Electronic Supplementary Information

Developing Bimetallic FeM-Organic Frameworks Based on Ferroalloy Trinuclear Clusters for High-Performance Supercapacitors

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1. Experiment

1.1 Materials

3,5-di (4′-carboxylphenyl) benozoic acid (DCPB) was purchased from Jinan Henghua Technology Corporation. $FeCl_3 \cdot 6H_2O$, $FeSO_4 \cdot 7H_2O$, $MnAc_2 \cdot 4H_2O$, $CoAc_2 \cdot 4H_2O$, $NiAc_2 \cdot 4H_2O$ were purchased from Aladdin Industrial Corporation, China. KOH and Ethanol (EtOH) were purchased from Sinopharm Chemical Reagent. All solvents and reagents were analytical grade and used as received without further purification.

1.2 General materials and methods

Single-crystal diffraction data were acquired using a BRUKER D8 Venture diffractometer at a temperature of 292 K, employing MoK_α radiation (wavelength λ = 0.71073 Å) at 40 kV and 40 mA. Powder X-ray diffraction (PXRD) patterns were obtained with a Ultima IV-185 powder diffractometer utilizing CuK_α radiation. Stepwise scanning was conducted with 2θ ranging from 5°to 50. Fourier transform infrared (FTIR) spectra were recorded on a VARIAN 660-IR Spectrometer, using KBr pellets within the range of 4000 - 400 cm^{-1}. Thermogravimetric analysis (TGA) was executed on a TGA/DSC 1 thermoanalyzer, heating from ambient temperature to 900°C at a rate of 2°C/min under a nitrogen atmosphere. Scanning electron microscopy (SEM) images and EDS were captured with a JSM-7500F microscope. XPS were captured with a K-Alpha+ X-ray Photoelectron Spectroscopy.

Table S1. Crystal data and structure refinement for Fe/Ni-MOF

Complexes	Fe/Ni-MOF
Formula weight	941.04
Empirical formula	$C_{42}H_{26}Fe_2NiO_{15}$
crystal system	trigonal
space group	R$\bar{3}$c
a (Å)	27.500(3)
b (Å)	27.500(3)
c (Å)	71.290(5)
α (deg)	90
β (deg)	90
γ (deg)	120
V (Å^3)	46691(10)
Z	18
Dcalcd (g cm^{-3})	0.602
m/mm^{-1}	0.483
F (000)	8604
R_1 [I > 2σ(I)][a]	0.0969
wR_2 [I > 2σ(I)][b]	0.2382
R_1 (all data)	0.1634
wR_2 (all date)	0.2690
GOF on F^2	1.352

[a]$R_1 = \sum||Fo| - |Fc||/|Fo|$. [b]$wR_2 = [\sum w (Fo^2 - Fc^2)^2/\sum w(Fo^2)^2]^{1/2}$

Table S2. Selected bond lengths (Å) and angles (deg) for Fe/Ni-MOF

Fe(1)−O(7)	1.888(3)	O(7)−Fe(1)−O(6)^{A}	95.00(17)
Fe(1)−O(3)	1.979(5)	O(3)−Fe(1)−O(6)^{A}	89.6(2)
Fe(1)−O(5)	1.994(4)	O(5)−Fe(1)−O(6)^{A}	89.1(2)
Fe(1)−O(8)	2.020(5)	O(8)−Fe(1)−O(6)^{A}	83.5(2)
Fe(1)−O(6) ^{A}	2.028(4)	O(7)−Fe(1)−O(1)	96.42(18)
Fe(1)−O(1)	2.036(5)	O(3)−Fe(1)−O(1)	91.6(2)
Ni(1)−O(7)	1.849(5)	O(5)−Fe(1)−O(1)	88.00(19)
Ni(1)−O(2)	1.976(4)	O(8)−Fe(1)−O(1)	85.1(2)
Ni(1)−O(4)	1.991(4)	O(6)^{A}−Fe(1)−O(1)	168.4(2)
O(7)−Fe(1)−O(3)	94.60(16)	O(7)−Ni(1)−O(2)^{A}	94.01(13)
O(7)−Fe(1)−O(5)	93.72(16)	O(2)−Ni(1)−O(2)^{A}	172.0(3)
O(3)−Fe(1)−O(5)	171.7(2)	O(7)−Ni(1)−O(4)^{A}	95.85(15)
O(7)−Fe(1)−O(8)	178.5(2)	O(2)^{A}−Ni(1)−O(4)^{A}	91.7(2)
O(3)−Fe(1)−O(8)	85.6(2)	O(2)−Ni(1)−O(4)^{A}	87.5(2)
O(5)−Fe(1)−O(8)	86.0(2)	O(4)^{A}−Ni(1)−O(4)	168.3(3)

