014	0.3868608115108400	0.6058477975517014
0.8311402504057459	0.4435365013653704	0.6043265979568603
0.9153521309755766	0.6105058199722131	0.6032162485085247
0.8311281493935017	0.5561433094843233	0.6043341125990217
0.9153499336492479	0.3891037458367171	0.6032155407387907
0.0004243721773896	0.7765717377167958	0.6028203651755382
0.0851819226227696	0.9421060750245039	0.6029206747782059
0.0004162976689369	0.8880436994561884	0.6029596356759447
0.0874631194301327	0.7224022906323225	0.6028943153446508
0.1741245532933050	0.7784780415614703	0.6028580290353818
0.1667711798221515	0.8883487455015440	0.6028161685987971
0.2634547963165308	0.7244226700064810	0.6040187053687515
0.3593072859700243	0.7643714881350762	0.6035028317065281
0.4409940908761173	0.7023856825785819	0.6085839037627729
0.5598298547087347	0.7023882876385535	0.6084750676370265
0.6414858500924919	0.7644543663553123	0.6033936208481329
0.7373647348927962	0.7245072440473553	0.6038369380916395
0.8267337874792281	0.7785299657123157	0.6027272045204205
0.9157201490958286	0.9421525858170990	0.6028905525989212
0.8341335878224603	0.8883975489993295	0.6026478176660296
0.9134006771694300	0.7223838740628440	0.6028566161838759
0.4185440113844831	0.5992970155392326	0.6155635008428261
0.4185709525161085	0.4004228952088950	0.6156062212310586
0.5823432318647821	0.5992650800065682	0.6152679432073489
0.5823590590840237	0.4004665889266157	0.6152887447793175
0.3698039916315017	0.8692801328818563	0.5981369861010970
0.6307204114410100	0.1304978137661061	0.5981416598486368
0.6306761797499484	0.8693908941005682	0.5981554322566246
0.3697616402537204	0.1305272061569141	0.5981493670403130
0.5005540398564131	0.4998607980710360	0.6281864886204873

**Table S13.** Atomistic coordinates for the FeN<sub>4</sub>-F<sub>8</sub> structure.

1.0000000000000000			
14.7677999999999994	0.0000000000000000	0.0000000000000000	
0.0000000000000000	12.8094000000000001	0.0000000000000000	
0.0000000000000000	0.0000000000000000	29.9093000000000018	
C	N	F	Fe
50	4	8	1
Selective dynamics			
Direct			
0.0003114513162955	0.1112831053600628	0.6117276568948965	
0.0875630663883358	0.2761866850409470	0.6072075924071236	
0.0003866621607717	0.2224463229030400	0.6084933751058983	
0.0842159819812282	0.0557984087733535	0.6091886887383591	
0.1630401454298600	0.1113736806360431	0.5994623626377926	
0.2643881958804741	0.2737797119261070	0.6037850160153405	
0.1745891790010255	0.2205614165335672	0.6045605895632121	
0.4420016921999774	0.2976795760684350	0.5994778906201629	
0.3611726860011450	0.2350530545577481	0.6062258802355880	
0.5589672460046832	0.2977120026768537	0.5994228848525405	
0.7365150680263961	0.2737451464091682	0.6037104717971911	
0.6396980130224773	0.2350317052767376	0.6061240875085959	
0.8375771115685536	0.1113683900357319	0.5995801067902274	
0.9132854360925291	0.2762438186877045	0.6071387311491877	
0.8262275856492700	0.2206207049623515	0.6045153149946492	
0.9163525246427109	0.0557553804070331	0.6093043600129058	
0.0004969049178316	0.4427311840431976	0.6059421510103824	
0.0857863081880188	0.6095239974057678	0.6050188583394289	
0.0004664854782797	0.5550018153259044	0.6049006210434422	
0.0858204013763499	0.3881398430160145	0.6061647914114131	
0.1701778010889938	0.4424916191377173	0.6040008393955399	
0.2548998231634489	0.6122829377854238	0.6034415272390379	
0.1702169225272467	0.5552022400934867	0.6042570941390881	
0.2548053469491003	0.3855451610984306	0.6018122005560683	
0.3342916374255667	0.4430727203553286	0.5960714742096186	
0.3342990467721247	0.5547005965686456	0.5970729565566795	
0.6667306132657236	0.4430727738142221	0.5961755340952670	
0.7459628958443264	0.6122173883100169	0.6036823961393388	
0.6666241487170445	0.5546588073567136	0.5972655046004259	
0.7461869912199128	0.3855242669920123	0.6018266777187679	
0.8307720333332114	0.4425085039048877	0.6040236950088970	
0.9151270890747811	0.6095147219255290	0.6050816084115674	
0.8307173788546542	0.5552074556885479	0.6043678371365674	

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0.9151203095896306	0.3882102346340027	0.6061148778054855
0.0004006012121000	0.7750604344248126	0.6066939512050298
0.0840426462533011	0.9413777635170699	0.6098080364375471
0.0003259669300250	0.8862429432473964	0.6059773119224477
0.0875931831231943	0.7213765017114268	0.6065803665005539
0.1746302195147181	0.7766029834271797	0.6108710450619714
0.1624914592144842	0.8848222660735905	0.6191661745037262
0.2647001066969324	0.7238419639982353	0.6077471227369554
0.3613930561757177	0.7630720623335280	0.6067805603991403
0.4422348609927201	0.6997096842223240	0.6011419952795242
0.5587569584234459	0.6996545063138188	0.6012285706022519
0.6394415865124267	0.7630829209652147	0.6069131355990238
0.7361374841074366	0.7237692169841897	0.6079658836199880
0.8262015700495877	0.7764265163468111	0.6110349323622181
0.9165576272653140	0.9413002437506690	0.6099322453691628
0.8381823532584056	0.8846215945399362	0.6193065842510780
0.9132518278456785	0.7213220757693012	0.6066548990930948
0.4189093854057614	0.5974459009239490	0.5931796572805237
0.4185895290863519	0.3999809149721852	0.5906845265729772
0.5820446238467682	0.5973999851667997	0.5933061834890656
0.5824083580479725	0.4000228776296719	0.5907344795883597
0.3752960383652614	0.8670789195512144	0.6093787870801590
0.6264409011944736	0.1335334475327272	0.6165541775080224
0.6252077919575956	0.8670609209030570	0.6093791537444587
0.3742019010462990	0.1336091671811207	0.6168353853717232
0.2311404892640813	0.9346151575717598	0.6401199402110753
0.7692195950281627	0.9342538244089749	0.6400861026018947
0.2331873161759251	0.0596742500606111	0.5804197107013588
0.7671533048192527	0.0597679009662204	0.5807240091578036
0.5005170750345918	0.4993676777954179	0.5784314176081599

**Table S14.** Atomistic coordinates for the FeN<sub>4</sub>-aO structure.

1.0000000000000000				
14.7677999999999994		0.0000000000000000		0.0000000000000000
0.0000000000000000		12.8094000000000001		0.0000000000000000
0.0000000000000000		0.0000000000000000		29.9093000000000018
H	C	N	O	Fe
9	50	4	1	1
Selective dynamics				
Direct				
0.3670748737470889		0.8498427031217995		0.6109479863617292
0.6333724515870522		0.8499953328846407		0.6102598436959922
0.2303707456054654		0.9308246926446154		0.6042694075454883
0.7699306397636850		0.9306738904469867		0.6045301786976133
0.3671459105460273		0.1499794794606230		0.6095221089445191
0.6328326056975607		0.1501544310908095		0.6103533231804363
0.2303277787531889		0.0690205511604142		0.6042303097096433
0.7698392619560745		0.0689332651528618		0.6040224153767719
0.4554354477524787		0.5604549785979740		0.5042836233455621
0.0000983474177935		0.1114808406057678		0.6056790699725338
0.0869930264415921		0.2777892483635840		0.6077031110033286
0.0000804365810076		0.2228279269587867		0.6070033763052133
0.0851074829177830		0.0568662518487556		0.6050875574888835
0.1671457395630776		0.1125895900631763		0.6052556682692006
0.2639441753113759		0.2764015978738705		0.6067075684818916
0.1741363693503322		0.2212243748759671		0.6068122007580382
0.4392692384084237		0.2984123114661238		0.6031961407916316
0.3589275577880581		0.2343713109347808		0.6067179724783989
0.5610088715641345		0.2982531218159625		0.6027625133570518
0.7363956557393228		0.2763139311294104		0.6064156320211379
0.6411113352525433		0.2343712409082474		0.6067917922361382
0.8330272145831338		0.1124855143391079		0.6052053668782369
0.9132054187645476		0.2777602746568162		0.6076444816483400
0.8259689445778728		0.2212253575655733		0.6066983760840452
0.9150022413017830		0.0568438694528101		0.6051101957596045
0.0001131925851734		0.4440595446752806		0.6094018275021155
0.0852778304088553		0.6110246274280802		0.6089760144473594
0.0000887367097054		0.5556865434412006		0.6094633286649853
0.0852488688272764		0.3887762930026271		0.6088397025153749
0.1697873035761061		0.4442113815455803		0.6082911484329804
0.2545378769136561		0.6127946996663228		0.6067041382970728
0.1697448077284277		0.5555911079904049		0.6083641572934064
0.2545755084105736		0.3871295677544549		0.6066705789967985
0.3350062316507498		0.4448303291978362		0.6030817664918122

