Supplementary Information

Shape controlled growth of pyrite FeS2 crystallites via a polymer-assisted hydrothermal route

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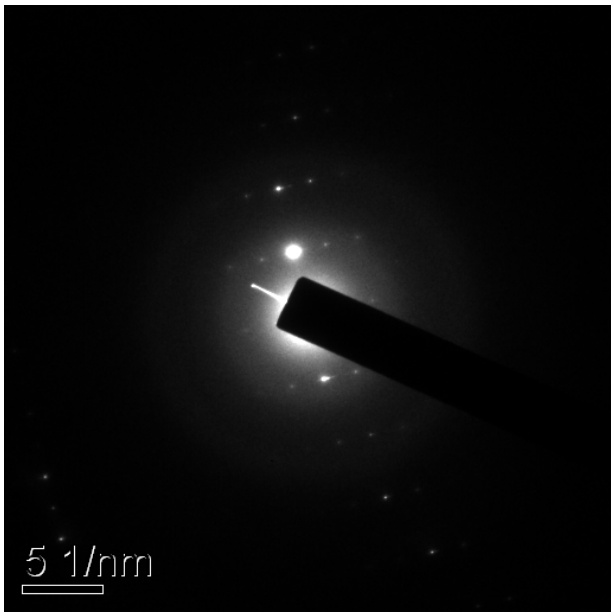


Fig. S1 Selected-area electron diffraction (SAED) pattern of the FeS_2 microcubes.

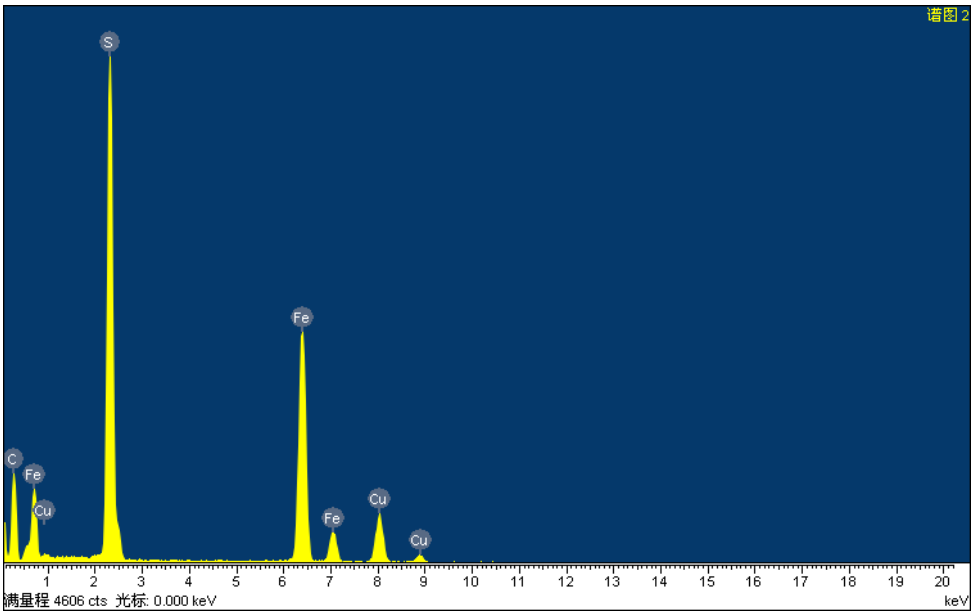


Fig. S2 Energy-dispersive spectroscopy (EDS) of the FeS_2 microcubes.

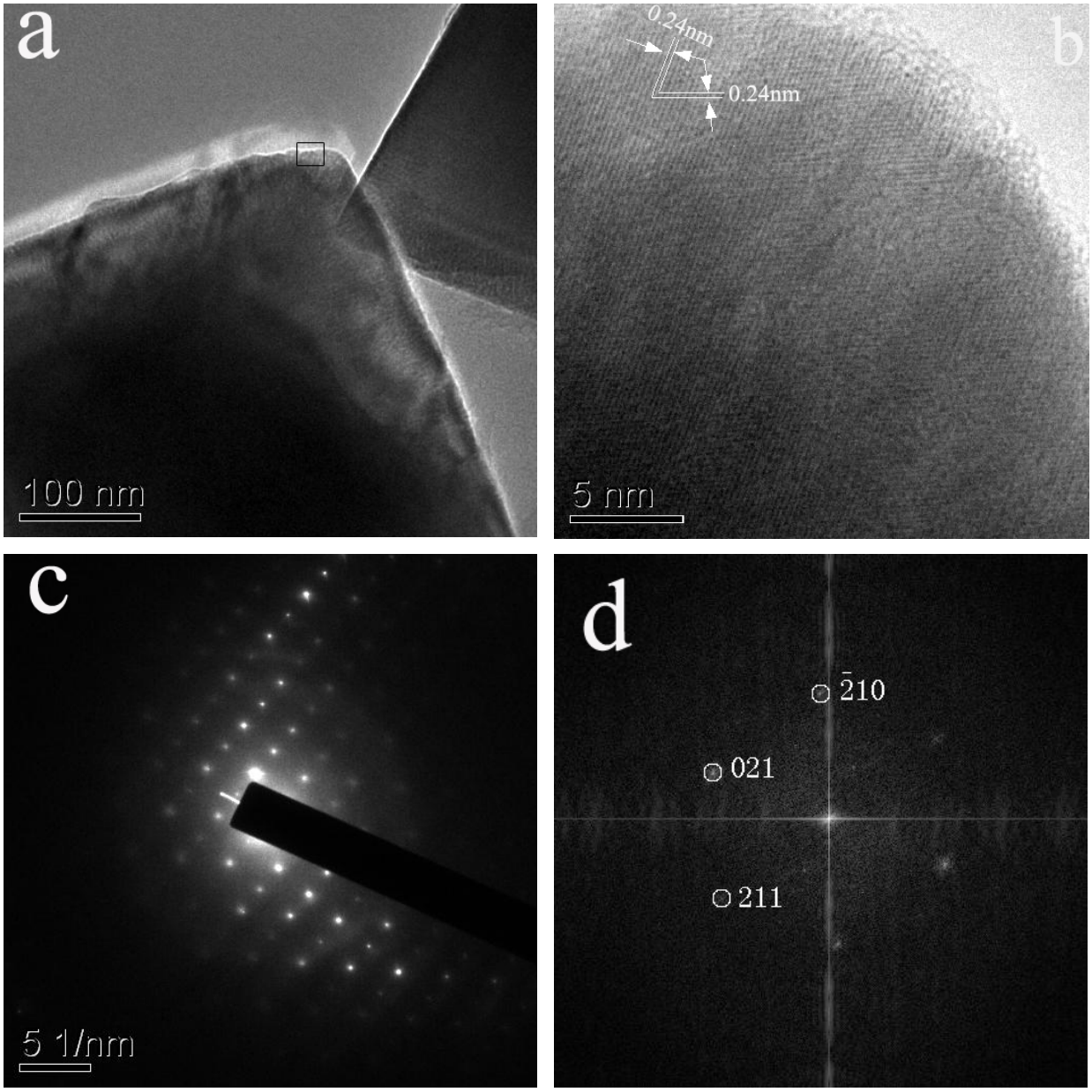


Fig. S3 (a) TEM image of the FeS_2 micro-octahedron, (b) (HR) TEM image of the edge of the octahedron, taking from the selected area marked by a square in (a), (c) SAED pattern and (d) corresponding FFT taking from (b).

