# Dynamic behavior of metal nanoparticles in MOF materials: analysis with electron microscopy and deep learning

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## 1. TEM analysis of MOF materials

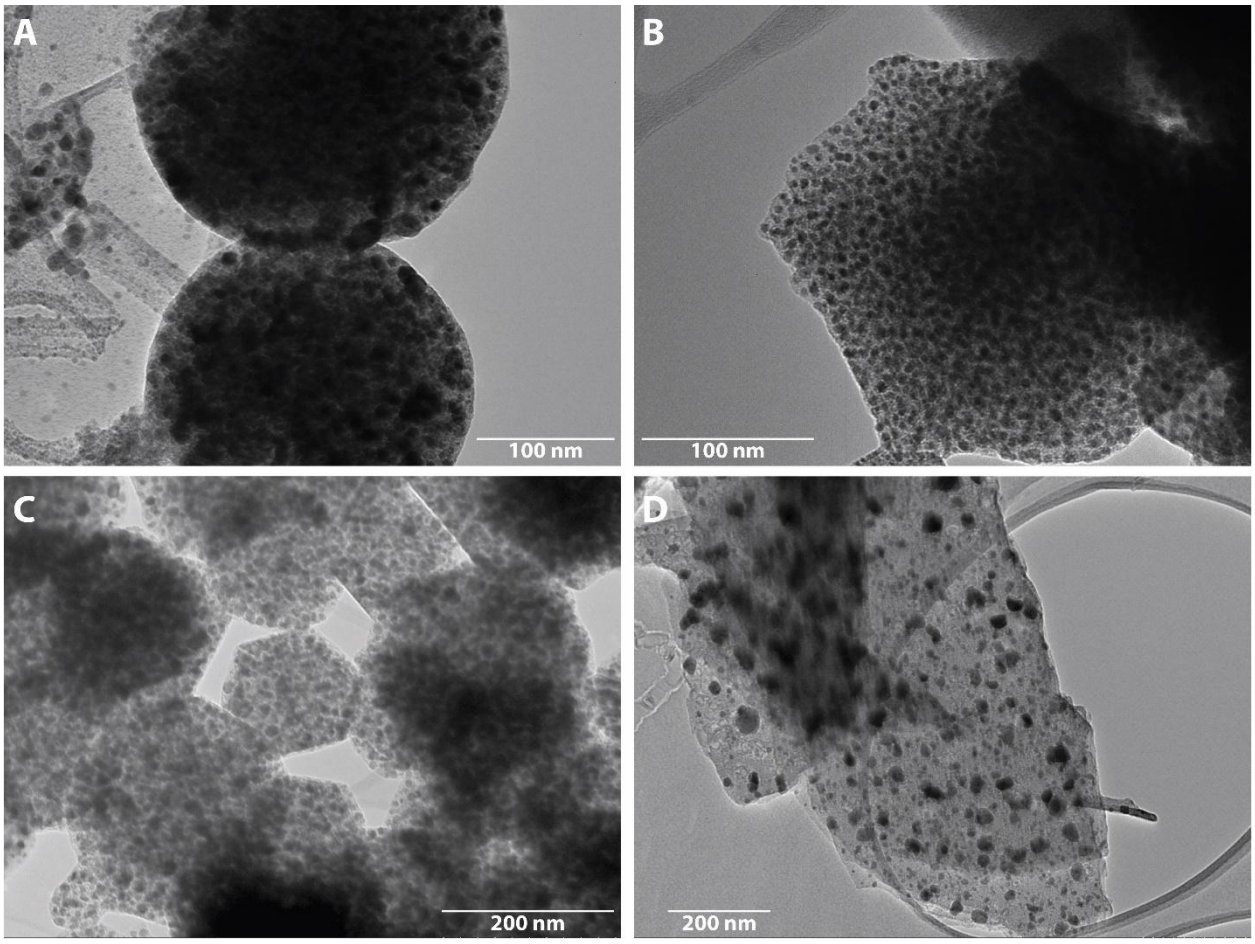


**Figure S1.** TEM images of MOFs, which are unstable under an electron beam: (A) MIL-101(Fe); (B) $NH_2$-MIL-101(Fe); (C) ZIF-67(Co); (D) BIF-66(Co). Electron beams cause MOF decomposition and the formation of nanoparticles.