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0.3348766939328001	0.5552707183776394	0.6029226450735147
0.6653097989631706	0.4447125696976798	0.6022053458855643
0.7456750179787029	0.6126921965779503	0.6066712522497050
0.6652420442633868	0.5551560099393489	0.6028499177917618
0.7455996415855584	0.3871132546354245	0.6061341401085778
0.8304291804160979	0.4442084387038746	0.6081090249495253
0.9149670926637625	0.6109502081460620	0.6089382219443149
0.8304435967459646	0.5555740577526515	0.6082391538286466
0.9148965672109318	0.3887692511053634	0.6087855670927160
0.0001600675024670	0.7769689176593382	0.6071155212179359
0.0851482028853490	0.9429755858618092	0.6050850078976624
0.0001352518351887	0.8882980442272406	0.6056846330204710
0.0870319813149589	0.7220399187207119	0.6078341603041815
0.1741665098881225	0.7786499556064949	0.6069653603881158
0.1671515358172956	0.8873238761960871	0.6053342319047749
0.2637914454777950	0.7235895063486343	0.6069517669029392
0.3589689525790211	0.7655978341996964	0.6073900769112983
0.4393594329371073	0.7018766066242507	0.6035088306853361
0.5610063825116202	0.7016282167135107	0.6037310640003638
0.6414750324922143	0.7656207626747406	0.6072449293964739
0.7364442663989861	0.7234726152710464	0.6070169549213380
0.8262070892229204	0.7785232287980381	0.6070580784376938
0.9150891325035388	0.9429333573939344	0.6051552196023954
0.8331430242679423	0.8871693931402799	0.6054927220949664
0.9133133738943738	0.7219597916017597	0.6078444056298351
0.4191956361791717	0.5985807123414026	0.5977287174323890
0.4193447983495420	0.4017314325289048	0.5984381683938850
0.5808621685988389	0.5984763890453014	0.5987240548642531
0.5810477330563589	0.4013989631599305	0.5968903743778569
0.4963048847470248	0.5085203233297971	0.5168486216651463
0.4998213359978734	0.5005616814998448	0.5779319479930071

**Table S15.** Atomistic coordinates for the FeN<sub>4</sub>-aO-F<sub>2</sub> structure.

1.0000000000000000					
14.7677999999999994		0.0000000000000000		0.0000000000000000	
0.0000000000000000			12.8094000000000001		0.0000000000000000
0.0000000000000000			0.0000000000000000		29.9093000000000018
H	C	N	O	F	Fe
7	50	4	1	2	1
Selective dynamics					
Direct					
0.6328860386029869		0.8502993950154195		0.6102849122902764	
0.2292241256992942		0.9319206099606925		0.6050181637423350	
0.7700331838199068		0.9313058295068728		0.6043343762808446	
0.3670800129784322		0.1498037087677092		0.6097522406465926	
0.2299069551643981		0.0685958528492133		0.6041994356134099	
0.7706645410286481		0.0682810732179021		0.6045559543377620	
0.4581762596125237		0.5570202043209626		0.5034795221877160	
0.0001700907201632		0.1117408606539597		0.6054250233039582	
0.0870542214144711		0.2776062110011122		0.6076249674932518	
0.0000549274536113		0.2231962113541602		0.6068420350159027	
0.0850845759342496		0.0577004569660247		0.6049071132549055	
0.1667324387525740		0.1120617294690039		0.6051548420310819	
0.2631756629914230		0.2763292176885422		0.6067480755660334	
0.1738432228818295		0.2217093872097070		0.6067578046145042	
0.4384604632428662		0.2981524750290978		0.6030778770936300	
0.3587315401699105		0.2341068232594407		0.6067772063600662	
0.5593480911062265		0.2982600318293337		0.6029683167618951	
0.7373469969766761		0.2761303070811292		0.6066681229479765	
0.6405237551371497		0.2362247403475679		0.6065058730948960	
0.8336160527981002		0.1116680842487313		0.6052144064485686	
0.9131227717516054		0.2775378674742899		0.6076166666030703	
0.8262560060599742		0.2214227900016549		0.6067436338854517	
0.9151926369436051		0.0575942200261747		0.6048755290445357	
0.0001037178868507		0.4441530974119152		0.6093846792198081	
0.0853412633983348		0.6108996415324593		0.6089809537439187	
0.0000571221844250		0.5558611832860484		0.6094524972360315	
0.0853701732553852		0.3893272380695222		0.6088352362326207	
0.1695268609056574		0.4439985107483496		0.6084393182885012	
0.2544104487597857		0.6129966292792696		0.6067957030354546	
0.1695265828813974		0.5562610729634252		0.6085152232201256	
0.2542555901357823		0.3871771954767998		0.6067739939423615	
0.3347148454530929		0.4447808993353514		0.6028495987575511	
0.3347388736091626		0.5553258620408443		0.6027944958576907	
0.6653682978858458		0.4447793258178144		0.6029749050474431	

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0.7458500322759167	0.6128233518407200	0.6069228003655318
0.6654480319625306	0.5552000352844172	0.6032114838139322
0.7457003868107892	0.3871264860250645	0.6067537403032455
0.8306424381169212	0.4438176425081676	0.6084326129393799
0.9148107778139798	0.6106840060310152	0.6089676398236368
0.8306349409352527	0.5559950521940071	0.6084863466687348
0.9148215704314643	0.3891591270894549	0.6088346212421586
-0.0000494859694279	0.7768889586622224	0.6070443301115847
0.0846740284948000	0.9424559939071501	0.6050112027474521
-0.0001905717152216	0.8883375783142555	0.6055376866977561
0.0869492131864458	0.7225900610960094	0.6078237141207157
0.1737581622456159	0.7787823154171540	0.6069793725980589
0.1663347011430619	0.8884486094839830	0.6055295690925176
0.2627937115977200	0.7239928011407556	0.6068398931807373
0.3594649988912628	0.7637894419550669	0.6066252001965109
0.4408562984556946	0.7018760872880553	0.6031424071576021
0.5614830145122441	0.7018631675474365	0.6034923695720881
0.6411948513209441	0.7660142773964632	0.6071498533392484
0.7368991111577944	0.7237183235849608	0.6070193543643319
0.8261465187679862	0.7781757892321957	0.6069903955307715
0.9148041079522773	0.9423334224729495	0.6049334532096430
0.8332598409966342	0.8878953751643339	0.6052835990941992
0.9130319972189973	0.7223704469162848	0.6078390635597603
0.4190032932393368	0.5983370914834761	0.5976931963046673
0.4188852759956077	0.4017988494636397	0.5979490076121052
0.5811126803612194	0.5982436522278192	0.5985366978989518
0.5810785612905157	0.4017279865772871	0.5979028701783000
0.4990385844657416	0.5065208032415187	0.5170690875693134
0.3697283728216589	0.8693992032621625	0.6102121827927423
0.6302897810443213	0.1306063195422098	0.6101502870609552
0.5001864265815433	0.5003400004092450	0.5781422576532149