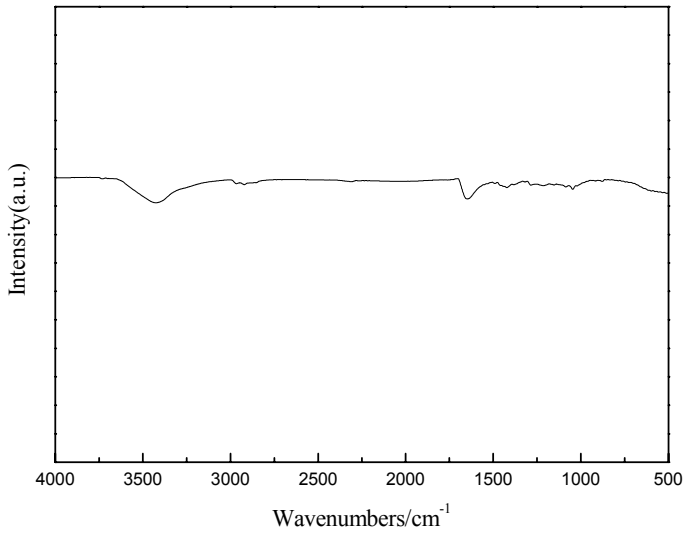


Fig. S4 FT-IR spectra of the as-obtained FeS_2 micro-octahedrons.

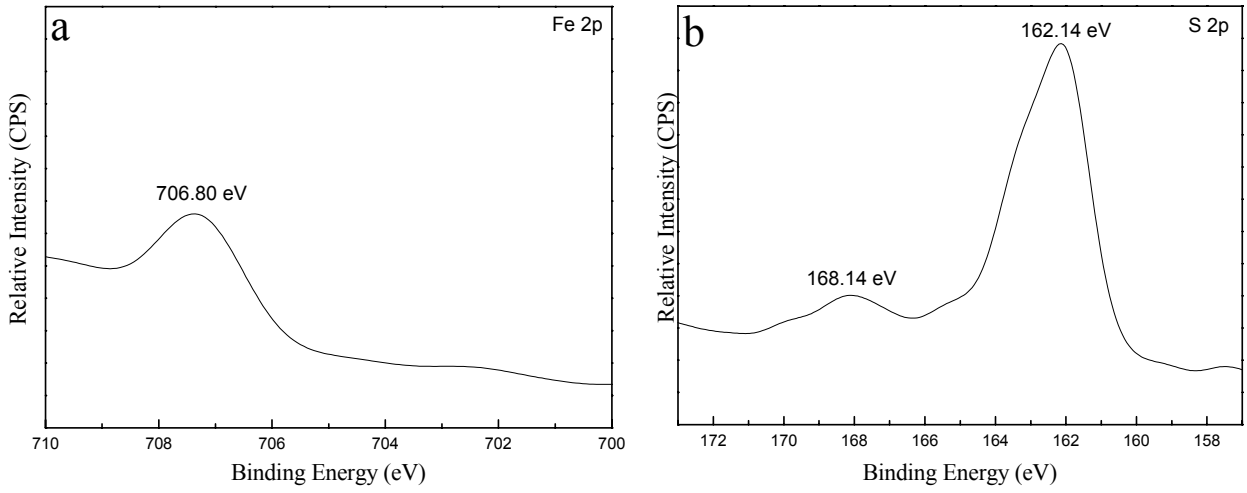


Fig. S5 XPS studies of the as-obtained FeS_2 micro-octahedrons, (a) iron region and (b) sulfide region.

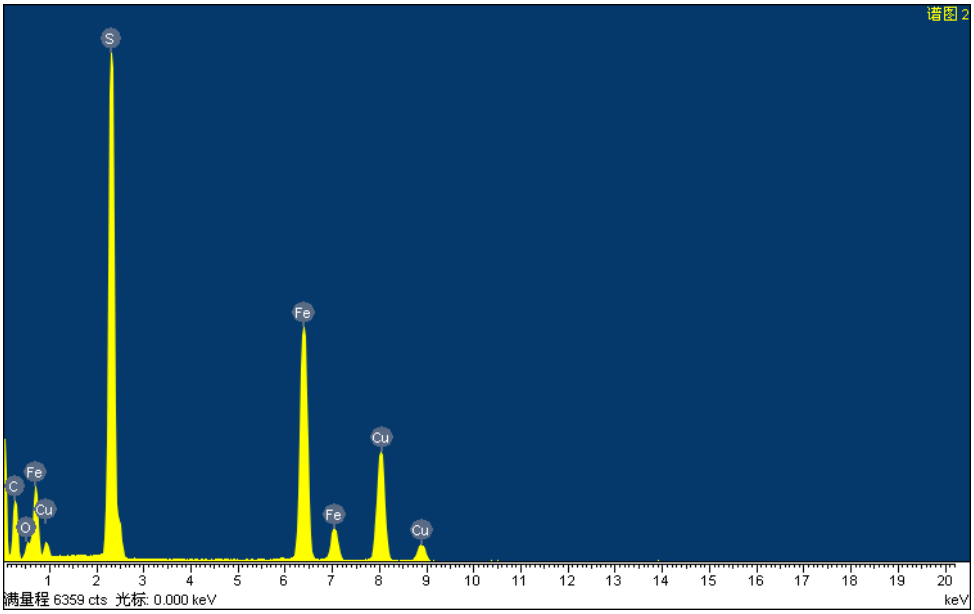
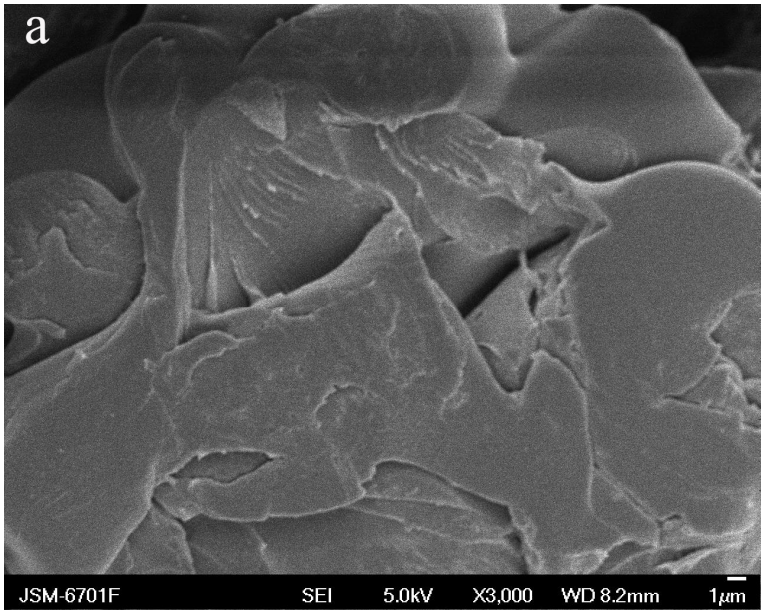


Fig. S6 Energy-dispersive spectroscopy (EDS) of the FeS_2 micro-octahedrons.



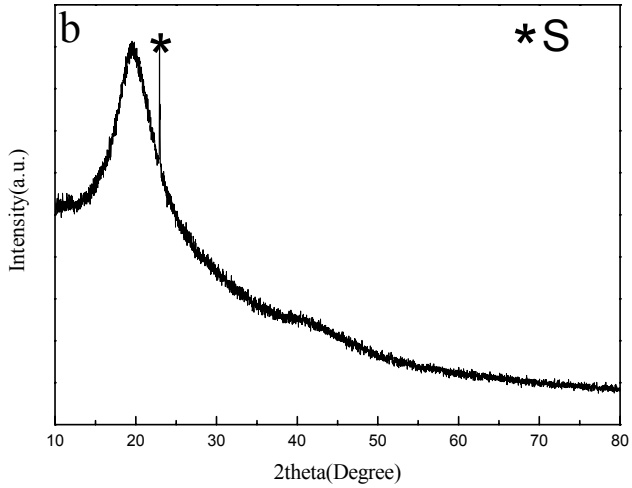


Fig. S7 FESEM image and XRD pattern of the product in the absence of NaOH.

