

Supporting Information

Laser-Driven Rapid Synthesis of Metal Organic Frameworks, Quantum Chemical Analysis and Investigation of UV-NIR Optical Absorption, Luminescence, Photocatalytic Degradation, and Gas and Ion Adsorption Properties

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Supplemental experimental procedures

S.1. Experimental Section

S.1.1. Synthesis of Lg-Based MOF (bpeMOF)

Zn(NO₃).H₂O and 1,2-bis(4-pyridyl) ethane (bpe) (14.04 mg, 0.066 mmol) were mixed in solvents [DMF/H₂O = 1:1 (v/v)]. The resulting solution was stirred for 5 minutes. Whitish in color bpeMOF crystals was synthesized in 70 minutes using a laser beam source at 88-90°C.

S.1.2. Synthesis of H₂L Based MOF (H₂LMOF)

Zn(NO₃)₂·6H₂O (10 mg, 0.033 mmol) and H₂L (11.46 mg, 0.033 mmol) were mixed in solvents [DMF/H₂O = 1:1 (v/v)]. The resulting solution was stirred for 5 minutes. Yellow colored H₂LMOF crystals was synthesized in 70 minutes using a laser beam source at 88-90°C

S.2. Material Characterization of Laser-Driven bpe(MOF) and H₂L(MOF)

2.1. Structure Characterization

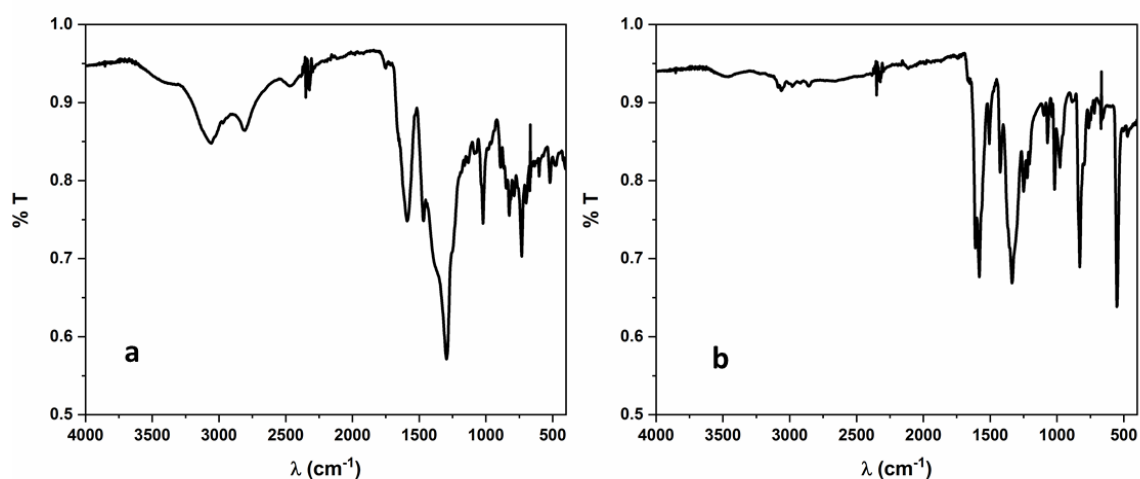


Figure S1. FTIR spectrum of H₂L(MOF) (a) and bpe(MOF) (b)