**Table S16.** Atomistic coordinates for the FeN<sub>4</sub>-aO-F<sub>4</sub> structure.

1.0000000000000000					
14.7677999999999994		0.0000000000000000		0.0000000000000000	
0.0000000000000000		12.8094000000000001		0.0000000000000000	
0.0000000000000000		0.0000000000000000		29.9093000000000018	
H	C	N	O	F	Fe
5	50	4	1	4	1
Selective dynamics					
Direct					
0.4608368471089862		0.5695234877788243		0.5049808528950859	
0.2301893801015499		0.9309074357760143		0.6055360667208703	
0.7712651565841750		0.9307904344882525		0.6054588579279173	
0.2302288474466170		0.0671597633634756		0.6052267554077442	
0.7711748819217386		0.0670815675665481		0.6050537442808984	
0.0007329927314156		0.1108051612632605		0.6054637757923249	
0.0877038370496641		0.2765700816236645		0.6071337093808338	
0.0006071329092693		0.2223077779363573		0.6065334282905721	
0.0855243909954870		0.0566683863241207		0.6051863094202424	
0.1673198548997731		0.1106266733224880		0.6055571167029208	
0.2636984936741410		0.2753148331683061		0.6064893824867311	
0.1745604112671453		0.2202691240540858		0.6065798544672971	
0.4414852681173754		0.2975972707966039		0.6030578737149747	
0.3601299450840748		0.2352692637534267		0.6064441657114018	
0.5597211287616792		0.2976043923197573		0.6026696395145431	
0.7376861836667730		0.2752346176551572		0.6061768298260175	
0.6408118556764140		0.2352819674120654		0.6061999716631900	
0.8341148065096692		0.1105584658042056		0.6054565434938267	
0.9135630319082803		0.2766279725795305		0.6070901736650183	
0.8266632048681626		0.2203594690884663		0.6064521928244784	
0.9158269846240750		0.0566201655649756		0.6051345381667965	
0.0006653708987888		0.4431390219990052		0.6085662761749480	
0.0860195061071270		0.6098446949741919		0.6083517763293128	
0.0006471156992615		0.5548445648785660		0.6087351720046829	
0.0860359653032257		0.3882175923954526		0.6080698318892429	
0.1702366375854079		0.4429859885351097		0.6078027367542471	
0.2551080337494686		0.6121307724997032		0.6067094676187526	
0.1702270786560702		0.5552368491708050		0.6079729877443206	
0.2551073303052968		0.3862562247750383		0.6064739501443600	
0.3355712252585002		0.4439438324999213		0.6030647356721478	
0.3354738008624488		0.5545541579903405		0.6031382284109756	
0.6657750102619019		0.4439756933323828		0.6024539257825992	
0.7461435754927430		0.6121021595946357		0.6066825652066259	
0.6657862722295831		0.5544764525247464		0.6030078580996852	



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0.7460877271755915	0.3862520221515375	0.6061474925011148
0.8310230793870402	0.4430113879501769	0.6078600179235166
0.9153540043693035	0.6097984158082508	0.6084723870642937
0.8310426570647697	0.5552171786328637	0.6080595104850222
0.9152238053124890	0.3882521881050403	0.6081262278682523
0.0006699809582353	0.7758434005557374	0.6069364093748550
0.0855199875211133	0.9414558798233342	0.6052921408744907
0.0007214829039615	0.8872980520239181	0.6056709723607977
0.0876807412778609	0.7214982080896394	0.6075227468757854
0.1744946253999572	0.7778005941790134	0.6069728663155981
0.1672366459732085	0.8874831672210275	0.6057916643065652
0.2635494666979255	0.7231129211145071	0.6068729165013992
0.3602088222147316	0.7632918020486882	0.6069581172202598
0.4415371448233309	0.7011432687943314	0.6035523296551001
0.5598711192901303	0.7009404312968615	0.6036415731169406
0.6411793089478102	0.7633873272215695	0.6069385178963532
0.7377496892778646	0.7231083966845028	0.6069228695389993
0.8268703841009162	0.7776886424480868	0.6070716774505763
0.9158798953595926	0.9414164740551201	0.6052545769277464
0.8342296241111963	0.8873785340676492	0.6058257904028708
0.9137134973295065	0.7214166813357485	0.6076583882800285
0.4195688407165634	0.5975987703469149	0.5983959731110201
0.4196260558754240	0.4010860734233536	0.5984509832321233
0.5815754462922088	0.5975179723693618	0.5987225238231044
0.5815923488451217	0.4011053979858343	0.5973288359544106
0.4947521965291808	0.5111500778923583	0.5173909673334532
0.3703835094957198	0.8684889104601889	0.6106628781404886
0.6304991617699094	0.1302540258178804	0.6101639342911509
0.6308249615879187	0.8686867424692178	0.6105890692928554
0.3700658634326343	0.1301267678055005	0.6101567366857286
0.5002833676425109	0.4999829710122849	0.5782036110095279

**Table S17.** Atomistic coordinates for the FeN<sub>4</sub>-aO-F<sub>8</sub> structure.

1.0000000000000000					
14.7677999999999994		0.0000000000000000		0.0000000000000000	
0.0000000000000000		12.8094000000000001		0.0000000000000000	
0.0000000000000000		0.0000000000000000		29.9093000000000018	
H	C	N	O	F	Fe
1	50	4	1	8	1
Selective dynamics					
Direct					
0.4624452476629722		0.5590735573407870		0.4976871418038394	
0.0003988608852319		0.1117125497843047		0.6115699938082748	
0.0876667204521038		0.2768540586832847		0.6083891450860139	
0.0004309734033906		0.2229350814558227		0.6091430181038400	
0.0844373713424125		0.0562486150328280		0.6093237485191610	
0.1635356684893292		0.1122334002083117		0.6000871594492851	
0.2645414334905838		0.2753209034026334		0.6045411383278787	
0.1748253419656675		0.2211979158570802		0.6054027663652126	
0.4423226740214419		0.2997235266085266		0.6000405942553036	
0.3620207123723263		0.2368386512887218		0.6065837729723202	
0.5586065876173075		0.2992294196482509		0.5997704171984271	
0.7365802054793013		0.2749230136370216		0.6039926924846497	
0.6387354995547238		0.2360793397186539		0.6058886166763293	
0.8375336945871378		0.1121072752975075		0.5991327297008733	
0.9132502671800755		0.2768773330569195		0.6080726731414036	
0.8260830622312801		0.2212170961770142		0.6046819980572791	
0.9162551024175821		0.0562071445173022		0.6088574443857220	
0.0005406107086348		0.4433887969575216		0.6082657249117596	
0.0861431980903951		0.6099962319517536		0.6069557789213875	
0.0004859218547858		0.5551338527188927		0.6070916360404918	
0.0861437529185302		0.3886374023596042		0.6080804000015996	
0.1704787927605954		0.4432997909514992		0.6059594824426763	
0.2556132700967427		0.6128271907148340		0.6049527427112303	
0.1705437008616383		0.5555602972178747		0.6062726872296392	
0.2553894916852487		0.3863285718798819		0.6033282041072597	
0.3351927435753077		0.4443833129720465		0.5976304922622379	
0.3351167278259258		0.5548941144168194		0.5981938094187765	
0.6658587182127611		0.4440504743142372		0.5980503145875911	
0.7452266331484038		0.6125727883987173		0.6053640632406465	
0.6655520255174914		0.5544897035386382		0.5994684533013078	
0.7455645033494626		0.3860546823230845		0.6033694692198927	
0.8304950083254521		0.4431994302868433		0.6060616306642769	
0.9148265346198005		0.6099079236382621		0.6069577104716266	
0.8303604296022181		0.5554636138974597		0.6064052256939142	

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0.9148084233136281	0.3886134645304531	0.6080273175518771
0.0003666896054353	0.7754561769027194	0.6078170671524710
0.0842178795587132	0.9418370122585862	0.6102595203064232
0.0003578464890589	0.8866154309874861	0.6065783583961480
0.0876485933465674	0.7216578651879411	0.6080485660012853
0.1748578106733162	0.7770722649135993	0.6121494095379417
0.1626947614450359	0.8853321710697717	0.6199451962983822
0.2648973796498614	0.7236816979663969	0.6090270043409258
0.3626555714871619	0.7624330097389790	0.6080150720861667
0.4427725540475461	0.6991944121880342	0.6016224513242947
0.5580723051678156	0.6989781098757056	0.6022433061389262
0.6384302886481991	0.7627735199865892	0.6071968418245068
0.7358434715586510	0.7235861524793362	0.6087781118883909
0.8258424145703698	0.7770386544387223	0.6116613857642903
0.9163967379212540	0.9418587367375908	0.6097772986299305
0.8376263814392542	0.8854917859071433	0.6190616037340105
0.9131319433410032	0.7215842931356977	0.6079026746728668
0.4195104322564416	0.5971508312078940	0.5929279465329332
0.4194039338182280	0.4020360986903793	0.5919308166792371
0.5809546144729357	0.5964863563167884	0.5955535296107716
0.5817651949779404	0.4015737494485410	0.5917104756076654
0.5052459294127822	0.5114559004020098	0.5117359071654577
0.3771565874179001	0.8658453208965494	0.6124148791440546
0.6262278983311497	0.1343796959597278	0.6160753873071650
0.6244412922072252	0.8667211106544787	0.6091751806574032
0.3750369522991656	0.1357459272832550	0.6175066995547740
0.2312275682596247	0.9357454159278344	0.6408394645451210
0.7683538233286884	0.9365043069664009	0.6390881670388809
0.2341077981561336	0.0605255758810904	0.5813739694236248
0.7674657710594023	0.0607289493194103	0.5798433823838181
0.5009336654332653	0.5006099424879332	0.5726751331381328