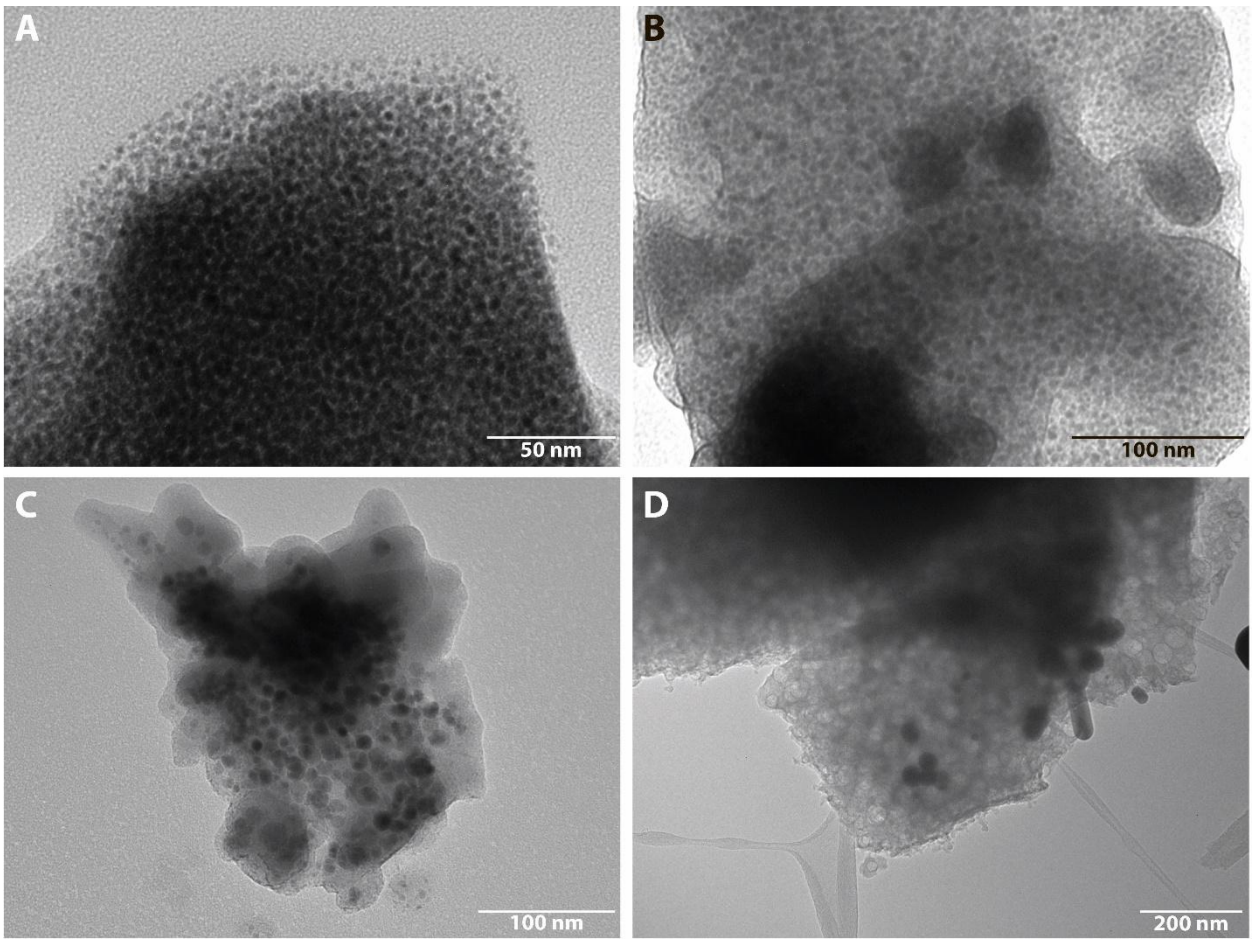


**Figure S2.** TEM images of MOFs unstable under an electron beam: (A) Ni(BDC); (B) Ni(BTC); (C) MOF-74(Ni); (D) HKUST-1(Cu). Electron beams cause MOF decomposition and the formation of M-NP.