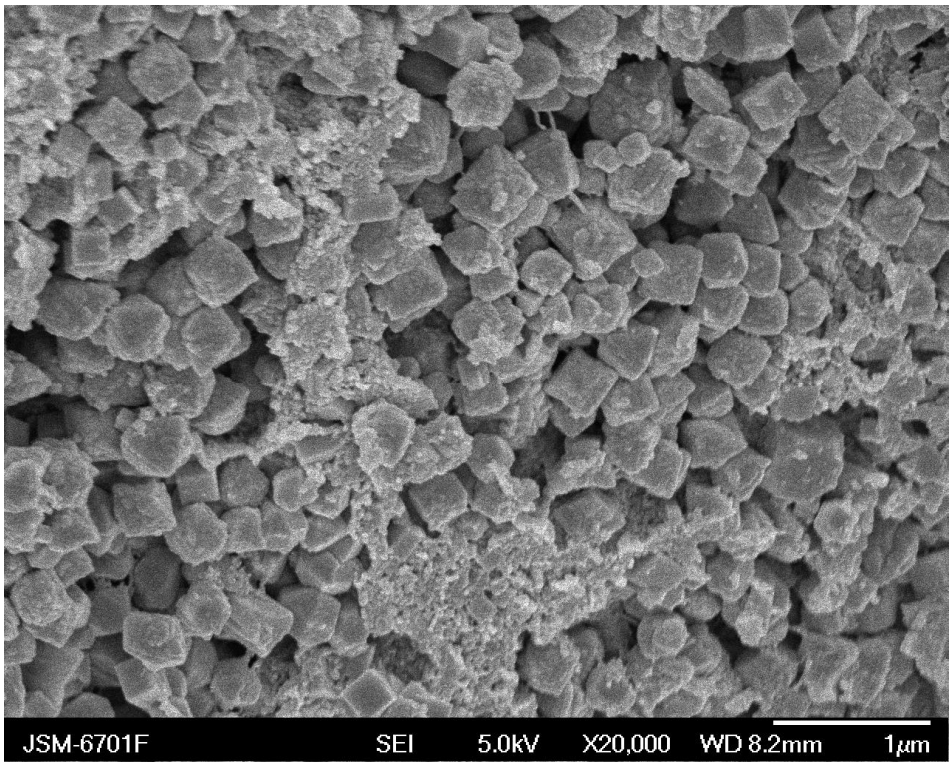


Fig. S8 FESEM image of the product, [NaOH]=0.21 M，PVA=10 mL, PVP=0.20 g.

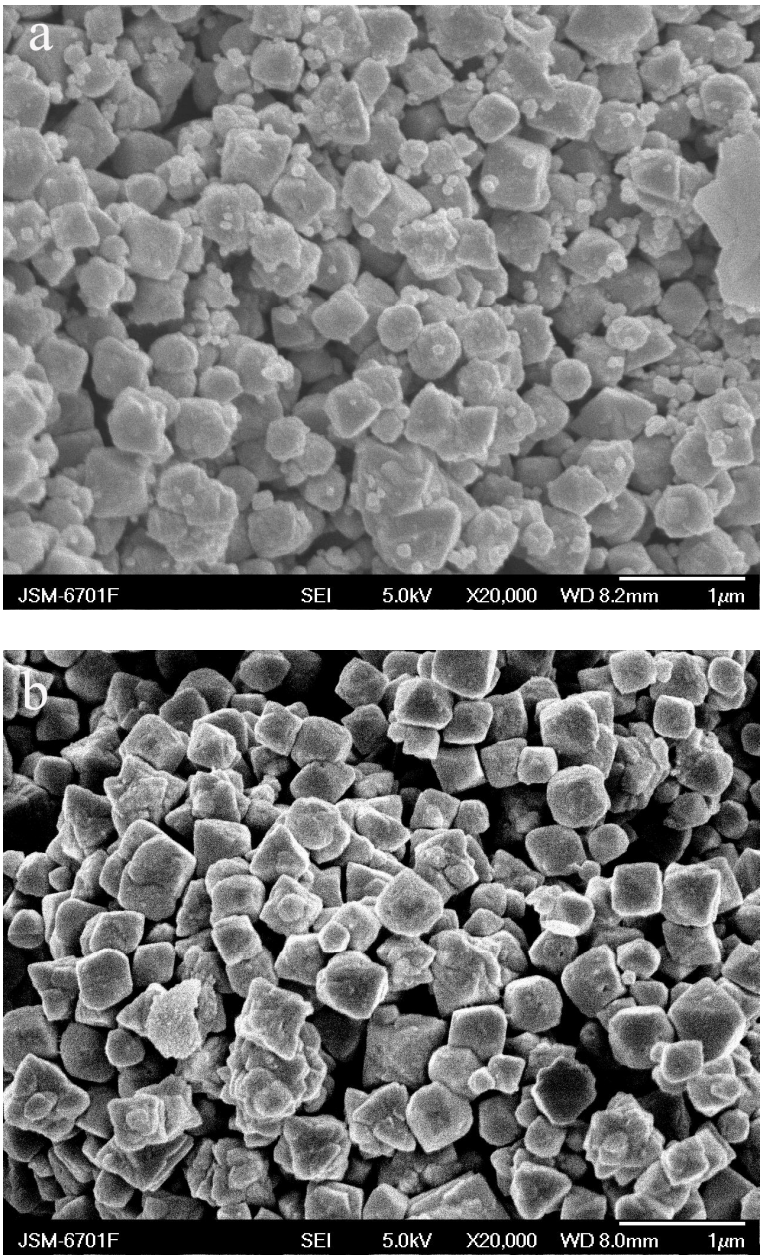


Fig. S9 FESEM image of the product in the absence of PVA (a) PVP=0.20 g, [NaOH] =0.11 M, and (b) PVP=0.20 g, [NaOH] =0.14 M.

