Supporting Information

Stability assessment in aqueous and organic solvents of metal-organic framework PCN 333 nanoparticles through a combination of physicochemical characterization and computational simulations

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KEYWORDS

metal-organic frameworks (MOF), stability, aqueous environment, molecular dynamics simulation, umbrella sampling

Method

Preparation of PCN-333(Al) and PCN-333 (Fe):

As previously reported,[1] 10 mL DMF solution of $AlCl_3 \cdot 6H_2O$ (1.5 mg mL^{-1}), 5 mL DMF solution of H_3TATB (1 mg mL^{-1}), 15 mL DMF and 50 μL TFA was mixed and heated at 95 °C for 24 h. nPCN-333 (Al) was collected by centrifugation.

10 mL DMF solution of $FeCl_3$ (1.5 mg mL^{-1}), 5 mL DMF solution of H_3TATB (1 mg mL^{-1}), 15 mL DMF and 50 μL TFA was mixed and heated at 120 °C for 24 h. nPCN-333 (Fe) was collected by centrifugation.

Result

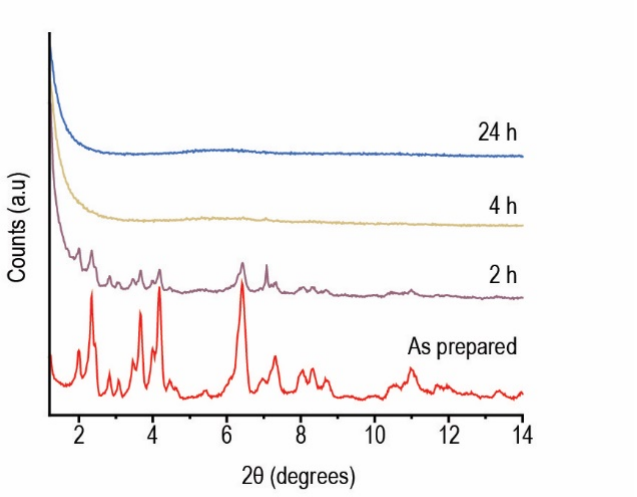

Figure S1 The change of the XRD patterns of nanosized-PCN-333 (Al) while soaking in water over time.

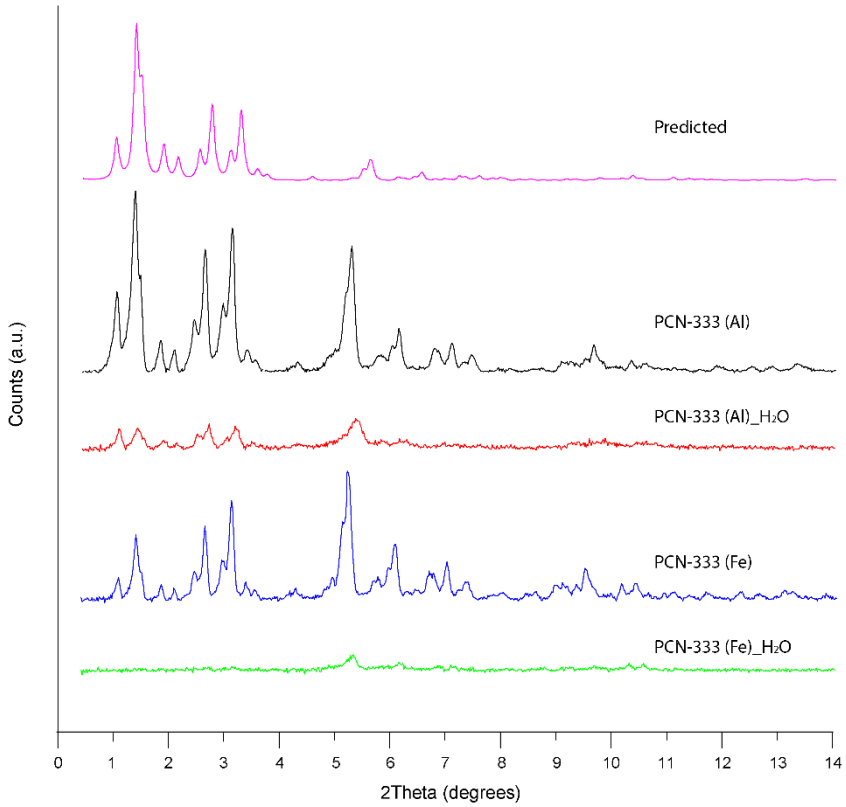

Figure S2 The XRD patterns of PCN-333(Al) and PCN-333 (Fe) particles before and after soaking in H_2O for 4h.

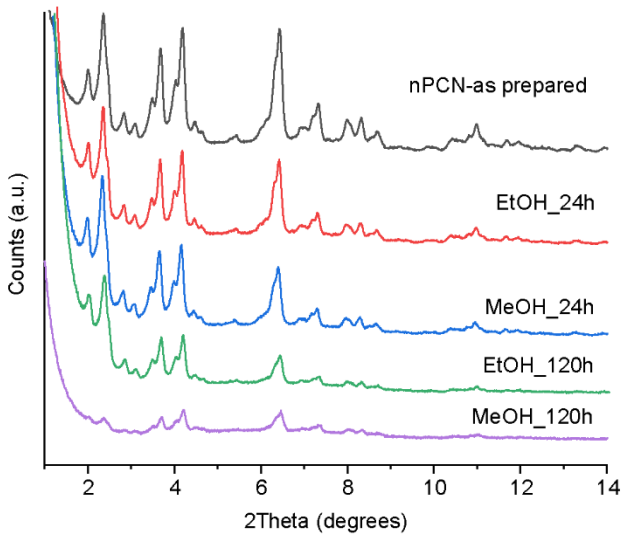

Figure S3 The XRD patterns of nPCN soaking in EtOH and MeOH at 60 ℃ for 24h and 120h.

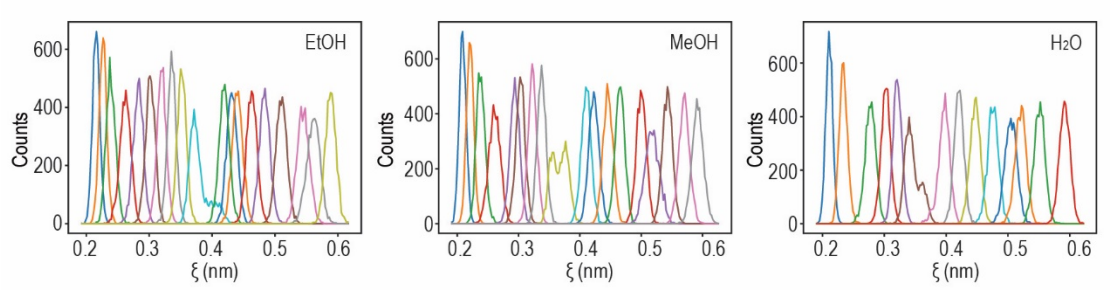

Figure S4 The histograms for each umbrella sampling simulation.

Reference

(1) Lian, X.; Erazo-Oliveras, A.; Pellois, J. P.; Zhou, H. C. High Efficiency and Long-Term Intracellular Activity of an Enzymatic Nanofactory Based on Metal-Organic Frameworks. *Nat Commun* 2017, *8* (1) 6969-6973. https://doi.org/10.1038/s41467-017-02103-0.