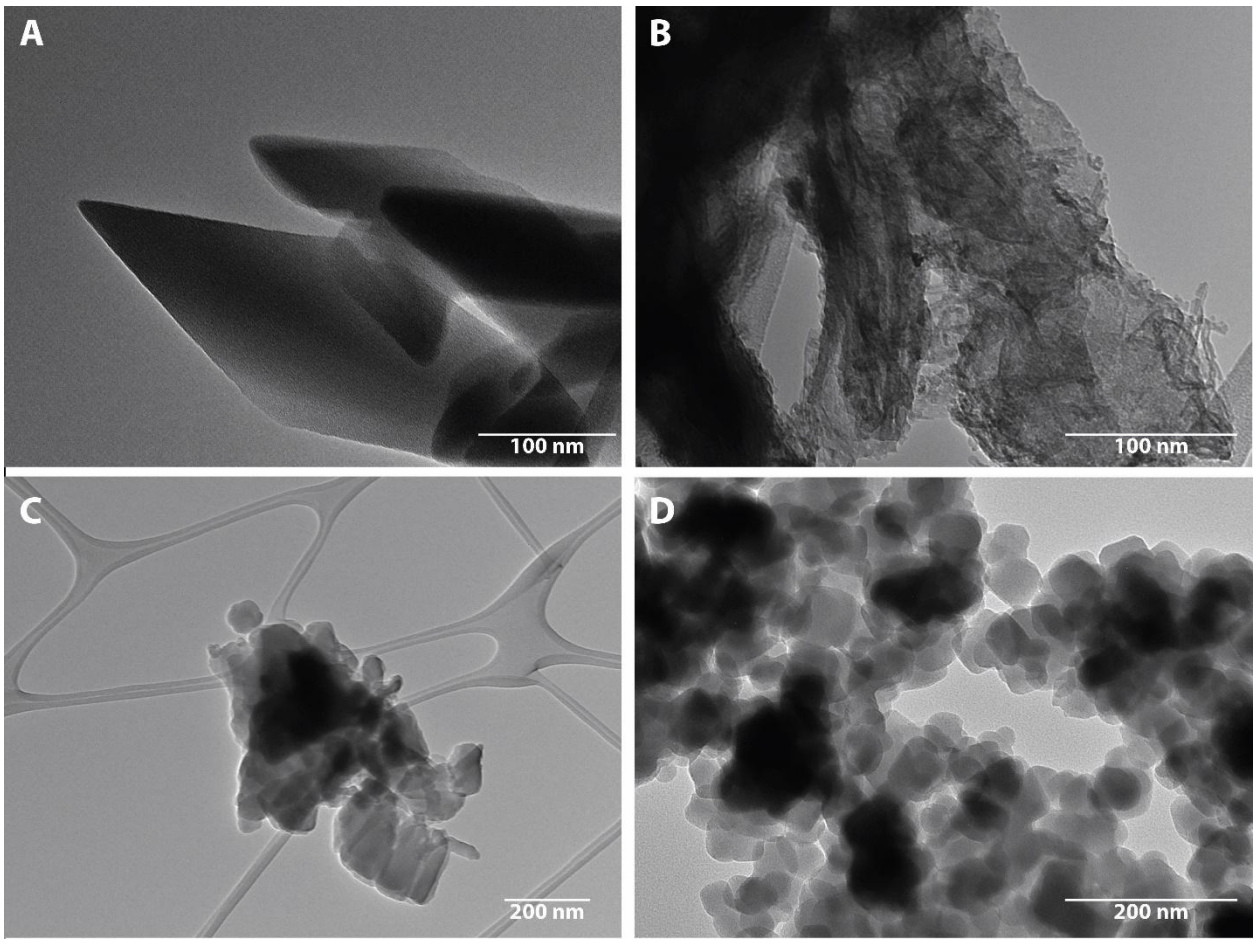


**Figure S3.** TEM images of MOFs stable under an electron beam: (A) MIL-53(Al); (B) $NH_2$-MIL-53(Al); (C) $NH_2$-MIL-101(Al); (D) ZIF-8(Zn).