**Table S18.** Atomistic coordinates for the FeN<sub>4</sub>-aN structure.

1.0000000000000000			
14.7677999999999994	0.0000000000000000	0.0000000000000000	
0.0000000000000000	12.8094000000000001	0.0000000000000000	
0.0000000000000000	0.0000000000000000	29.9093000000000018	
H	C	N	Fe
13	55	5	1
Selective dynamics			
Direct			
0.3672939798349400	0.8487341711926063	0.6130192316354923	
0.6345000856581959	0.8491692849237964	0.6119787545457083	
0.2308997399471945	0.9301064881040881	0.6099068758846733	
0.7707112312616343	0.9300509607869266	0.6094951728985860	
0.3676172755817578	0.1503152820669230	0.6154003501251769	
0.6338409519960240	0.1495643423143237	0.6145550720651169	
0.2310103124506945	0.0684495254651967	0.6107508586278652	
0.7706479312901540	0.0682430406616406	0.6107435473318789	
0.5224484068937603	0.6627531523238157	0.4290727218368648	
0.5209880962132932	0.4922388981124243	0.3866372661869802	
0.5093958581076704	0.3252249132658241	0.4312208202119437	
0.5006490135534594	0.3352230737523246	0.5141082889434119	
0.5128434292873539	0.6594305791813551	0.5120286043987218	
0.0008444173466407	0.1107999954868817	0.6105830774427247	
0.0877009434302210	0.2769136107125008	0.6101896340190351	
0.0007771342296237	0.2220737094809553	0.6104961001405224	
0.0858925665698236	0.0562972191209963	0.6106150683298665	
0.1677061440955986	0.1117635560575966	0.6107541261195905	
0.2642507708401827	0.2756286581688455	0.6087435890829119	
0.1747469308992127	0.2207214896256024	0.6104003354547481	
0.4394393104337926	0.2971732751599062	0.6036334413203107	
0.3593452137063220	0.2338956757202533	0.6096221159071462	
0.5619503278899628	0.2970589332079461	0.6041761688645353	
0.7371845729981180	0.2753139242128516	0.6092748398042818	
0.6420539151567620	0.2334803208169204	0.6096800823168551	
0.8339265034341961	0.1116083315452278	0.6107320018199252	
0.9138792400727191	0.2768106173128392	0.6103916154409719	
0.8267639150352110	0.2205144342834929	0.6105835131366526	
0.9158149879647093	0.0561992838133832	0.6105629307780687	
0.0007757479821194	0.4432991635305611	0.6098492250450007	
0.0857995017279015	0.6102271150721523	0.6088751840629391	
0.0007804551906868	0.5549679698975821	0.6094922475980880	
0.0858564825812609	0.3881482683850051	0.6095664719623598	
0.1701003969011341	0.4434225502938409	0.6076765318037755	

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0.2548087744414660	0.6120812885805925	0.6050827324275174
0.1700920063471572	0.5549919755012542	0.6073394150917405
0.2548959756814359	0.3864021302242606	0.6058180569420346
0.3345139672327402	0.4438393359638514	0.5998915922160571
0.3344651692408176	0.5545324215069860	0.5995277780657798
0.6669483791854272	0.4437947869760240	0.6020280823013416
0.7467676739276617	0.6119960374217458	0.6063831856219869
0.6670053075271123	0.5543567878808324	0.6015697357779444
0.7466437422495928	0.3861509498822365	0.6071848200031658
0.8314574039204353	0.4432739074673779	0.6087509170875229
0.9157519356282480	0.6101645003253285	0.6092556444228597
0.8314813888021740	0.5548545010563416	0.6083753439847639
0.9157535106292422	0.3880182040220549	0.6099728650922625
0.0008339601914285	0.7762498408550377	0.6094882664569816
0.0858452159402340	0.9421472620299535	0.6102984254918613
0.0008241079949955	0.8875354285957215	0.6100254832941406
0.0876547705099551	0.7214341372270124	0.6090775950987317
0.1746602477935440	0.7777345513827345	0.6091768557642551
0.1676318923106143	0.8867080766717484	0.6099776039743872
0.2640742441429148	0.7229232330082227	0.6074263825636254
0.3590624222437790	0.7648872911213379	0.6079369824963087
0.4391081651229682	0.7014647945256679	0.6023434649633108
0.5623375337988485	0.7015380891714088	0.6027744072995542
0.6425258257008956	0.7650283528563743	0.6077810486770135
0.7375422865829813	0.7228743266035755	0.6077294647937069
0.8269545794745884	0.7776574573852147	0.6091858315073999
0.9158357638200962	0.9420605694497515	0.6101663422537129
0.8339670664944366	0.8866426509623039	0.6097239237481707
0.9139659552585837	0.7213745119751587	0.6092509326063189
0.5177580796639932	0.5880577232926312	0.4464014975633827
0.5168467825163349	0.4936744511625403	0.4230010399489599
0.5104577714187928	0.4012076970900667	0.4476176592171148
0.5055043442253087	0.4058374956583376	0.4939255251481103
0.5124911713723466	0.5871930087241832	0.4927490915597687
0.4193276766559154	0.5983254293526638	0.5945941020115876
0.4194294762459844	0.4000459166493784	0.5951532734955267
0.5822672464050320	0.5980796671555654	0.5960971238701159
0.5821527173339016	0.4001998005568446	0.5968255310392158
0.5065512843311218	0.4974506024947397	0.5167821774335977
0.5013423870745664	0.4989779931763499	0.5812949335454252

**Table S19.** Atomistic coordinates for the FeN<sub>4</sub>-aN-F<sub>2</sub> structure.

1.0000000000000000				
14.7677999999999994	0.0000000000000000	0.0000000000000000		
0.0000000000000000	12.8094000000000001	0.0000000000000000		
0.0000000000000000	0.0000000000000000	29.9093000000000018		
H	C	N	F	Fe
11	55	5	2	1
Selective dynamics				
Direct				
0.6343423322908277	0.8496941612676905	0.6115698411701902		
0.2301080835850970	0.9309985050148419	0.6100313544289401		
0.7712539047918295	0.9307331370581964	0.6094467971841743		
0.3677864376930140	0.1489923200446589	0.6140060289707312		
0.2308521661010325	0.0674472818289928	0.6105478834992111		
0.7719726703863504	0.0670500174137927	0.6102364793752606		
0.5210092802385530	0.6640960814330907	0.4304657434608039		
0.5210606602187624	0.4941953624075237	0.3877902778129849		
0.5095526802800913	0.3265136536377915	0.4317088303501190		
0.4997915393450561	0.3354152007833774	0.5148637642675609		
0.5101966537654258	0.6595014431968067	0.5136503735585640		
0.0012469850661354	0.1107839598399689	0.6102042417460980		
0.0881607799854666	0.2763925809333163	0.6095428645700043		
0.0010288904454685	0.2221882970249185	0.6098174503030337		
0.0861845430883422	0.0568442480623800	0.6104429338973939		
0.1676389392219769	0.1109233202017205	0.6104670193710371		
0.2643557066667986	0.2749538237149816	0.6083489065385055		
0.1748907444097917	0.2209230502362268	0.6098276159931622		
0.4400608584960651	0.2962785684075009	0.6038121331004609		
0.3596481948080312	0.2328666597657904	0.6090506971243856		
0.5595322317920414	0.2966432652488583	0.6040929669097205		
0.7378720954469303	0.2746663136982088	0.6082748039834648		
0.6415310193697454	0.2350929699516526	0.6078573874731913		
0.8348898528728219	0.1105163424558964	0.6100566871168023		
0.9139181171426214	0.2762917293244900	0.6094794947341909		
0.8272162287564854	0.2204061158975648	0.6094281500285827		
0.9164135408765873	0.0567867804305059	0.6102225925729847		
0.0009780023087706	0.4430436976224293	0.6091562139157242		
0.0861939932893941	0.6097764561574234	0.6084164323585840		
0.0009868603284083	0.5550095420935732	0.6089521068393815		
0.0862055027750340	0.3884316288851051	0.6089407040226439		
0.1702575130573680	0.4428396964108430	0.6075385659030506		
0.2552636264196980	0.6119629272138115	0.6055908029758044		