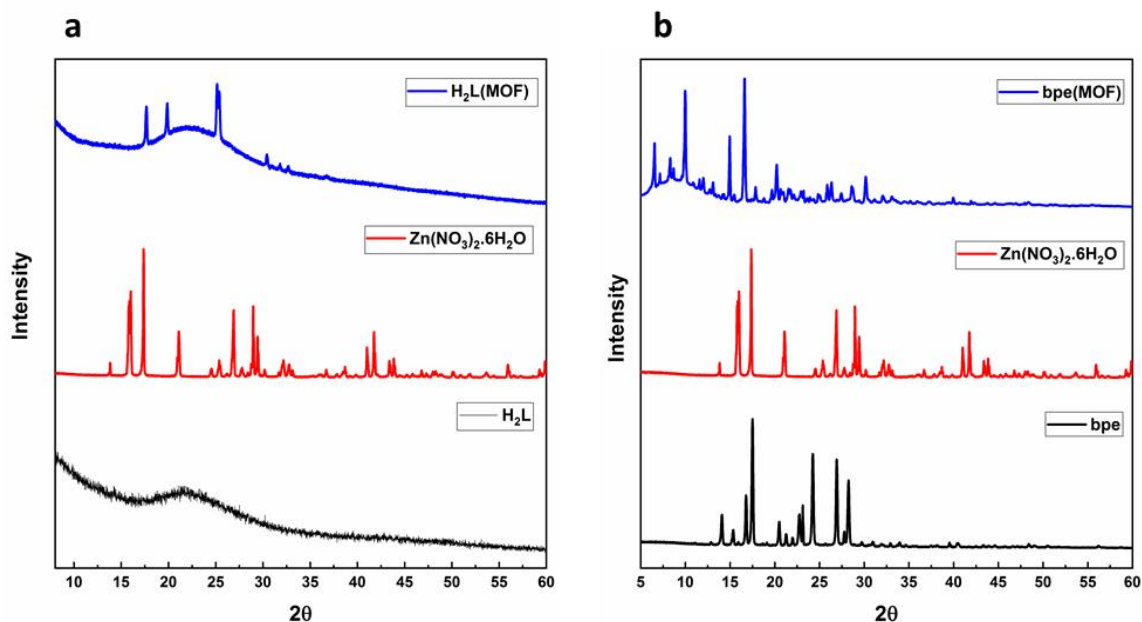


Figure S2. XRD spectrum of zinc salt, a H₂L and H₂L(MOF) structures (a) XRD spectrum of zinc salt, bpe and bpe(MOF) (b)

It is seen that the crystal structure formation is more in bpe(MOF), while the amorphous structure of H₂L(MOF) is exhibited.