## 2. TGA analysis

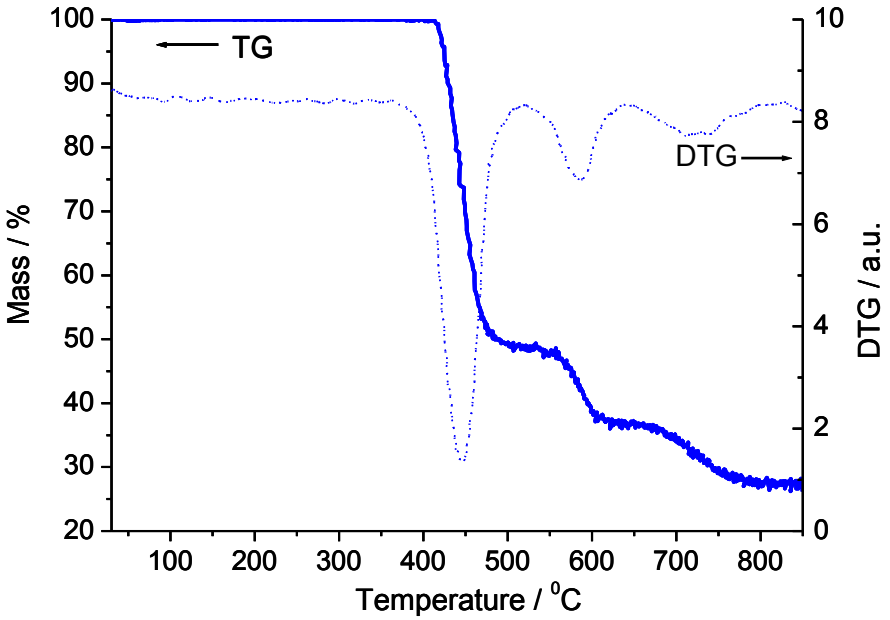


**Figure S4.** TG, DTG curves for sample BIF-66.

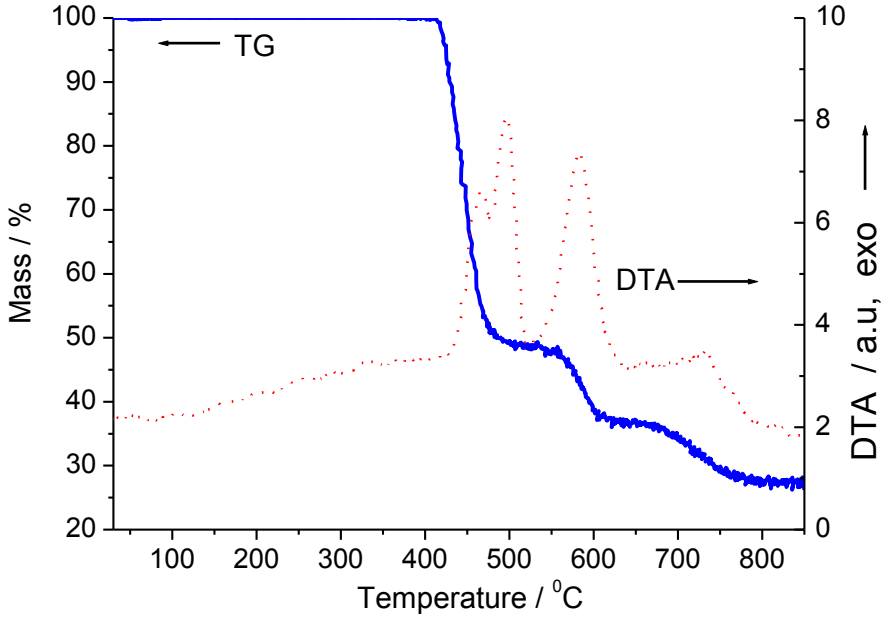


**Figure S5.** TG, DTA curves for sample BIF-66.

## 3. Powder XRD analysis

For MOF samples MIL-53(Al), $NH_2$-MIL-101(Al), $NH_2$-MIL-53(Al), ZIF-8(Zn), MIL-101(Fe), $NH_2$-MIL-101(Fe), BIF-66, ZIF-67, and HKUST-1, X-ray powder diffraction data were collected (22°C) in a reflection mode utilizing a Panalytical EMPYREAN instrument equiped with a linear X'celerator detector and non-monochromated Ni-filtered Cu $K_\alpha$ radiation ($\lambda$=1.5418 Å). Measurement parameters are as follows: tube voltage/current 45 kV / 40 mA, divergence slits of 1/8 and 1/4$^o$, 2$\theta$ range 3-40$^o$, speed 1$^o$ min$^{-1}$.

PXRD patterns of NiBTC and MOF-74(Ni) were collected with a diffractometer DRON-2 using the following mode: 2$\Theta$=10-60° range, rate 1°/min, Cu $K_\alpha$ radiation (30 kV, 30 mA), Ni-filter.

Micro-powder X-ray diffraction was used for NiBDC analysis and was carried out on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (kappa geometry, shutterless $\omega$-scan technique), using monochromatized Cu $K_\alpha$ radiation (50 kV, 1 mA). Samples were fixed on the loop utilizing grease (Dow corning). Data were collected at 22°C, exposure time was 300 s and detector distance was 120 mm in 2$\theta$ range 0-50°.