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0.1703343693768084	0.5555173689048656	0.6072771978008075
0.2550203850277543	0.3861168224007469	0.6060543296365862
0.3349406228326457	0.4434960422491761	0.6011081336326810
0.3350529041231166	0.5542484717085745	0.6009987787559168
0.6669201370437935	0.4437582098548377	0.6028423130996046
0.7469831327250697	0.6120171900484992	0.6065304831417123
0.6671139977062227	0.5544132690464847	0.6023494586171549
0.7467242684800296	0.3860707833504616	0.6071352173879612
0.8316461765368750	0.4426146440442595	0.6083543532864281
0.9157756371614361	0.6096474139637041	0.6088576503123257
0.8316827953945541	0.5552875600295152	0.6081677957099622
0.9157824692898375	0.3883102422613684	0.6092294477977519
0.0009527310305190	0.7759265731606827	0.6092684407706960
0.0857020007825257	0.9412958000131001	0.6102024657135001
0.0008592585093591	0.8873501578039487	0.6099412659184096
0.0880229711397157	0.7217676955992957	0.6087635212936904
0.1747595770964417	0.7775639512988738	0.6088079897225791
0.1672068674404512	0.8875020165207432	0.6098553699270383
0.2640830913483798	0.7233185850387146	0.6072138273557047
0.3603885993623260	0.7628830265285235	0.6070649245236155
0.4423632594013706	0.7015192715906076	0.6028001868895864
0.5620201638504416	0.7018840466637393	0.6032460393844443
0.6424299649476445	0.7654854978544975	0.6077986290119278
0.7377504277096709	0.7232436699509927	0.6077169121144738
0.8271863846295453	0.7771361033964558	0.6091344406916545
0.9159325665777036	0.9412580773447261	0.6101258684240769
0.8344594810807260	0.8872199966854580	0.6097243558657446
0.9138654044949504	0.7216493728068558	0.6090490310838843
0.5163528499369213	0.5893304908855082	0.4476873559951322
0.5163561235311839	0.4951347521363734	0.4241514988316625
0.5100930655655971	0.4021503814992828	0.4483867394019403
0.5044903262402530	0.4061739081516818	0.4946934291369263
0.5102442682042366	0.5877192302677174	0.4940230891384323
0.4200305043814142	0.5975334424701876	0.5964065655980495
0.4197618496829640	0.4000855481815865	0.5964242012444707
0.5823419139196426	0.5976825556054823	0.5970741616030510
0.5819498776002053	0.4006527402790599	0.5981153989987512
0.5049075605143232	0.4975208966213665	0.5175138691449328
0.3709389861057020	0.8686059877244222	0.6110802539116962
0.6309436759927709	0.1291576911561922	0.6108778613759657
0.5013977179048453	0.4988153772375056	0.5826520021923368

**Table S20.** Atomistic coordinates for the FeN<sub>4</sub>-aN-F<sub>4</sub> structure.

1.0000000000000000					
14.7677999999999994		0.0000000000000000		0.0000000000000000	
0.0000000000000000			12.8094000000000001		0.0000000000000000
0.0000000000000000			0.0000000000000000		29.9093000000000018
H	C	N	O	F	Fe
9	55	5	1	4	1
Selective dynamics					
Direct					
0.2299749130332933		0.9307983023910219		0.6045745666247644	
0.7720783631282713		0.9306198472569619		0.6048159110314693	
0.2299670393419723		0.0671057765926171		0.6049354890981696	
0.7720759899952884		0.0670578823290732		0.6043919542597280	
0.5213208725160317		0.6648972403861814		0.4462314456803119	
0.5218777552932290		0.4955670728125496		0.4031312523153403	
0.5110968181512043		0.3275039262999491		0.4468332569853450	
0.5010048092303306		0.3355751865116275		0.5295128891575253	
0.5103606074875793		0.6590876845267536		0.5289669526115937	
0.0010608642913972		0.1105041933691397		0.6041971135997486	
0.0873202322506252		0.2764952631378825		0.6040584166751835	
0.0010437104677452		0.2220536066003675		0.6041819526432874	
0.0854334816213283		0.0560231022813948		0.6042853188700421	
0.1670771597106297		0.1104019432231806		0.6044485365226541	
0.2618174621563866		0.2739306518624975		0.6041290072766070	
0.1735504120732149		0.2194861701719502		0.6041752445409333	
0.4368882656322684		0.2945065158209709		0.6051654780729867	
0.3556817319457824		0.2316513607099178		0.6044210468066344	
0.5650653860719858		0.2945980359234250		0.6056861128648144	
0.7401979482908475		0.2738917433273001		0.6043538085265693	
0.6462222236436832		0.2316420706221650		0.6044387784799589	
0.8350048472774706		0.1103666164935630		0.6042342410120937	
0.9148003012194311		0.2764624799280152		0.6041598955267853	
0.8285361379230265		0.2194703508875964		0.6042000920475397	
0.9166763725746722		0.0560193651140810		0.6042030552597584	
0.0010685095753250		0.4428617188405813		0.6040265200880977	
0.0856764957443264		0.6100876006913604		0.6041585343367187	
0.0011117981528896		0.5548778109390783		0.6041149429587297	
0.0856419082324366		0.3877011924954294		0.6039426103934041	
0.1695387956033052		0.4429368626660807		0.6038018829471229	
0.2535281976376157		0.6120403826488607		0.6038955147818120	
0.1695850129417801		0.5548174464469727		0.6039313233770822	
0.2534565117440923		0.3856704813637403		0.6037992013344118	
0.3339932908467366		0.4426593510064710		0.6040333453286104	



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0.3340421565676553	0.5549928908457293	0.6039145876398101
0.6681705069416658	0.4426811754057494	0.6058524460627922
0.7487061158460954	0.6120565802032814	0.6046424504798285
0.6681878529258707	0.5549928465777677	0.6057615903373669
0.7486890778456522	0.3856748863677056	0.6045917021167851
0.8326445133178647	0.4429269556265371	0.6042561481308765
0.9165783651174211	0.6100794656703250	0.6042308578442098
0.8326695486110464	0.5548682673436446	0.6042992968797855
0.9165153133485311	0.3876634026606755	0.6041029798637366
0.0011315508030423	0.7756470098548035	0.6044165202996353
0.0854244390666782	0.9416979221126838	0.6043154868782787
0.0010364394898233	0.8872353124546815	0.6043300308228083
0.0873914840289614	0.7212069734534616	0.6043618633971042
0.1736395952467288	0.7782381760919268	0.6044264647822999
0.1671035167952799	0.8873864143153408	0.6043813697709371
0.2619354673507656	0.7237809458727925	0.6043851402047160
0.3558586100360907	0.7660297669756596	0.6049076771690260
0.4369442510339808	0.7030803042866608	0.6049595416764324
0.5651658332410819	0.7030999712067749	0.6056945309901463
0.6463301315699794	0.7660134109954650	0.6047423454781033
0.7402511039457822	0.7238011559853252	0.6045906117956046
0.8285731497549588	0.7782113554648933	0.6044511795231750
0.9166705326986698	0.9416853632582255	0.6042850029546833
0.8350073453070126	0.8873451471762345	0.6044646283659842
0.9148758394430003	0.7212169529199141	0.6043839191410323
0.5169738792727760	0.5898079310576715	0.4632008670370826
0.5172696713253390	0.4960828926896088	0.4395028160871743
0.5112164472212745	0.4030986446795870	0.4635366228482709
0.5055547129240883	0.4072617856266881	0.5100087602588947
0.5109249472874881	0.5869676534064018	0.5096538529145923
0.4163966427634581	0.6014119498826597	0.6041717582628164
0.4163326688834389	0.3962165904149672	0.6046917056508365
0.5857623415787745	0.6013581048258755	0.6063408687979541
0.5857266799075583	0.3962900784866550	0.6065944401982659
0.5055981668073127	0.4974538511471031	0.5330572616601302
0.4969187730351634	0.4997171600241234	0.6668816619178555
0.3660859571823777	0.8714710127918194	0.6058875782233196
0.6358821453193788	0.1260876257285141	0.6039455182045252
0.6362197486503692	0.8715429384753430	0.6042897454928814
0.3655991560995219	0.1260906268730742	0.6043115852584623
0.5008050956018448	0.4988242650848967	0.6106408925459550