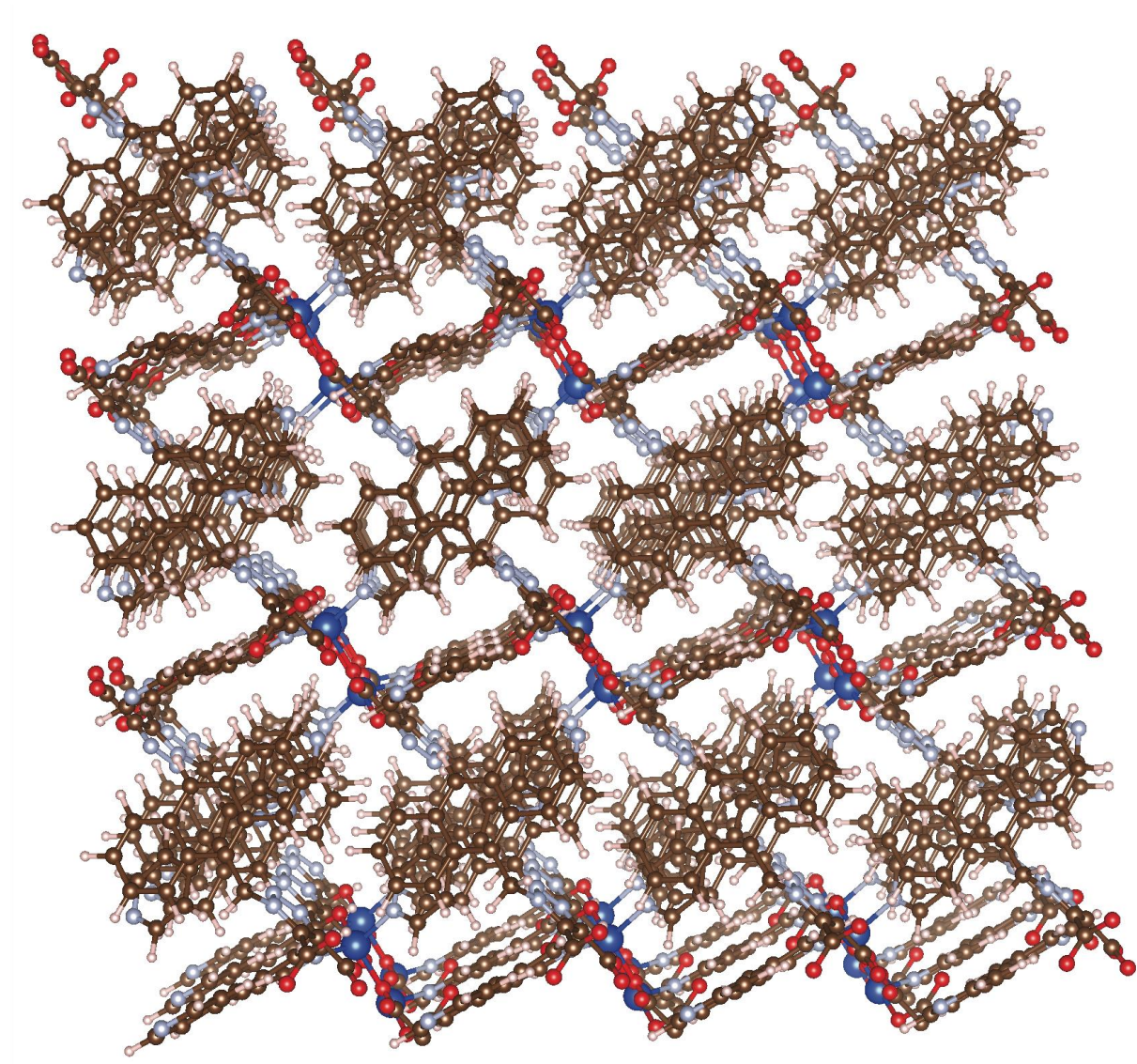


Figure S3: The 3D crystalline structure of ZnMOF. The dark blue, light blue, red, brown, and white spheres represent Zn, N, O, C, and H atoms respectively.