XRD patterns of the synthesized MOF samples, i.e., $NH_2$-MIL-101(Al), BIF-66, ZIF-67, HKUST-1, NiBTC, and MOF-74(Ni) are consistent with those reported in literature.[1-4]

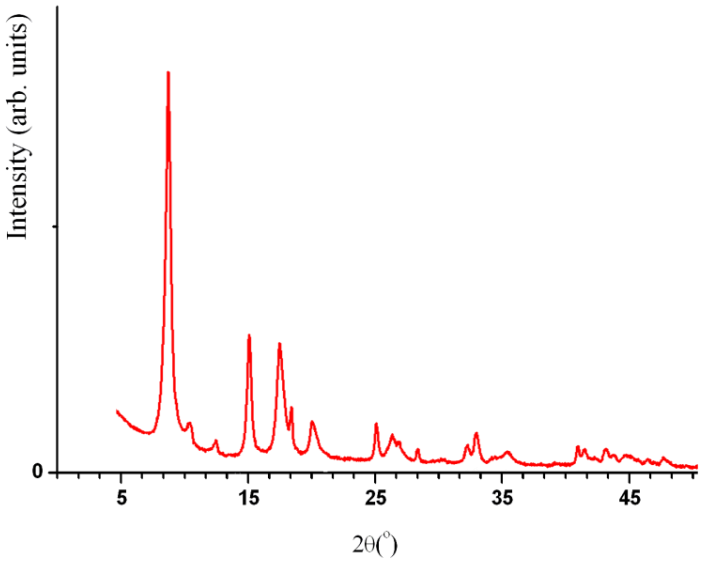


**Figure S6.** PXRD pattern of MIL-53(Al).

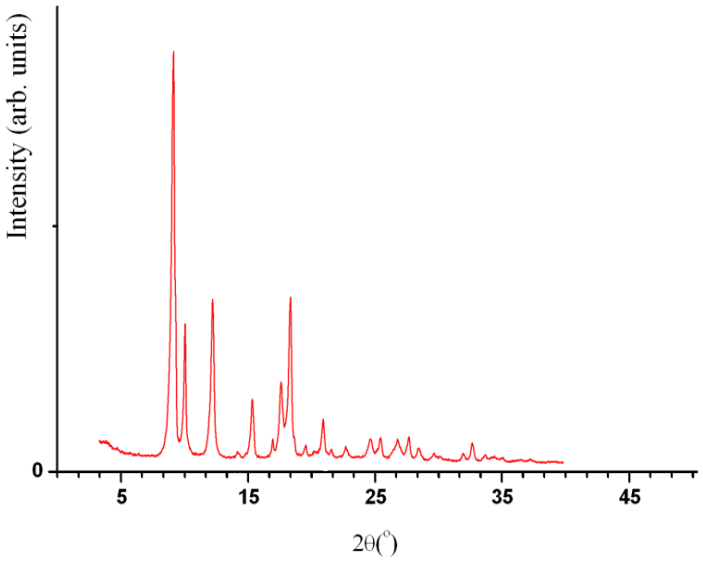