**Table S21.** Atomistic coordinates for the FeN<sub>4</sub>-aN-F<sub>8</sub> structure.

1.0000000000000000				
14.7677999999999994		0.0000000000000000		0.0000000000000000
0.0000000000000000		12.8094000000000001		0.0000000000000000
0.0000000000000000		0.0000000000000000		29.9093000000000018
H	C	N	F	Fe
5	55	5	8	1
Selective dynamics				
Direct				
0.5224131720893824		0.6697451257573973		0.4295192745673401
0.5228775821796563		0.5010449767611193		0.3860086173366153
0.5121010086728628		0.3320828996672913		0.4290489859398139
0.5023303019640729		0.3385950891114851		0.5121751972052796
0.5118589933675636		0.6627291047209897		0.5127394445076381
0.0010678201403536		0.1102535668207150		0.6133613344975433
0.0883346702259882		0.2751199101708430		0.6101174989406216
0.0010554792355196		0.2213178228428749		0.6110989280851177
0.0849953768693616		0.0548898200961505		0.6103355146807941
0.1636715107960205		0.1107521951627499		0.6010598304075546
0.2651851291775989		0.2729053908272878		0.6065646953609313
0.1752390448975913		0.2197557232469586		0.6069789913641308
0.4432480806149492		0.2966881422417100		0.6029751143462168
0.3621235467453836		0.2340255234407766		0.6088371457415110
0.5586781493983404		0.2968461351820532		0.6034480519686134
0.7367564481173863		0.2728456658871187		0.6070789530382663
0.6397142653652673		0.2340148543430206		0.6088901140915436
0.8383689546581310		0.1108427193780283		0.6010745538950656
0.9137451509041730		0.2751280760178993		0.6102936263233741
0.8268107022679855		0.2197423804958915		0.6071645039638440
0.9171251976937477		0.0549716158646508		0.6102538722969245
0.0010638775755860		0.4417663062694132		0.6100046233316376
0.0865687889013057		0.6084411943540300		0.6082567898154441
0.0010698437977569		0.5538334276046137		0.6087149680169169
0.0865982871118143		0.3872719947720817		0.6097470132919961
0.1708453054819565		0.4415476186798943		0.6074426828902734
0.2559696018496960		0.6114825058563441		0.6065957426892781
0.1709577304189636		0.5543790893820744		0.6076009006338302
0.2556854074665588		0.3845212129037683		0.6051566436565143
0.3350836891953331		0.4425473781238316		0.6000256332669299
0.3351973120897964		0.5533077698941277		0.6008163228218287
0.6670068641840292		0.4425791476709903		0.6017296607799191
0.7461916912754040		0.6115234272373850		0.6076576793380848
0.6669262869109569		0.5532978445595644		0.6023713893454927

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0.7463938764144000	0.3844917400474535	0.6064102841718608
0.8312599762793837	0.4415566284200237	0.6084595113885242
0.9155783016803257	0.6084826638496719	0.6086071767354896
0.8312005581469956	0.5544114414335232	0.6085437922911913
0.9155753215225575	0.3872723018771818	0.6101580692486613
0.0010855741847598	0.7742012115690182	0.6088509064726840
0.0849130330925218	0.9404411558581859	0.6107560125915640
0.0011027595758110	0.8852631647758845	0.6072134816946011
0.0883316162006760	0.7204540737971777	0.6091216801680287
0.1753125685856030	0.7756896005975380	0.6129316666388090
0.1632145492761886	0.8841987204895987	0.6204289047374175
0.2656511805210678	0.7230026597411895	0.6101735425842063
0.3626798087599478	0.7619950374274718	0.6090461874133301
0.4436455128451610	0.6988832750826388	0.6038130182588846
0.5586584017496929	0.6990193765118656	0.6041162884734285
0.6397043578104040	0.7624114780180495	0.6086854357086626
0.7366018489319964	0.7231358718411596	0.6104227714677392
0.8268399109071711	0.7757908256855860	0.6129795801340786
0.9172118993870734	0.9405024447427934	0.6107730963051324
0.8388755089009926	0.8843014620192866	0.6205508735420504
0.9137891421929538	0.7205220893391775	0.6092110384027892
0.5181172247739826	0.5945002646452094	0.4463844058097950
0.5182251062137285	0.5009853898481326	0.4223762884564768
0.5122255051952724	0.4072551275811356	0.4461000607756145
0.5067071834694935	0.4099824264516621	0.4924081667629983
0.5122614637926569	0.5914943496539301	0.4927386287564182
0.4202760845543669	0.5957729719838821	0.5961785496315332
0.4199328718899109	0.3997646353297892	0.5945016613639247
0.5819838503431949	0.5956254225849075	0.5974012867906862
0.5822557661401646	0.4000331550218192	0.5958557073787494
0.5068227181490086	0.5006268664890210	0.5157065302110686
0.3767901353389644	0.8661300513609074	0.6115199239123267
0.6263966814084334	0.1316924596758686	0.6177749189768146
0.6259318839964022	0.8667457267861137	0.6095156793457672
0.3748802128982000	0.1320199616086989	0.6187305885750181
0.2323270548123237	0.9342968828770012	0.6409093475058817
0.7697596054255543	0.9344376695230949	0.6411697510165821
0.2338852938837169	0.0598431868257166	0.5816269828031124
0.7677812288655325	0.0599475238497305	0.5818688363526159
0.5015431502429040	0.4983260494337681	0.5809370687086225

**Table S22.** Atomistic coordinates for the FeN<sub>4</sub>-aC structure.

1.0000000000000000			
14.7677999999999994	0.0000000000000000	0.0000000000000000	
0.0000000000000000	12.8094000000000001	0.0000000000000000	
0.0000000000000000	0.0000000000000000	29.9093000000000018	
H	C	N	Fe
11	51	4	1
Selective dynamics			
Direct			
0.3674397131203208	0.8490741967159354	0.5987927081608813	
0.6334444823373697	0.8488783961643315	0.5981822708367509	
0.2303545540328379	0.9304885197250210	0.6026453089048277	
0.7710026666195062	0.9304400433947172	0.6019030007589389	
0.3674332763020804	0.1491558909206269	0.5986417842148049	
0.6334302366471475	0.1492389857633207	0.5985562960691205	
0.2302947267271301	0.0676507032568701	0.6021187808963544	
0.7707974481411903	0.0675574897784497	0.6024906877706832	
0.4976179356833708	0.5988161984682944	0.7040776804460662	
0.5602740490173137	0.4787432162547214	0.7091537481764794	
0.4378514265862476	0.4765317471517770	0.7086258213660320	
0.0005533839004623	0.1106913255645294	0.6019570981826329	
0.0874385155029998	0.2765388193735422	0.6020628756825865	
0.0005132997011298	0.2221612031905061	0.6019316280970390	
0.0857026269919325	0.0567842750813524	0.6020093269703342	
0.1670714836720275	0.1110248894180560	0.6019284630545623	
0.2630076114728193	0.2754963817754308	0.6031788054063613	
0.1742309625060258	0.2210246818109486	0.6020757879777804	
0.4385287463752497	0.2967147821157425	0.6072879219479385	
0.3593256703240252	0.2332542452391198	0.6028342301197598	
0.5624936524735179	0.2967658500156050	0.6072940894831033	
0.7380215966931670	0.2755019141222495	0.6031428609243225	
0.6416438745628800	0.2333033647689899	0.6027532969698418	
0.8340230444569330	0.1109784317779638	0.6020955960929811	
0.9136236149178246	0.2765927445292594	0.6020282444149235	
0.8268094223050291	0.2210148339864647	0.6020541083791204	
0.9154228419139090	0.0567514620522958	0.6021359081144811	
0.0005788209857053	0.4432493947982100	0.6023918282484451	
0.0856072548887230	0.6098186679223245	0.6025045444752191	
0.0005698063644535	0.5548579568444759	0.6024572882812763	
0.0856571940469499	0.3883210711696062	0.6023578860835228	
0.1695174223215727	0.4429368961620203	0.6029826359664469	
0.2542316482316189	0.6120111664337290	0.6042006634960332	
0.1695276546654923	0.5553248742678565	0.6030046782174885	