2.2. Photophysical Properties

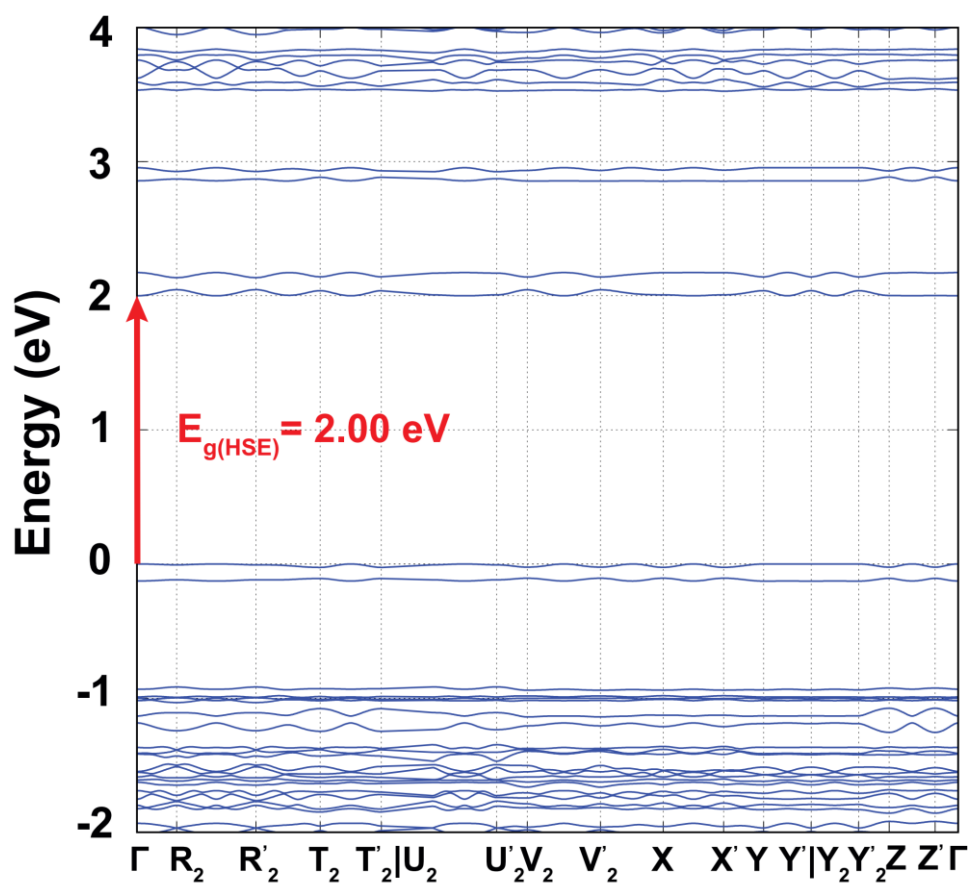


Figure S4. The electronic band structure of ZnMOF along all symmetry directions

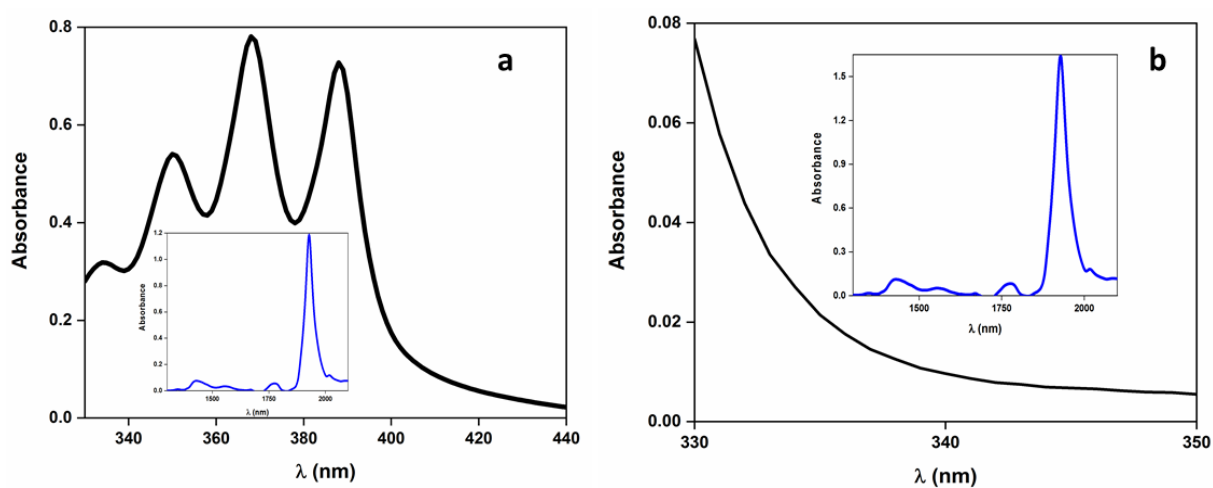


Figure S5. UV-Vis-NIR absorption spectrum in DMF (1mg/3ml) $\text{H}_2\text{L}(\text{MOF})$ (a) and $\text{bpe}(\text{MOF})$ (b)

In Figure S5B, while there are no absorption peaks in the Uv-vis region of BPE(MOF), the presence of absorption peaks belonging to both MOF structures in the NIR region is seen.