**Figure S7.** PXRD pattern of $NH_2$-MIL-53(Al).

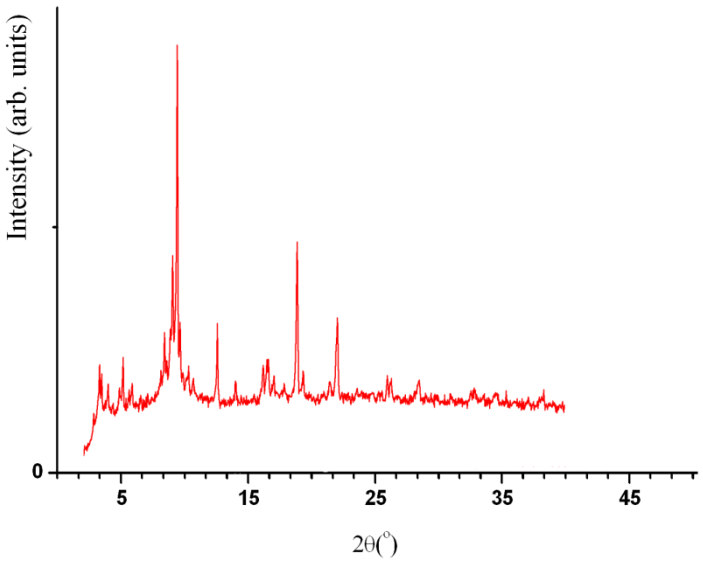


**Figure S8.** PXRD pattern of MIL-101(Fe).

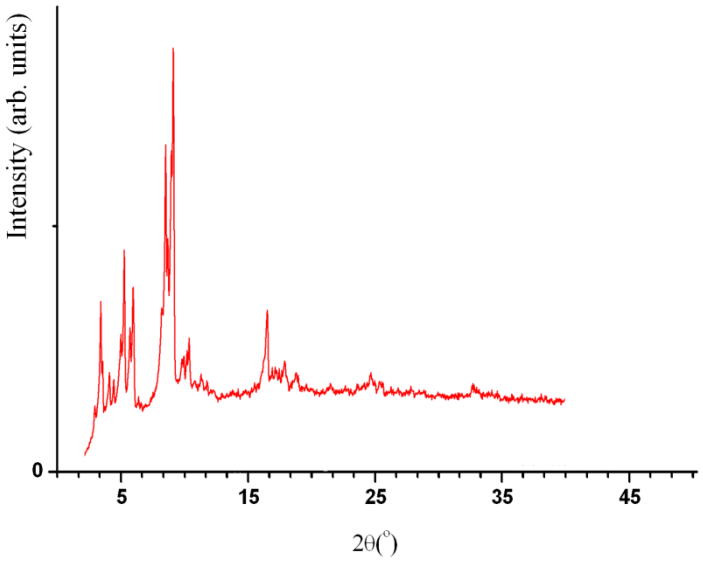


**Figure S9.** PXRD pattern of $NH_2$-MIL-101(Fe)

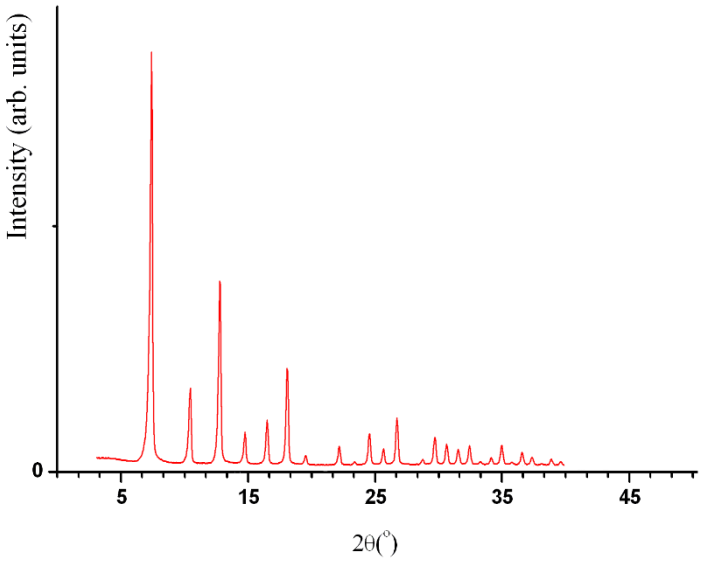