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0.2541511876189868	0.3861913134732980	0.6043384922646301
0.3342919190146399	0.4440613372354005	0.6084735015428913
0.3342796437304796	0.5540641846088133	0.6082724079391488
0.6668183630906558	0.4440694302818955	0.6087419108821329
0.7468050635626624	0.6119802024026285	0.6043269475694678
0.6667837693715500	0.5540877424429237	0.6086261791258086
0.7469476653991104	0.3862055561486256	0.6044587791947235
0.8315772002972808	0.4429628264209436	0.6030627042223400
0.9154864080644416	0.6097669977086124	0.6024683132383970
0.8315466267184549	0.5553157466767826	0.6030760505238156
0.9154452696221522	0.3883960538129528	0.6023466251252531
0.0005627881264582	0.7759986458744971	0.6023551469231548
0.0857434280635113	0.9413665288899548	0.6022870500736043
0.0006701327103941	0.8874252993048886	0.6023410017729341
0.0874165394284567	0.7215989647842364	0.6024224040944971
0.1742636200279735	0.7770646435861700	0.6023677652645608
0.1671279260758282	0.8870540303678418	0.6024217449770768
0.2631391718966176	0.7227373646456519	0.6030942781029336
0.3593494392856826	0.7648772212149605	0.6026396207522291
0.4387742159219539	0.7014350675582419	0.6069132830046571
0.5621417103998811	0.7014092206701437	0.6069646103847881
0.6415448093583562	0.7647843159502331	0.6024220140884922
0.7378956295166632	0.7226776523033893	0.6029500673238287
0.8268198496841328	0.7769435281837239	0.6020630436444947
0.9155276071298986	0.9412995286284417	0.6022224999053910
0.8342000046234083	0.8869747885652332	0.6020015603001353
0.9136922457266555	0.7215345699678570	0.6022569652768822
0.4987742392687547	0.5153881503613340	0.6956762069595434
0.4190148474111597	0.5974463589568877	0.6132243498874993
0.4189432487502194	0.4006219159609310	0.6135088430155294
0.5819928303558802	0.5975087928889269	0.6135702879208024
0.5821072179693132	0.4006152782479227	0.6136495104135860
0.5004337172894461	0.4996751218613363	0.6296519800976199

**Table S23.** Atomistic coordinates for the FeN<sub>4</sub>-aC-F<sub>2</sub> structure.

1.0000000000000000				
14.7677999999999994		0.0000000000000000		0.0000000000000000
0.0000000000000000		12.8094000000000001		0.0000000000000000
0.0000000000000000		0.0000000000000000		29.9093000000000018
H	C	N	F	Fe
9	51	4	2	1
Selective dynamics				
Direct				
0.6328612807734283		0.8486522121086914		0.5984359123295280
0.2304500625424107		0.9311901111143267		0.6018900995184208
0.7710856317338162		0.9306768497636529		0.6034736010099070
0.3680882347809301		0.1490254065614205		0.5981529275020494
0.2308067236295941		0.0676197037253637		0.6017713523896654
0.7715306297805175		0.0673130679257146		0.6010533043458787
0.4959691066374161		0.5983721532650018		0.7052222120615405
0.5570891811336093		0.4773377530396609		0.7104741606449894
0.4346581610010529		0.4770313240603368		0.7088580601900354
0.0010234402311225		0.1108030577827388		0.6017486467216061
0.0878995071346878		0.2766704168185176		0.6016869373171200
0.0008823799341784		0.2222851581533974		0.6016264561622717
0.0861165909012956		0.0569010869690336		0.6017357601875697
0.1675921816690769		0.1110258045693750		0.6015856760235293
0.2636440066507260		0.2755272443686488		0.6027648422361910
0.1747095478853612		0.2210898286768800		0.6016862618783407
0.4391305305682929		0.2965982731326150		0.6071048735966402
0.3599345095737950		0.2330565477295248		0.6024197864467765
0.5603489907714948		0.2968570669581249		0.6072304879233840
0.7384445487837203		0.2753830794638661		0.6027837313681703
0.6410844008767795		0.2354456632194108		0.6026867399356592
0.8345186556719063		0.1106442711560385		0.6013840975537189
0.9139847390767281		0.2766835324185244		0.6017513607546521
0.8271258770365417		0.2207055406583069		0.6015846788982105
0.9160153019197467		0.0567921360748187		0.6019155455970178
0.0010939262082968		0.4434207441026863		0.6020146287003935
0.0862869897210187		0.6100767403554213		0.6020592101794513
0.0010690341779052		0.5550491159011116		0.6021025184479201
0.0862298950761112		0.3885172440334603		0.6018344096718174
0.1701410740020279		0.4431508673085830		0.6024738547818262
0.2552597805149482		0.6121567859562907		0.6040517511567325
0.1702901332217468		0.5555977103092643		0.6025722972082590
0.2547631312220047		0.3862793125623475		0.6039666994484308
0.3349023482603823		0.4439755795520647		0.6084375892342637

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0.3351592669676003	0.5541032620349140	0.6084395021007815
0.6668693536452277	0.4439901453496204	0.6090403096282890
0.7469524625595751	0.6119872108872982	0.6047889860958532
0.6670103057447527	0.5540715217970178	0.6093350384027221
0.7469565467404293	0.3862373596613353	0.6043747765587072
0.8318196756937111	0.4429421051957100	0.6030491043772159
0.9157887580919030	0.6098293046361914	0.6023731247137609
0.8317961851864583	0.5552909085181711	0.6032301675977080
0.9158303890481243	0.3884698129728688	0.6021415276400041
0.0009678363091464	0.7761130101900383	0.6021628626913712
0.0858761670961108	0.9415186078329890	0.6019577439017775
0.0008989402652433	0.8875315592327654	0.6021530401292378
0.0880456018669560	0.7218620684612369	0.6020660485508826
0.1750184552408166	0.7777335462337235	0.6020204426050340
0.1675025674779340	0.8877289060897144	0.6019338443172121
0.2640318936320993	0.7230864695044643	0.6029607097447961
0.3615896367146788	0.7624978681762349	0.6029989029519216
0.4426091567910282	0.7008388172534830	0.6074407300595301
0.5619768636430387	0.7010216893917953	0.6077136119988458
0.6413573662213639	0.7646904503968239	0.6028970460641341
0.7378250177083024	0.7227828513974895	0.6034826642657204
0.8269228956285657	0.7771047363319267	0.6024876646429450
0.9157493148462104	0.9413540082608265	0.6022989747194886
0.8342542390369853	0.8871607481468522	0.6027113266320751
0.9139231133370926	0.7216445315182997	0.6022796946090024
0.4965079212958484	0.5150785882910781	0.6965406302119788
0.4198754638394222	0.5970225608440904	0.6137524418926670
0.4192960207294237	0.4004386370644771	0.6136996663541974
0.5823185887617859	0.5971410109439167	0.6147347025212502
0.5822793466073788	0.4004978231828272	0.6138536566808708
0.3721952610048742	0.8679219959182405	0.5981451058560737
0.6308954157521143	0.1300851146642293	0.5977324194985978
0.5006624394131517	0.4991233798241508	0.6304600605633718

**Table S24.** Atomistic coordinates for the FeN<sub>4</sub>-aC-F<sub>4</sub> structure.

1.0000000000000000				
14.7677999999999994		0.0000000000000000		0.0000000000000000
0.0000000000000000		12.8094000000000001		0.0000000000000000
0.0000000000000000		0.0000000000000000		29.9093000000000018
H	C	N	F	Fe
7	51	4	4	1
Selective dynamics				
Direct				
0.2295381971495794		0.9316202924183179		0.6038087263169370
0.7714696876991409		0.9316016524751194		0.6039423558017594
0.2294848021834694		0.0674936696101870		0.6039371987157103
0.7715441193061914		0.0675696781445729		0.6037218826468012
0.5003800019902964		0.5920683370687856		0.6934568780770571
0.5619223730418039		0.4707323595571197		0.6959380225143392
0.4398971650225315		0.4700351898451043		0.6959630031000458
0.0005340004081669		0.1113954586161244		0.6040382995217802
0.0873999685940705		0.2768875577823164		0.6038917299447198
0.0005666255231773		0.2227807957335757		0.6039305440356775
0.0850990820584333		0.0572252436863634		0.6040444371831717
0.1665297661638504		0.1108125110375013		0.6039860901056950
0.2626258151499950		0.2746116808365295		0.6042846857675915
0.1737400898273316		0.2207789431945610		0.6039424252723823
0.4397336288040656		0.2953703330881891		0.6066364125568489
0.3585575734329161		0.2332182456389038		0.6046615969554313
0.5616939218691578		0.2954000295062084		0.6065929458761883
0.7387095524898917		0.2747051603500613		0.6040577199656318
0.6428939296294613		0.2333549064982267		0.6041606639536833
0.8345783545717008		0.1107511494604385		0.6037667415532422
0.9138044825442397		0.2768590972314850		0.6037557124340316
0.8274871831975422		0.2207326146486071		0.6036983518605572
0.9159941481093964		0.0571850984771566		0.6039854397458148
0.0005629349524546		0.4436409488726635		0.6036654590951711
0.0856103186267516		0.6103314608131554		0.6036902890126914
0.0005785893765714		0.5555639642356903		0.6036515706483147
0.0855327160594620		0.3888539872300557		0.6037640645025583
0.1694554874005770		0.4432332402648563		0.6038975205587184
0.2542498638252618		0.6127887782348835		0.6045262193753491
0.1695638091074738		0.5559665546239692		0.6038849578621068
0.2539425398000073		0.3862114104173226		0.6045190543010087
0.3340240189167519		0.4436239849211752		0.6068094711447569
0.3341301868950039		0.5552343038409393		0.6068647182047415
0.6674123758539368		0.4436472810144283		0.6068641078011355