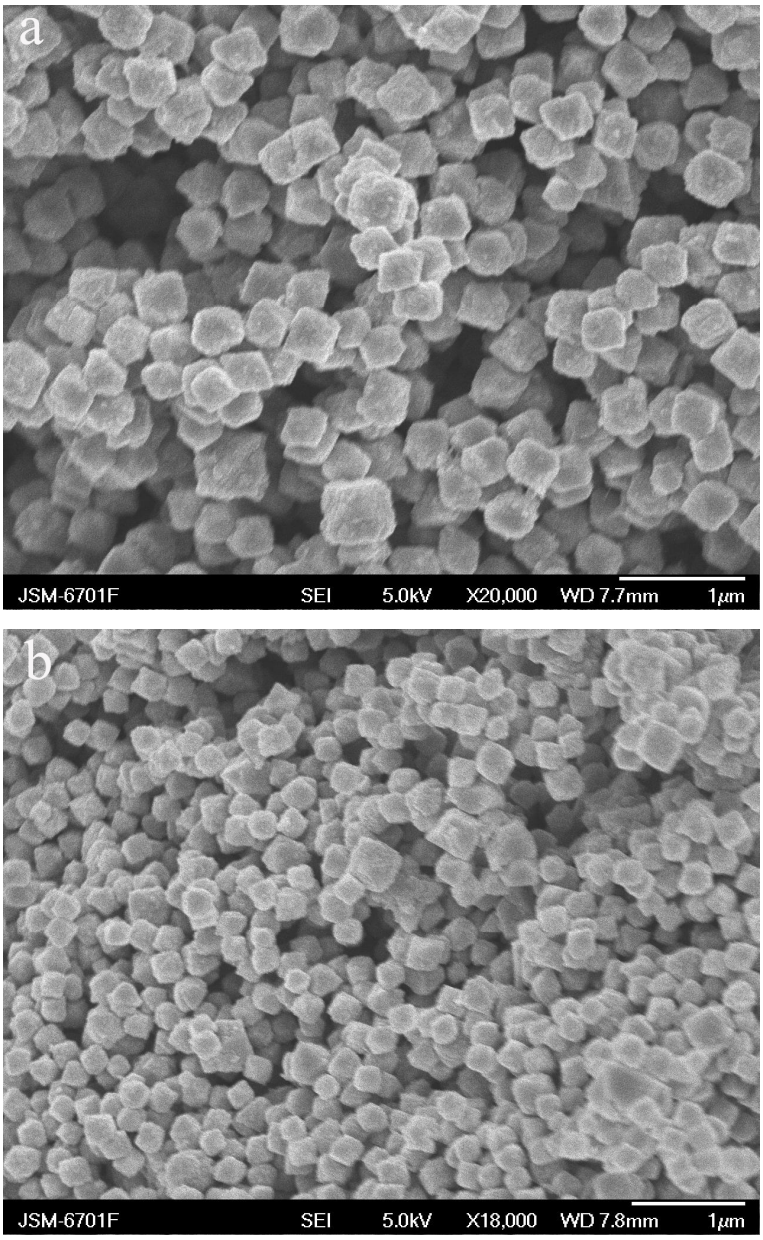


Fig. S10 FESEM image of the product in the absence of PVP (a) PVA=15 mL, [NaOH] =0.14 M, and (b) PVA=10 mL, [NaOH] =0.14 M.

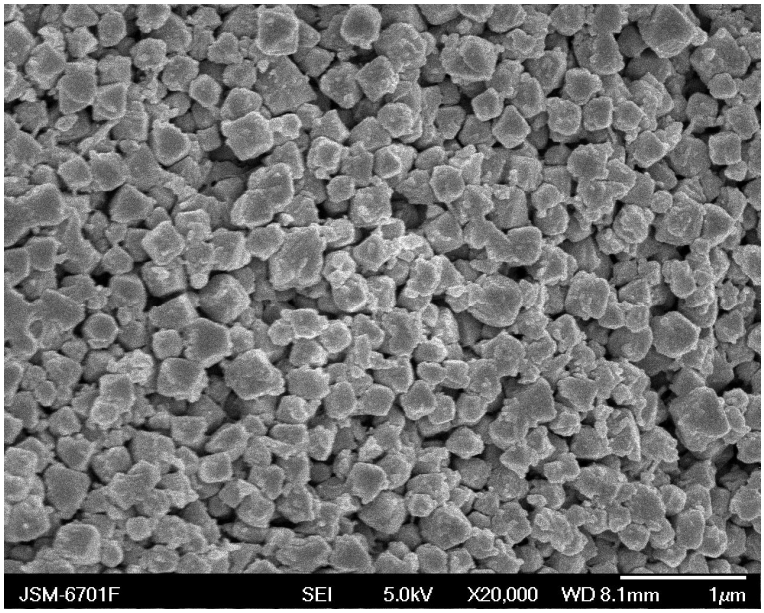


Fig. S11 FESEM image of the product, PVP=0.3 g, PVA=10 mL, and [NaOH] =0.14 M.

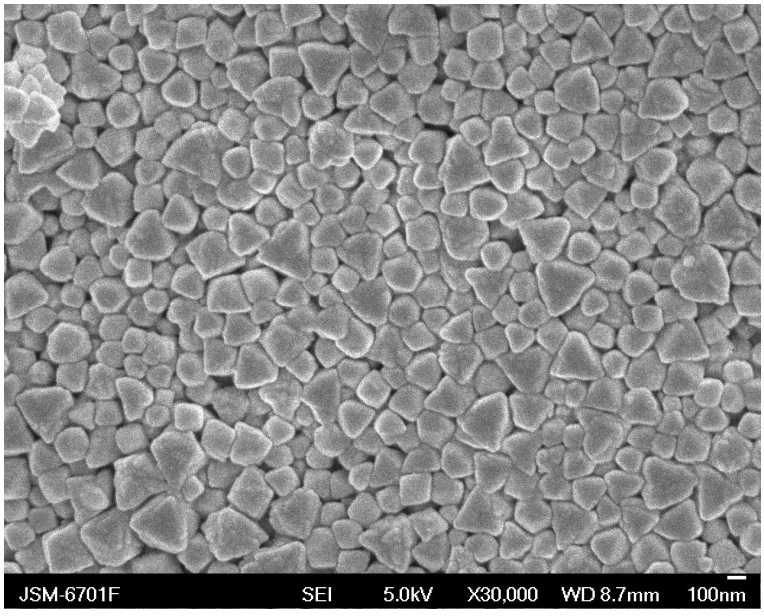


Fig. S12 FESEM image of the product, PVP=0.2 g, PVA=8 mL, and [NaOH] =0.14 M.

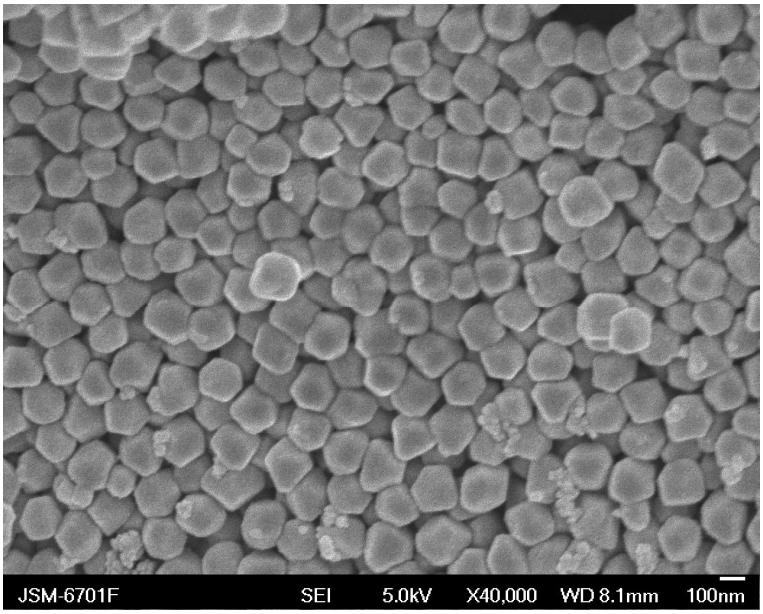
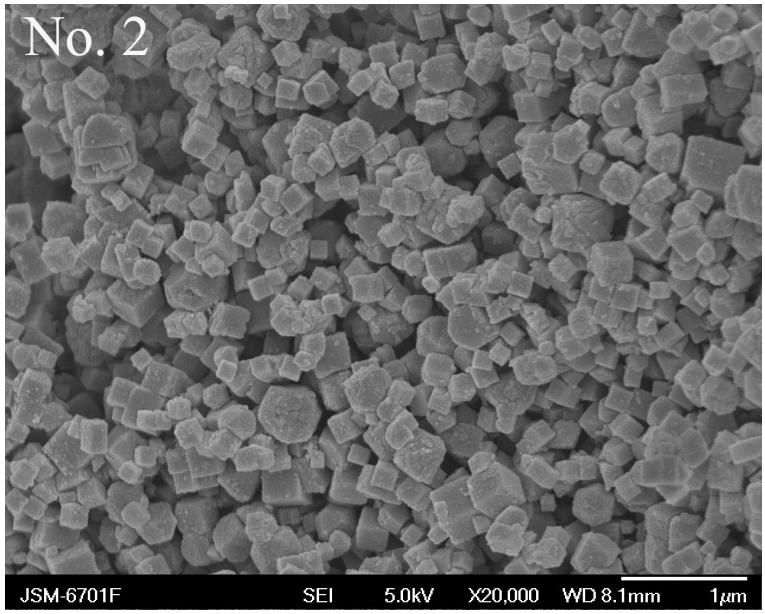