Symmetry operation code：A = −y+x+1/3, −y+2/3, -z+1/6; B = y−2/3,x-1/3,-z+1/6; C: -2/3 + y, -1/3 + x, 1/6 - z);

D =+y,-x+y,−z; E = -y+x,+x,-z; F =y+1/3,x+2/3,-z+1/6;

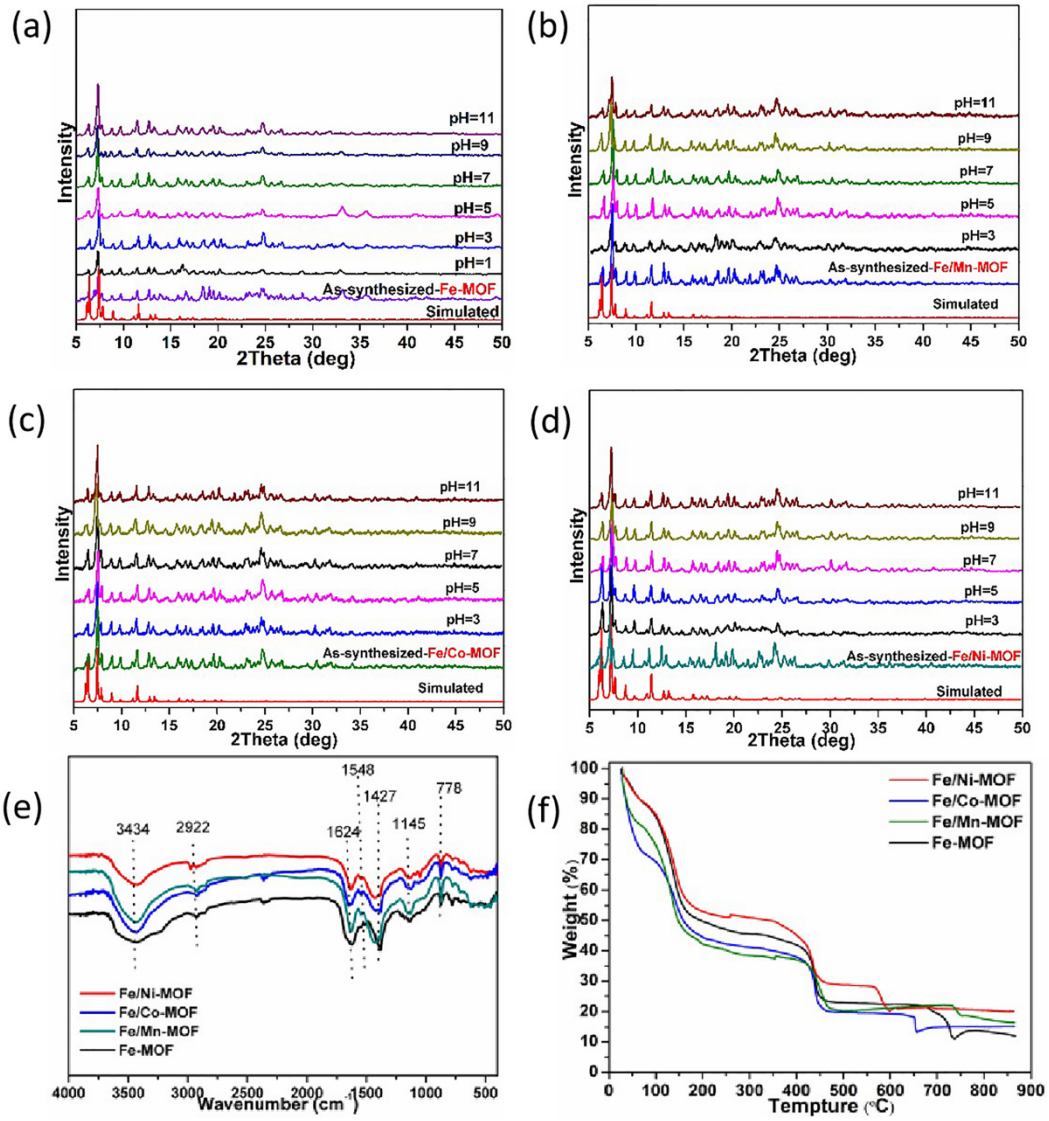

Figure S1. (a - d)The PXRD patterns of Fe_2M-MOF (M =Mn, Co, Ni) samples treated in water at different pH values for 12 h; (e) IR spectra of Fe/M-MOF (M =Mn, Co, Ni) materials and (f) TG curves.

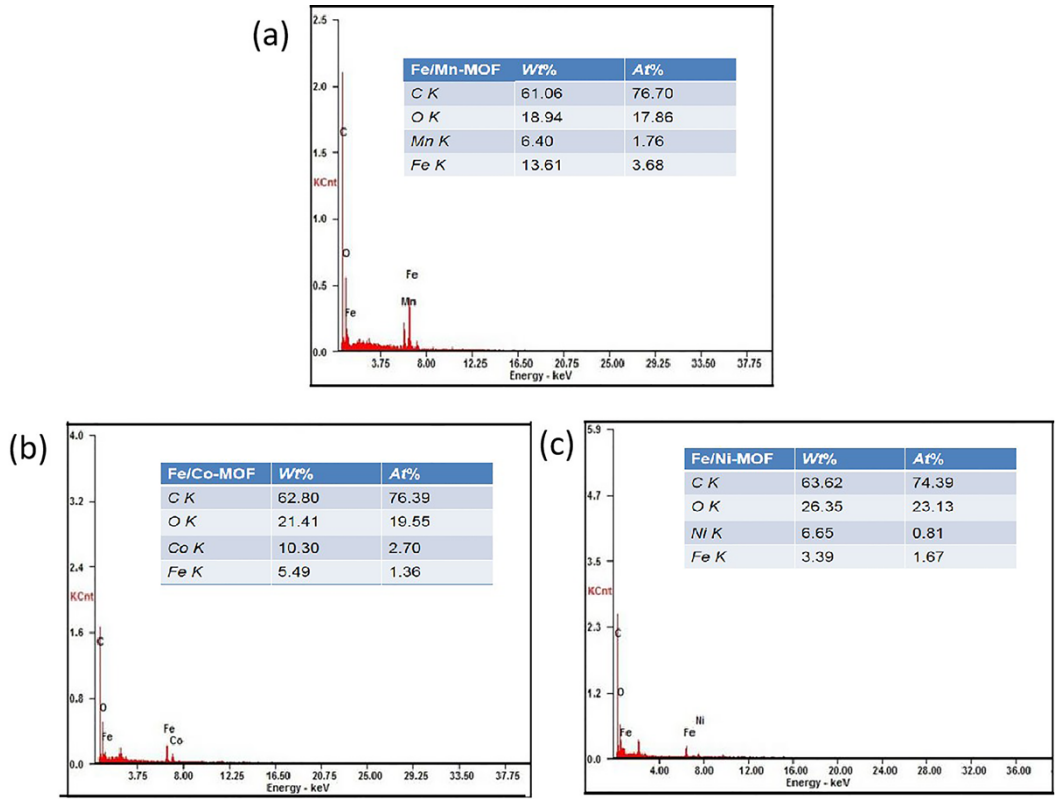

Figure S2. EDS spectra of (a) Fe/Mn-MOF; (b) Fe/Co-MOF; (c) Fe/NiMOF;