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0.7470470426499285	0.6127905785880744	0.6044925956711009
0.6672629926589619	0.5552327248436709	0.6068655751355270
0.7474161143283500	0.3862400051732408	0.6044989880795978
0.8318441799993745	0.4432400084947336	0.6038784934506211
0.9155607396105769	0.6103376412507544	0.6036497379966443
0.8317101921644970	0.5559280609884152	0.6038418724505853
0.9156687534239875	0.3887953590636810	0.6036749039996037
0.0005691866825242	0.7763793207407844	0.6038547438116681
0.0850935168642031	0.9418043329722486	0.6039928490844759
0.0005219120469343	0.8877503434373555	0.6040417153598922
0.0874845524073517	0.7223167069713802	0.6038092868218576
0.1739161381089674	0.7782923340008187	0.6038615749615088
0.1665846787583677	0.8882436901739529	0.6038472839740225
0.2630930098465987	0.7244530741336301	0.6042879357909992
0.3588941334037560	0.7653685740938535	0.6046553725103158
0.4406045667213994	0.7033630082562475	0.6067234116915434
0.5606824060378524	0.7033494172229482	0.6067080936020336
0.6423862227670465	0.7653326844622566	0.6043874113030369
0.7381236487833116	0.7244318375625132	0.6041590548653413
0.8271573706596579	0.7782983995726090	0.6038338367085652
0.9159480214443422	0.9417543211119037	0.6040624641837148
0.8344277444085400	0.8882502857013947	0.6039327865255188
0.9136647786109954	0.7223085733919559	0.6037509589677896
0.5007326380515444	0.5096119591468143	0.6833571875279693
0.4186329535550355	0.5991635829461106	0.6096473532321985
0.4180803524637875	0.3992458156172168	0.6095618014231534
0.5827281122319273	0.5991697544546126	0.6097123610761246
0.5833229600101185	0.3992442766943710	0.6096819126548136
0.3689367558724473	0.8709698174784362	0.6035050755368471
0.6335130424504462	0.1277967818848761	0.6019736392499264
0.6324231584472241	0.8709406931093749	0.6027341044237132
0.3685092175114051	0.1276097840439981	0.6035075073472491
0.5006965974378956	0.4995983330412030	0.6174148141703752

**Table S25.** Atomistic coordinates for the FeN<sub>4</sub>-aC-F<sub>8</sub> structure.

1.0000000000000000				
14.7677999999999994		0.0000000000000000		0.0000000000000000
0.0000000000000000		12.8094000000000001		0.0000000000000000
0.0000000000000000		0.0000000000000000		29.9093000000000018
H	C	N	F	Fe
5	55	5	8	1
Selective dynamics				
Direct				
0.5216499772927189		0.6686377450224866		0.4293964504720044
0.5227293744014064		0.4995403436968123		0.3861550133378133
0.5127509446160321		0.3309152518930881		0.4295519811081522
0.5030221132668541		0.3383340591946111		0.5126732070686844
0.5113946591322122		0.6624823098037336		0.5126151417390907
0.0011573088863155		0.1103519724815264		0.6132915062446574
0.0884023246848445		0.2751791859692809		0.6098434352789939
0.0011250921525293		0.2214270809337714		0.6109315638837417
0.0850837099161985		0.0549890096994551		0.6101275184994741
0.1636807409792878		0.1107523456161812		0.6005382540920466
0.2651677084680907		0.2730680592164514		0.6062310487345924
0.1752908069652379		0.2197794366378238		0.6065507517702352
0.4432292182100869		0.2968567954571222		0.6029319862421989
0.3620414985160430		0.2341920313119825		0.6085122916122829
0.5586591206090979		0.2969772691956171		0.6035356404417968
0.7367648519654272		0.2729511792393007		0.6071715764683315
0.6397233914910431		0.2340675918775455		0.6089525093843494
0.8383965309575425		0.1109440083232395		0.6011002892768483
0.9138023468044562		0.2752605164959174		0.6102331752139329
0.8268304325924060		0.2198668825024493		0.6071780727490740
0.9171473122933057		0.0550888165005844		0.6103372081054181
0.0011169395933420		0.4418876537856201		0.6099716097250295
0.0865671703967652		0.6085777281224403		0.6082590982852332
0.0010942356580302		0.5539650559918867		0.6087330373490795
0.0866455385355519		0.3873399129556410		0.6096397117559679
0.1708539956625468		0.4416747792552781		0.6073836897103202
0.2559484322750646		0.6115883655868037		0.6066133640445402
0.1709621411183634		0.5544824734459096		0.6075941664376774
0.2556939032359686		0.3846939951033956		0.6050341540922658
0.3351120465808403		0.4427031189537161		0.6000449806362439
0.3352073980671860		0.5534734566991806		0.6008994385308830
0.6669574116832558		0.4426958236417195		0.6020141144873753
0.7461985719093037		0.6116423971449972		0.6078063216281644
0.6668884046777956		0.5534321176283389		0.6026390615278200

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0.7463689669352709	0.3845999577326699	0.6065726861735476
0.8312548480278825	0.4416259166416684	0.6085469237361320
0.9155647223635952	0.6086032855988870	0.6086868022232051
0.8311895250820265	0.5544801595490888	0.6086594207645656
0.9156230637729471	0.3874088536217896	0.6101280095620291
0.0010852959210720	0.7743457137339737	0.6089190186290758
0.0849428407262990	0.9405707784808482	0.6107054393490650
0.0011136354207716	0.8854059902830789	0.6072995193666801
0.0883446315396404	0.7206073519559049	0.6091031973291837
0.1753170879074481	0.7758550611112781	0.6128077278740824
0.1632874144737596	0.8843850465444199	0.6203411706659065
0.2655694706131619	0.7231272050795587	0.6100485134179101
0.3625229020674433	0.7622891794061016	0.6088211180399793
0.4435923910295188	0.6991896006185186	0.6038219640731852
0.5587018308868072	0.6993204284329693	0.6042039648966664
0.6397606085952579	0.7626418280127999	0.6087767808127783
0.7366487549174640	0.7232890018947532	0.6105160574007766
0.8268559534912355	0.7759629617036369	0.6130854353379848
0.9172323323996219	0.9406170820231365	0.6109139948923488
0.8389026926306862	0.8844530671977276	0.6206861620632310
0.9137854971614376	0.7206537757179295	0.6092969810987816
0.5176595759979998	0.5935416124738135	0.4463796738664989
0.5182055683767223	0.4997920986342503	0.4225221742303556
0.5126268930497203	0.4063232365834795	0.4464121090656296
0.5071116872106147	0.4094963712607297	0.4927339214905411
0.5119315038899691	0.5910359746470789	0.4927358479493498
0.4202792842496701	0.5959886609863246	0.5963139802931122
0.4199706221594189	0.3999549520303727	0.5945855674158105
0.5819804942287693	0.5958655648140098	0.5976014704028383
0.5822216084658263	0.4001730450584152	0.5960939953685372
0.5068631754404876	0.5003704666163823	0.5158745863039829
0.3762577866627514	0.8665289980899049	0.6108252753144638
0.6264018326622526	0.1317050169285320	0.6177727492314209
0.6260672567783724	0.8669718511088514	0.6096615141483808
0.3747297739522392	0.1320295765388870	0.6180481307590444
0.2323714518811633	0.9345157601704132	0.6408547414514881
0.7698754998979244	0.9345724583307095	0.6413511704200651
0.2336483346163525	0.0596857133705361	0.5808470142205964
0.7678288879792844	0.0599708411537645	0.5818868026447670
0.5016026429419493	0.4985297864788908	0.5811690177817065

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