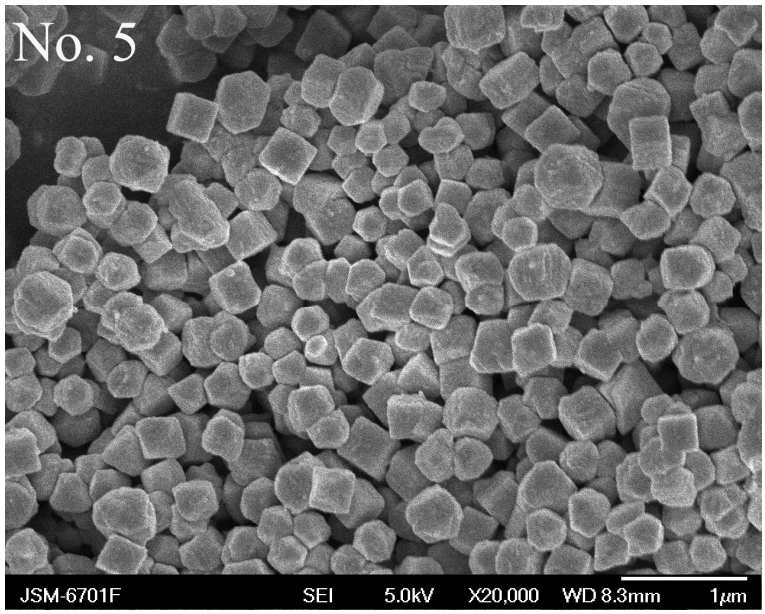
Fig. S13 FESEM image of the product, PVP=0.2 g, PVA=12 mL, and [NaOH] =0.14 M.

Table S1 Shapes of the product obtained at 453 K under different NaOH and polymers dosages.

No.	PVA/ mL	PVP/ g	NaOH/ M	Morphologies
1	8	0.2	0.14	octahedrons (a) and irregular particles
2	12	0.2	0.14	octahedrons and polyhedrons (a)
3	10	0.3	0.14	octahedrons (a) and irregular particles
4	10	0.1	0.14	octahedrons with broad size distribution
5	10	0.05	0.14	cubes and irregular particles
6	10	0.1	0.11	cubes and irregular particles (a)
7	8	0.2	0.11	cubes (a) and polyhedrons
8	12	0.2	0.11	cubes (a) and polyhedrons
9	10	0.3	0.11	cubes (a) and irregular particles
10	10	0.2	0.21	cubes and octahedrons
11	8	0.2	0.21	cubes and irregular particles (a)
12	10	0.1	0.21	irregular particles
13	10	0.2	0.12	cubes (a) and cuboctahedron

(a): denotes the predominant products.


No. 2
JSM-6701F SEI 5.0kV X20,000 WD 8.1mm 1μm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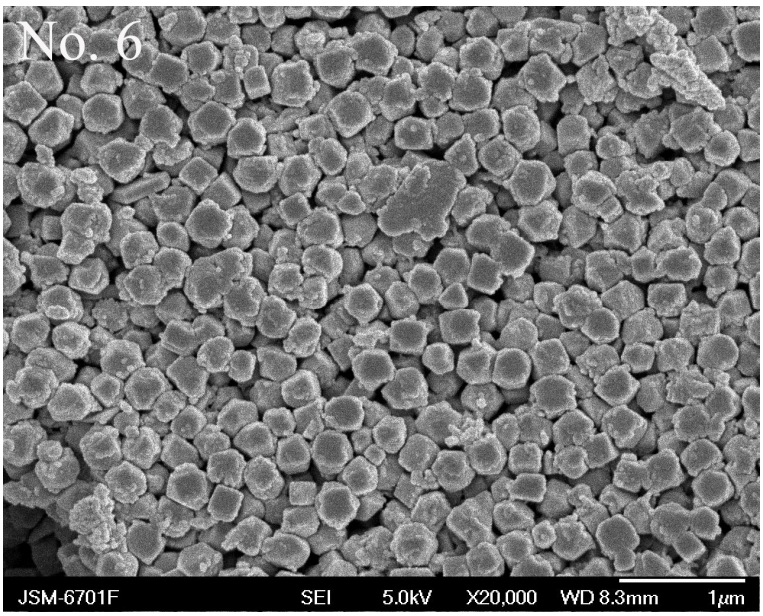
JSM-6701F SEI 5.0kV X20,000 WD 8.3mm 1μm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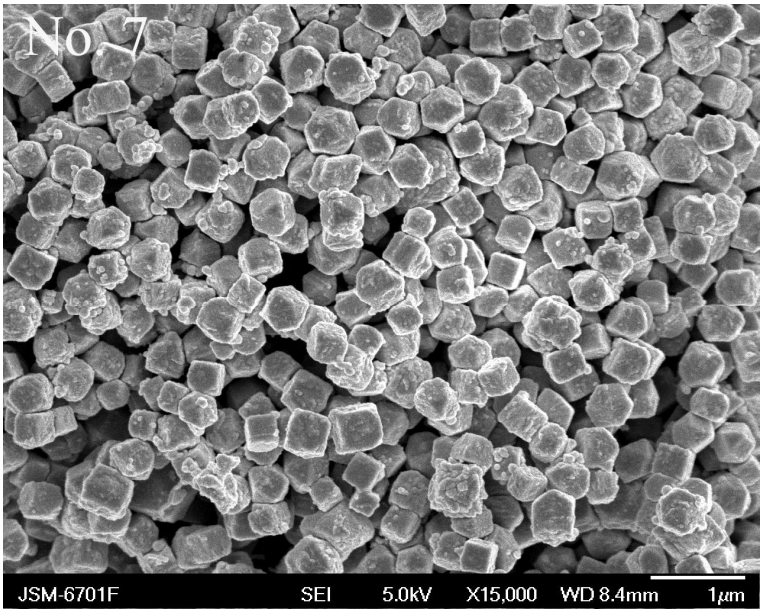
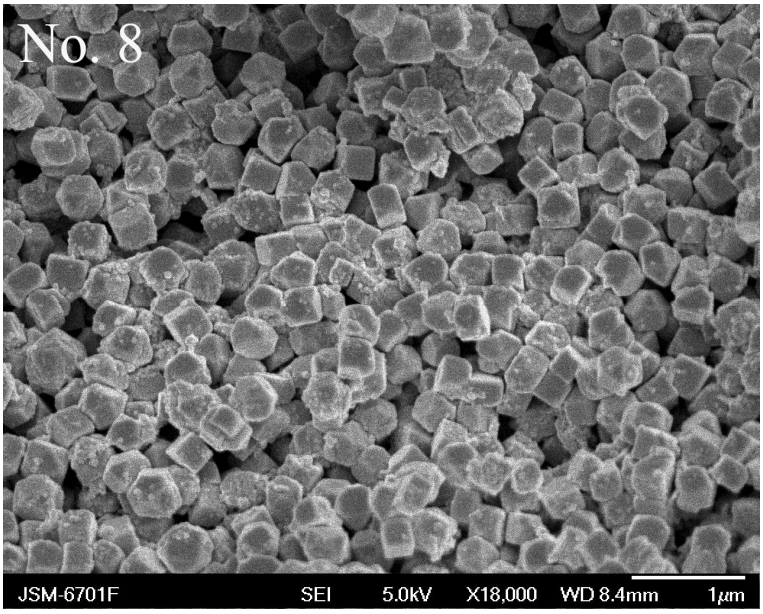
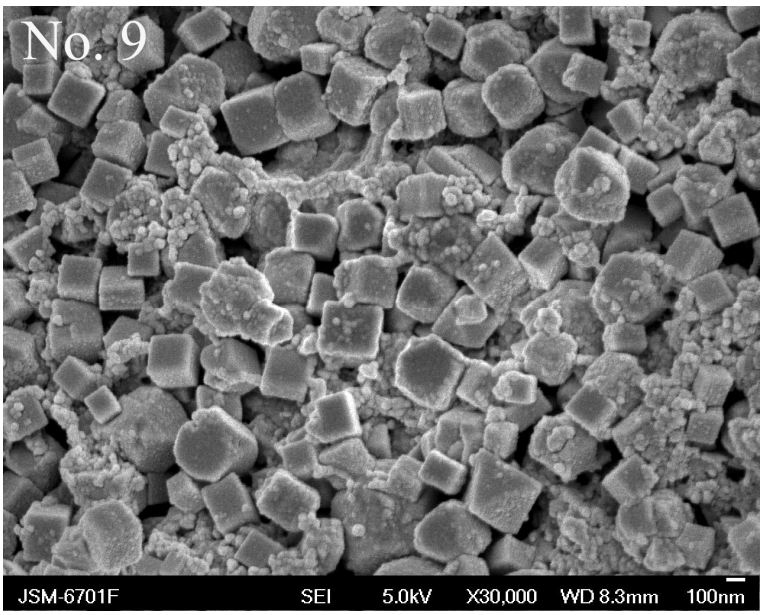
JSM-6701F
SEI
5.0kV
X20,000
WD 8.3mm
1μm