Figure S3 (a), (c), (e), (g) CV curves at different scan rates and (b), (d), (f), (h) GCD curves at different current densities of the Fe/M-MOF electrodes, respectively. (i) Plots of i_p vs $v^{1/2}$ for Fe/M-MOF.

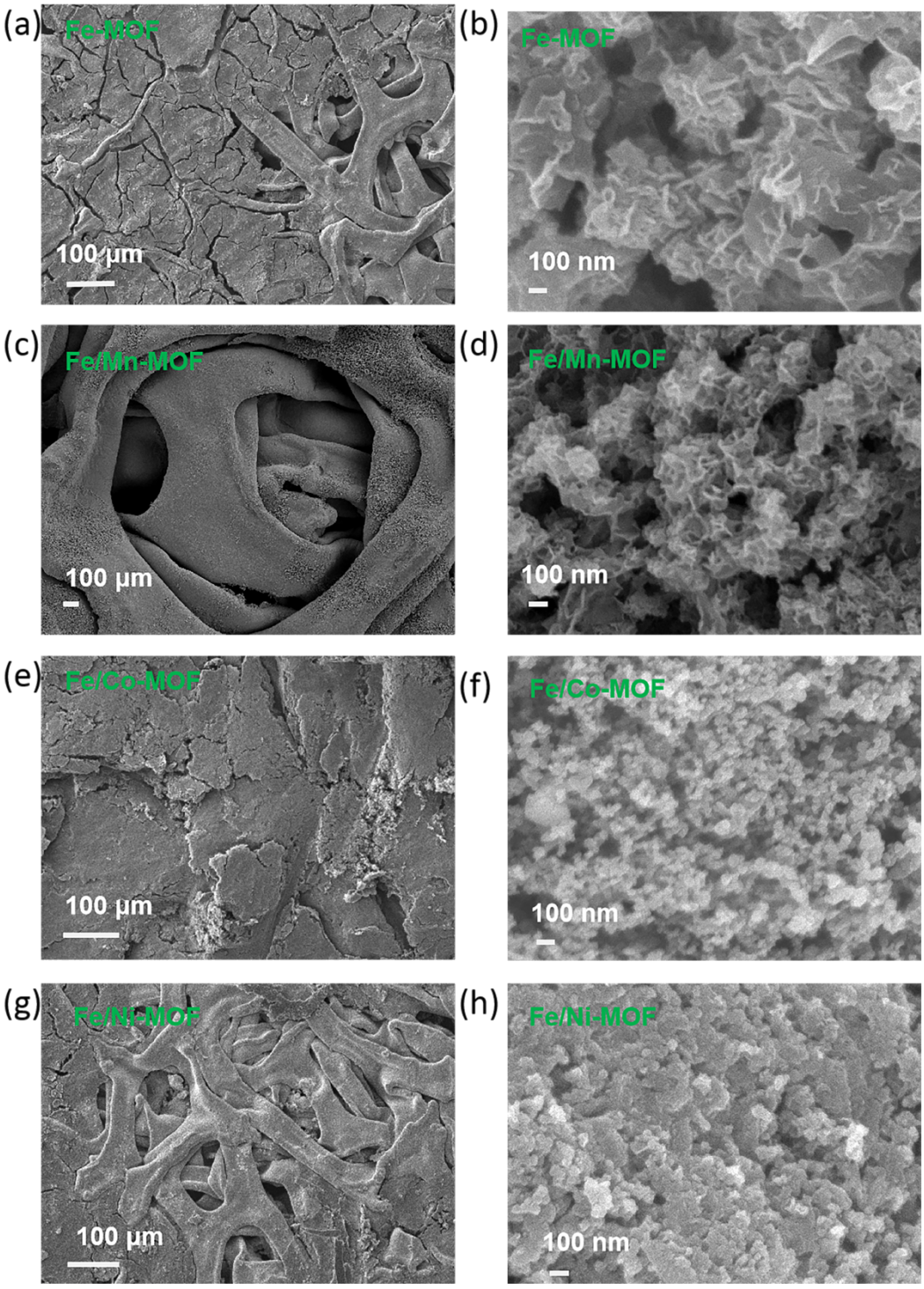

Figure S4. (a), (c), (e), and (g) samples loaded on foam nickel SEM images