**Figure S10.** PXRD pattern of ZIF-8.

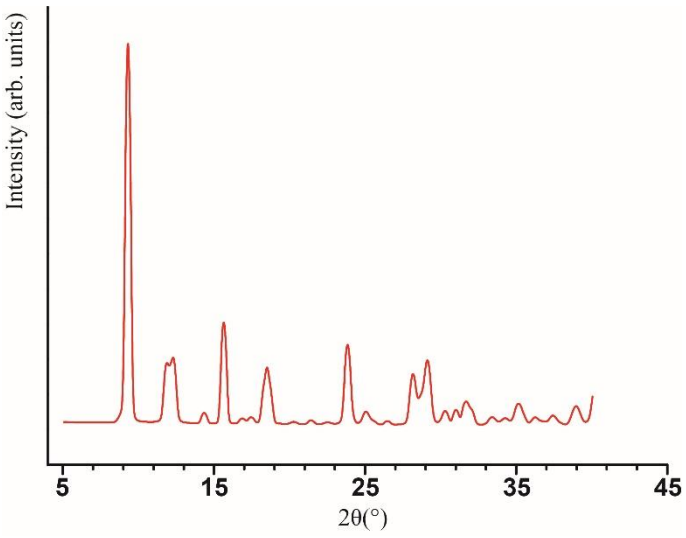


**Figure S11.** PXRD pattern of NiBDC.

## 4. Analysis with HR-TEM

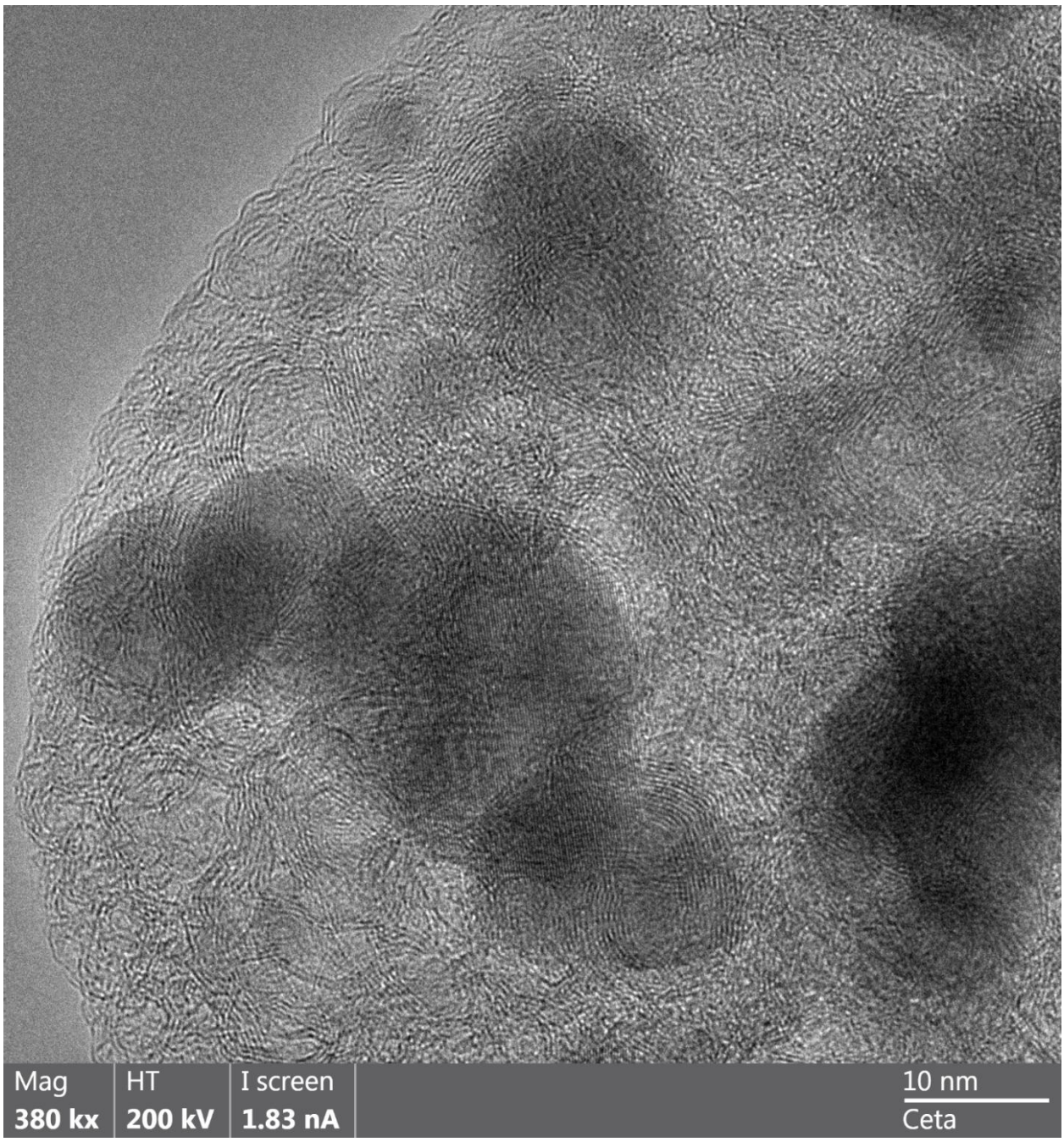


**Figure S12.** HR-TEM image of ZIF-67 with formed Co NPs.

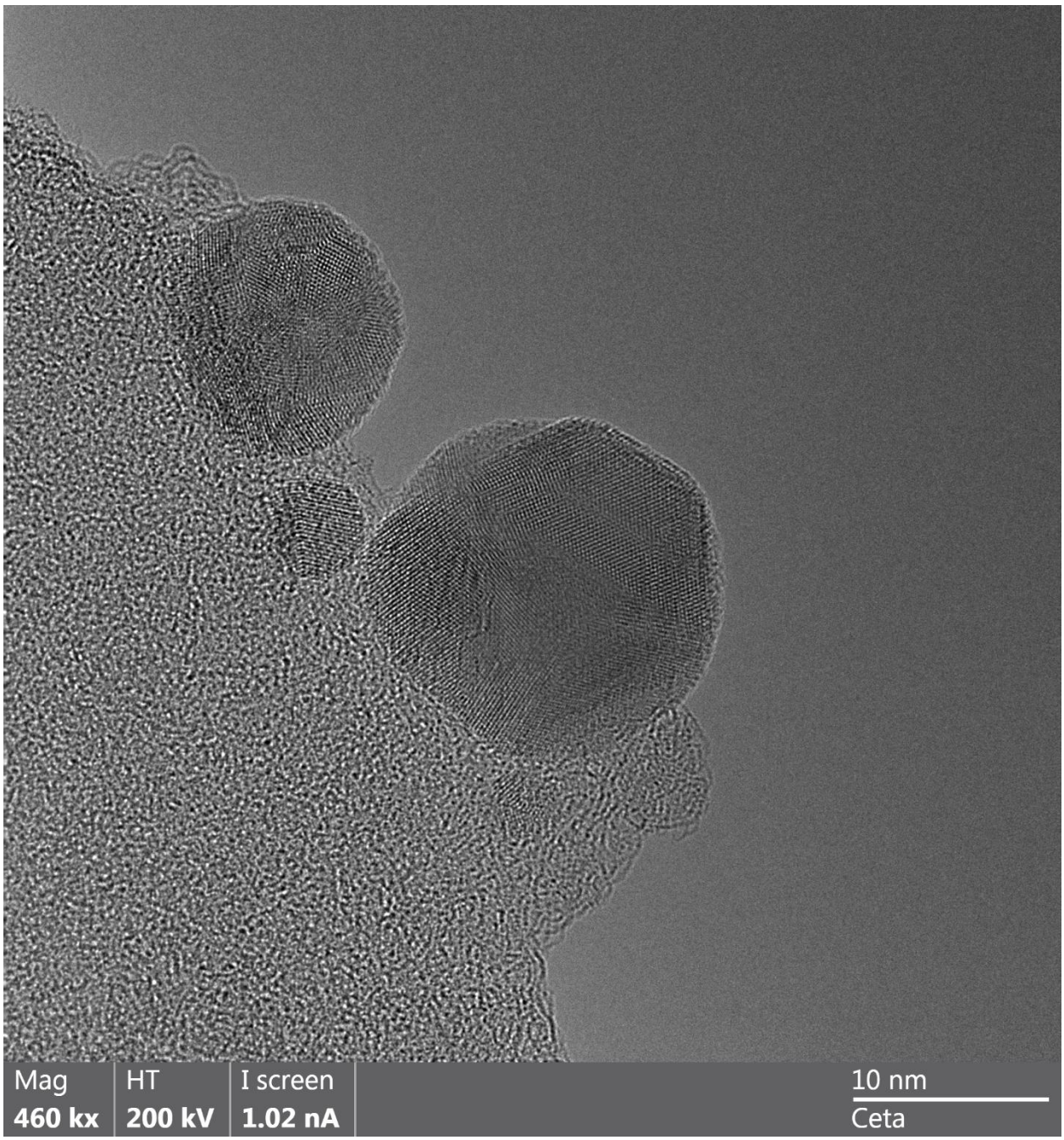


**Figure S13.** HR-TEM image of HKUST-1 with formed Cu NPs.

## 5. SAED analysis

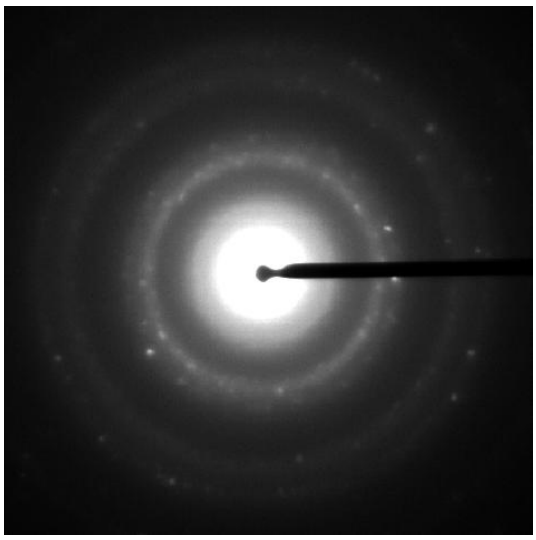

**Figure S14.** ED pattern of ZIF-67 particle with formed Co NPs.

## References


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