No. 7
JSM-6701F
SEI
5.0kV
X15,000
WD 8.4mm
1μm


No. 8
JSM-6701F SEI 5.0kV X18,000 WD 8.4mm 1μm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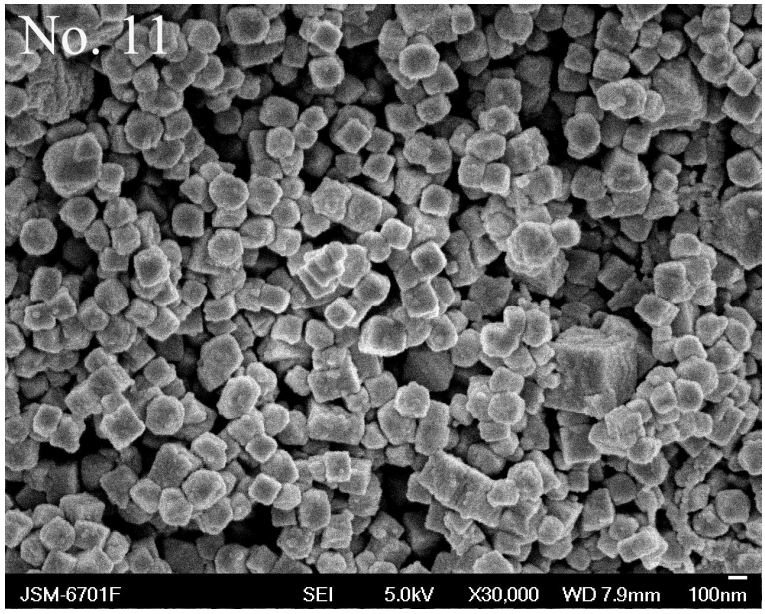
JSM-6701F SEI 5.0kV X30,000 WD 8.3mm 100nm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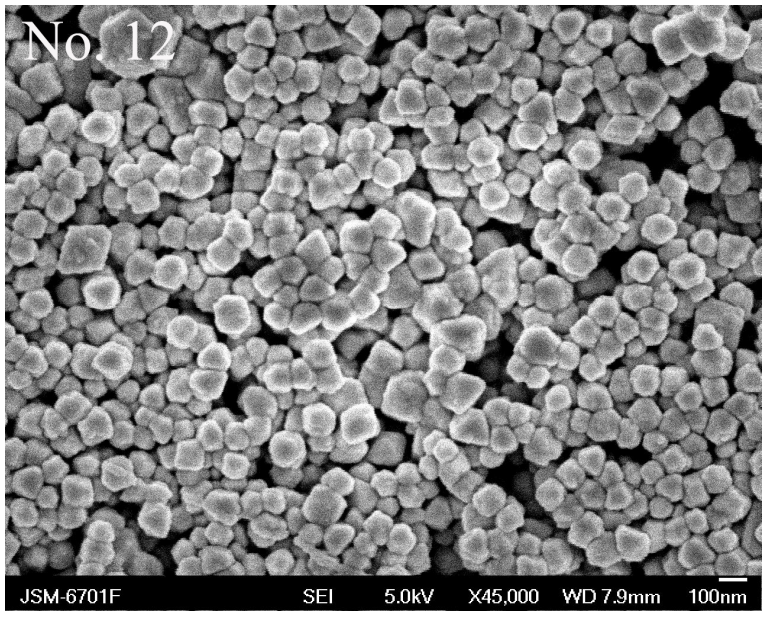
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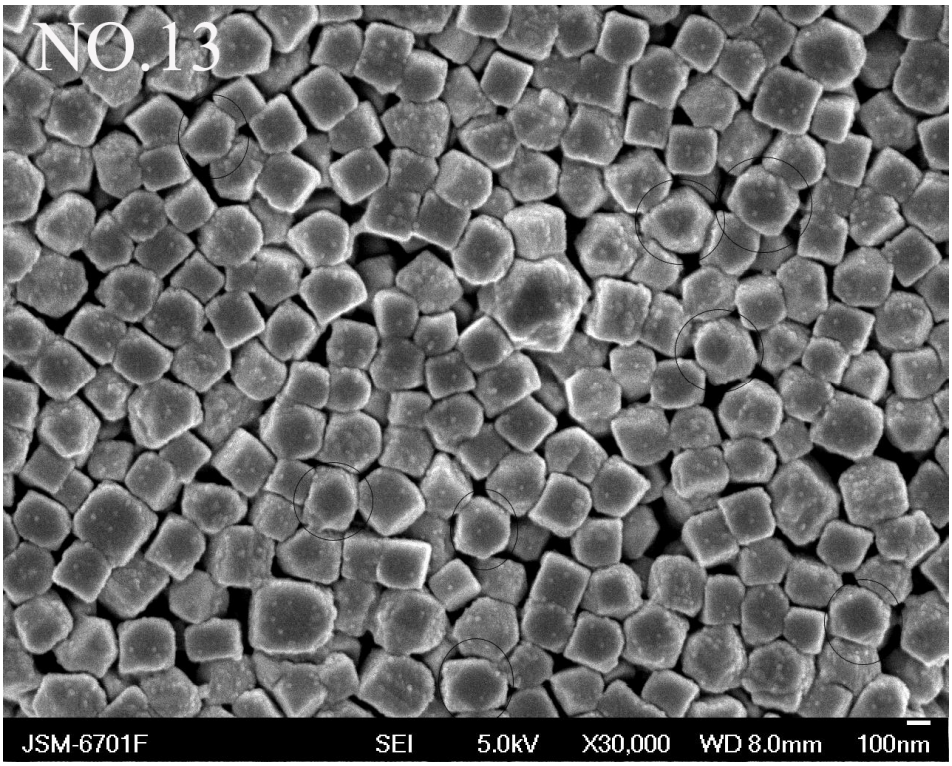
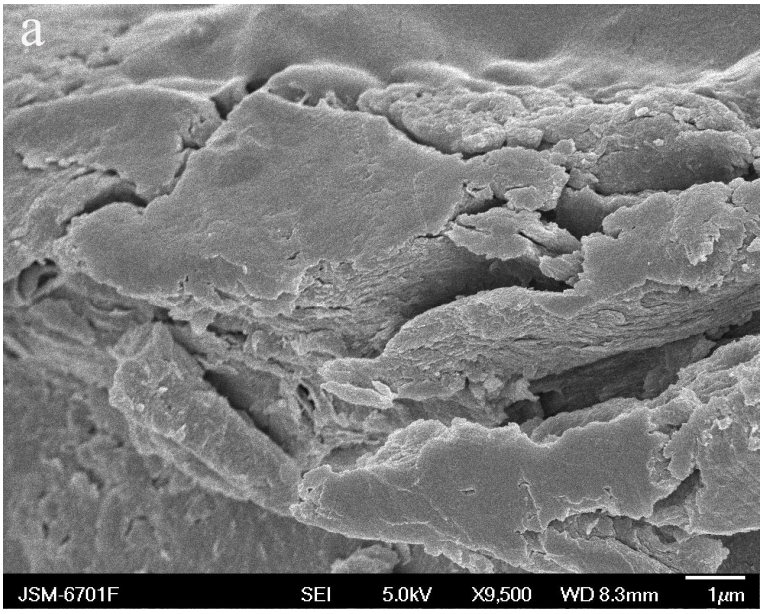