after 1000 Cycling and (b), (d), (f), and (h) samples of Fe-MOF, Fe/Mn-MOF, Fe/Co-MOF and Fe/Ni-MOF respectively.

Asymmetric supercapacitors

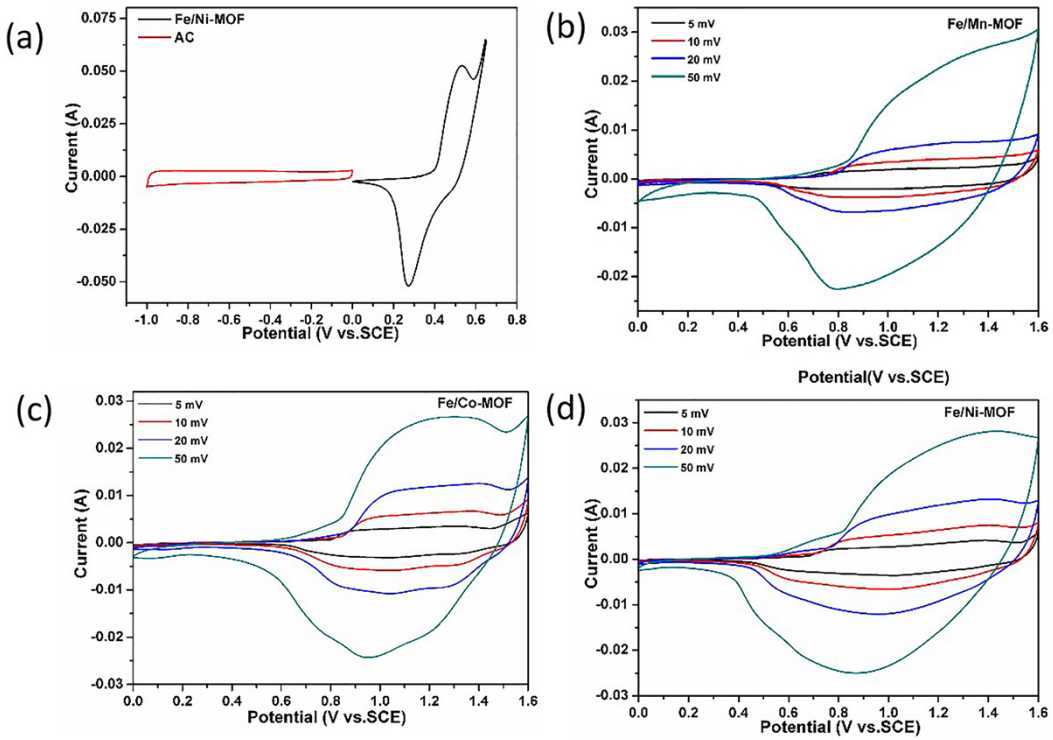

Figure S5. (a), (c), (e) CV curves at different scan rates and (b), (d), (f) GCD curves at different current densities of the Fe/M-MOF//AC, respectively.