Note: some cuboctahedron were marked with a circle, which gave direct evidence that the shape evolution from cube to octahedra.



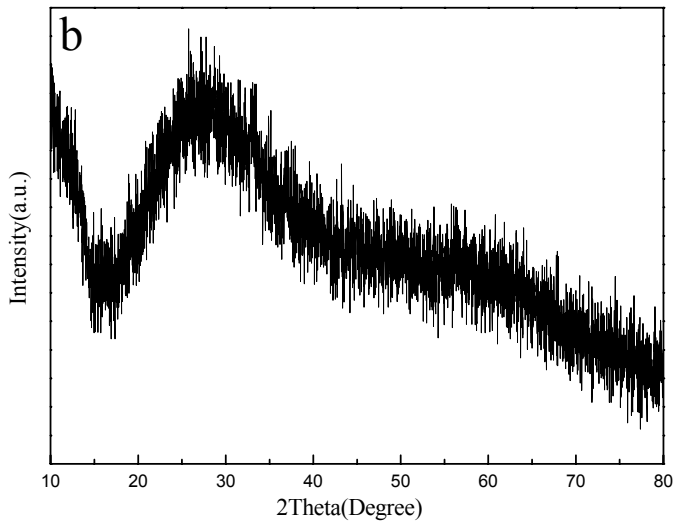
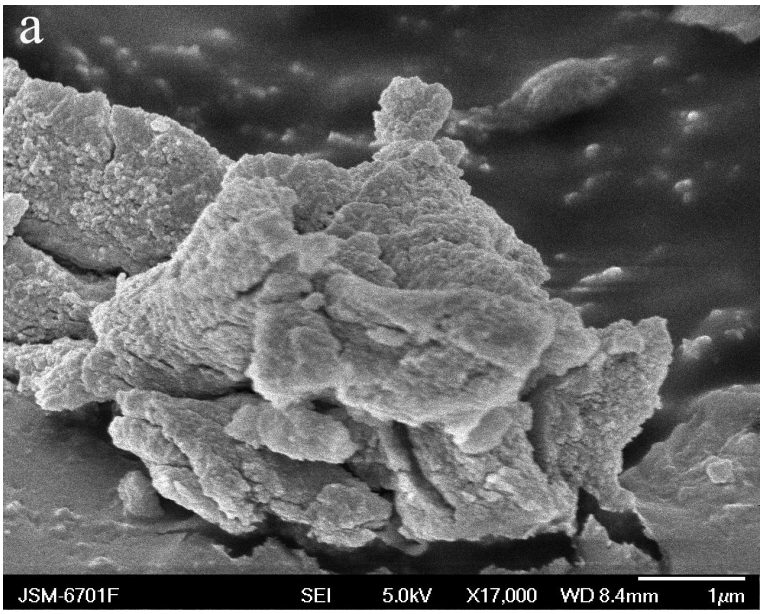


Fig. S14 FESEM image and XRD pattern of the product, TAA as the sulfur source, PVA=10 mL, PVP=0.20 g, and [NaOH] =0.14 M.



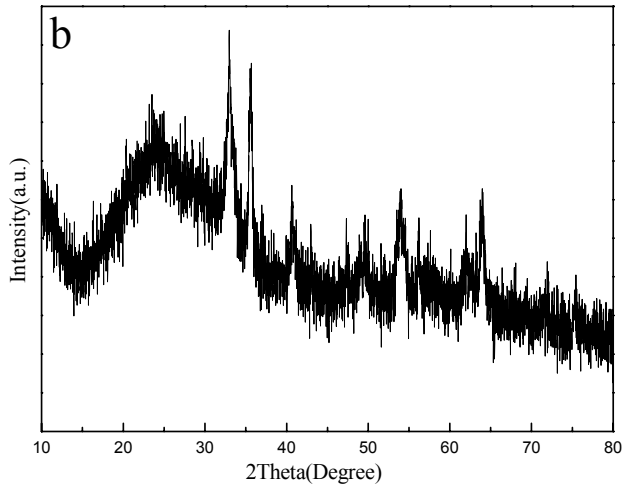
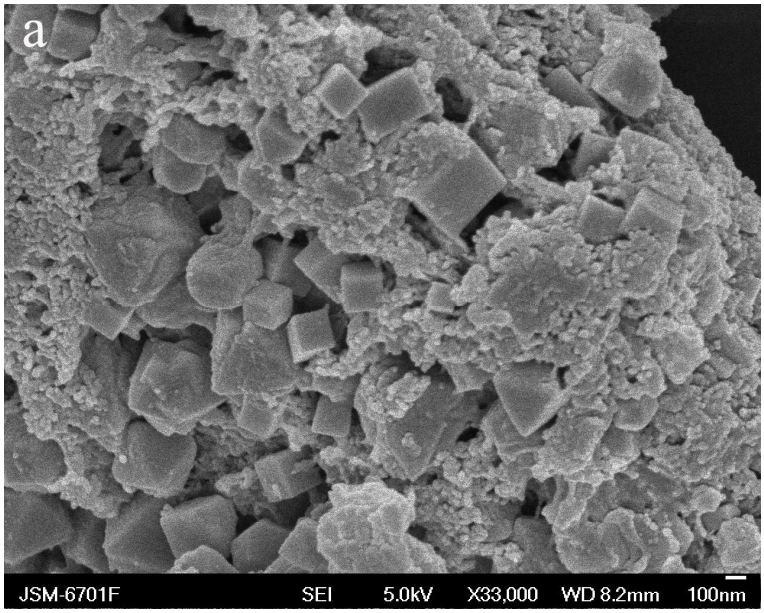


Fig. S15 FESEM image and XRD pattern of the product, S dosage is 0.10 g, PVA=10 mL, PVP=0.20 g, and [NaOH] =0.14 M.



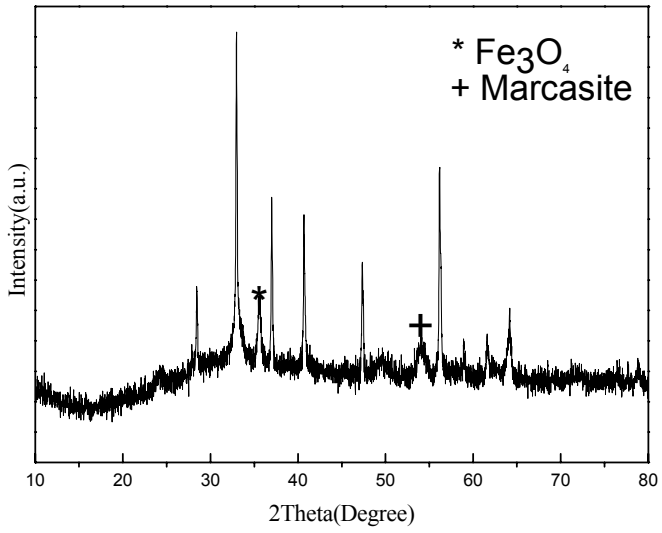


Fig. S16 FESEM image and XRD pattern of the product, S dosage is 0.16 g, PVA=10 mL, PVP=0.20 g, and [NaOH] =0.14 M.

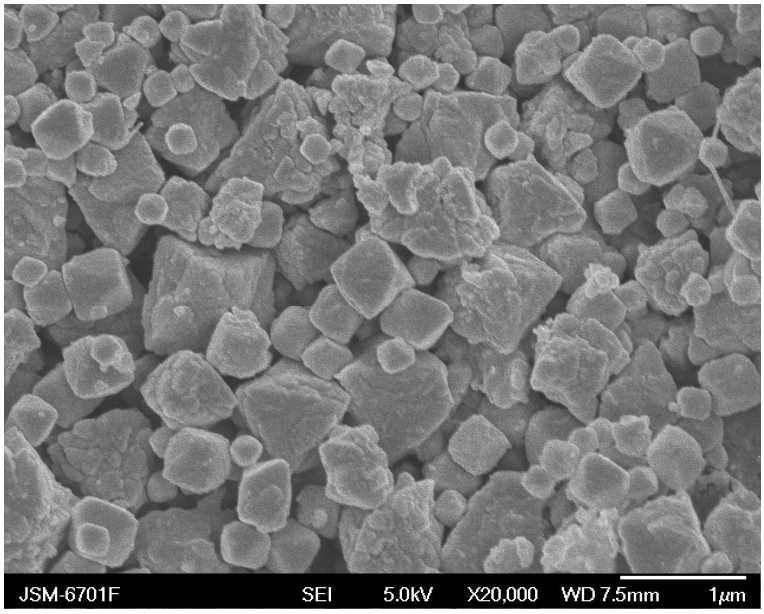


Fig. S17 FESEM image of the product, PVA=10 mL, PVP=0.2 g and [NaOH] =0.11 M at the temperature of 433 K.

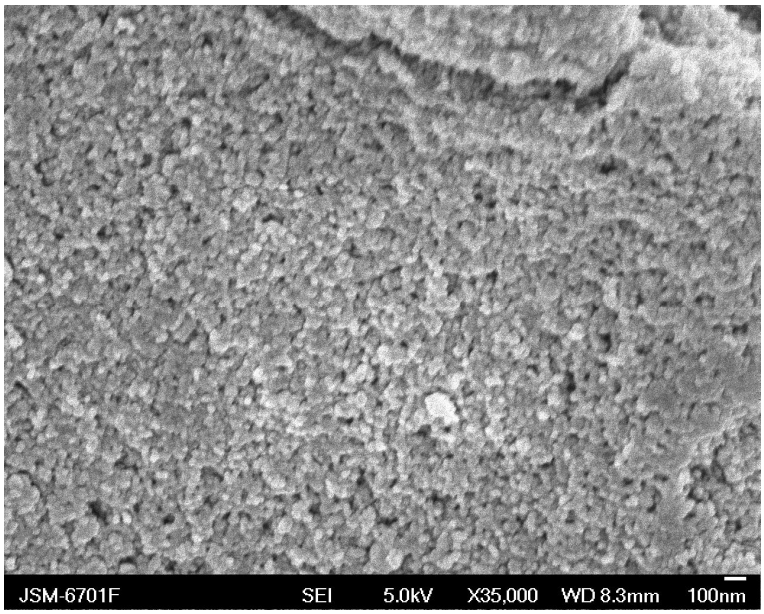


Fig. S18 FESEM image of the product, PVA=10 mL, PVP=0.20 g, and [NaOH] =0.29 M.

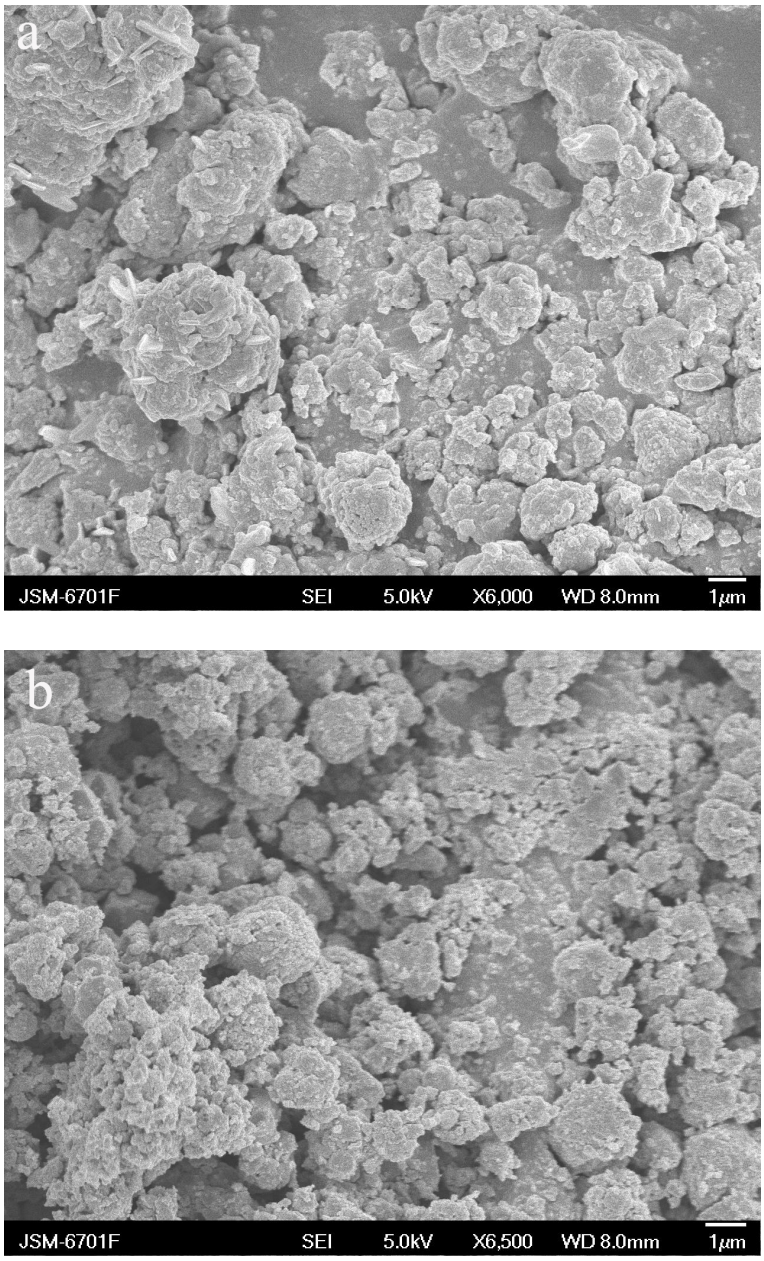


Fig. S19 FESEM images of the product with employing different surfactants (a) 0.3 g of CTAB, and (b) 0.3 g of SDBS.