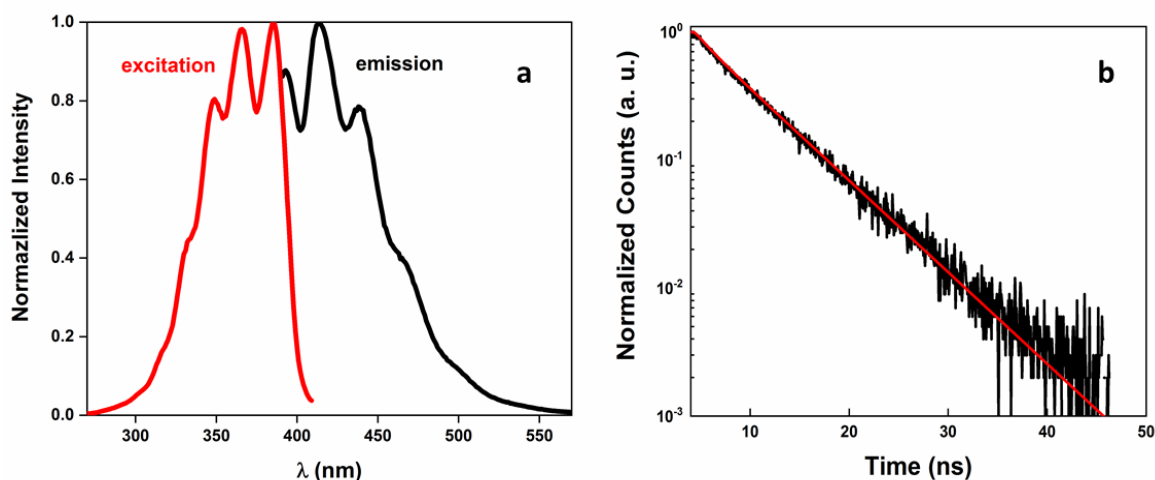


Figure S6. Fluorescence excitation (λ_{obs} 413 nm) and emission (λ_{exc} 366 nm) spectrum of H₂L (MOF) in ethanol at room temperature **(a)**. Time-resolved emission decay curves of H₂L (MOF) at 413 nm under ambient conditions, where the red line indicates the fitting curves and the black line indicates the experimental data **(b)**.

The singlet excited state energy of H₂L(MOF) was estimated 306.7 kJ mol⁻¹. Fluorescence quantum yield measurement was performed by using of 9,10-diphenylanthracene (ϕ_f = 0.95 in ethanol) as standard and ϕ_f was found to be 63.0%. It also has fluorescence lifetimes of 1.4 and 6.0 ns.

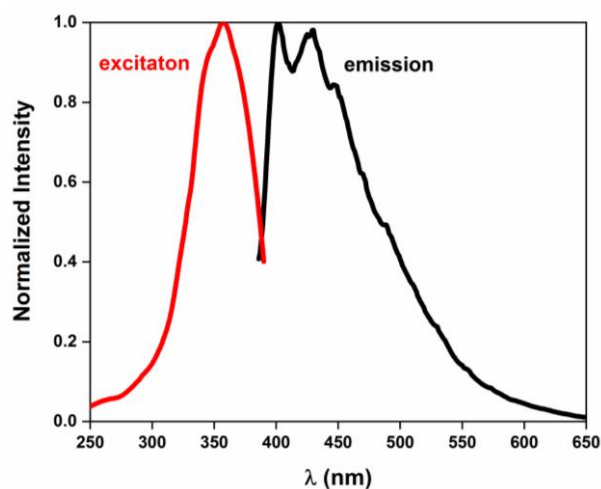


Figure S7. Fluorescence excitation (λ_{abs} 355 nm) and emission (λ_{exc} 398 nm) spectrum of bpe(MOF) in ethanol at room temperature

The singlet excited state energy of bpe(MOF) was estimated 309.11 kJ mol⁻¹. The ligand, which does not have photoluminescent chromophore groups, has no fluorescence quantum efficiency and lifetime of the metal organic framework structure.

2.3. Morphological Characterization

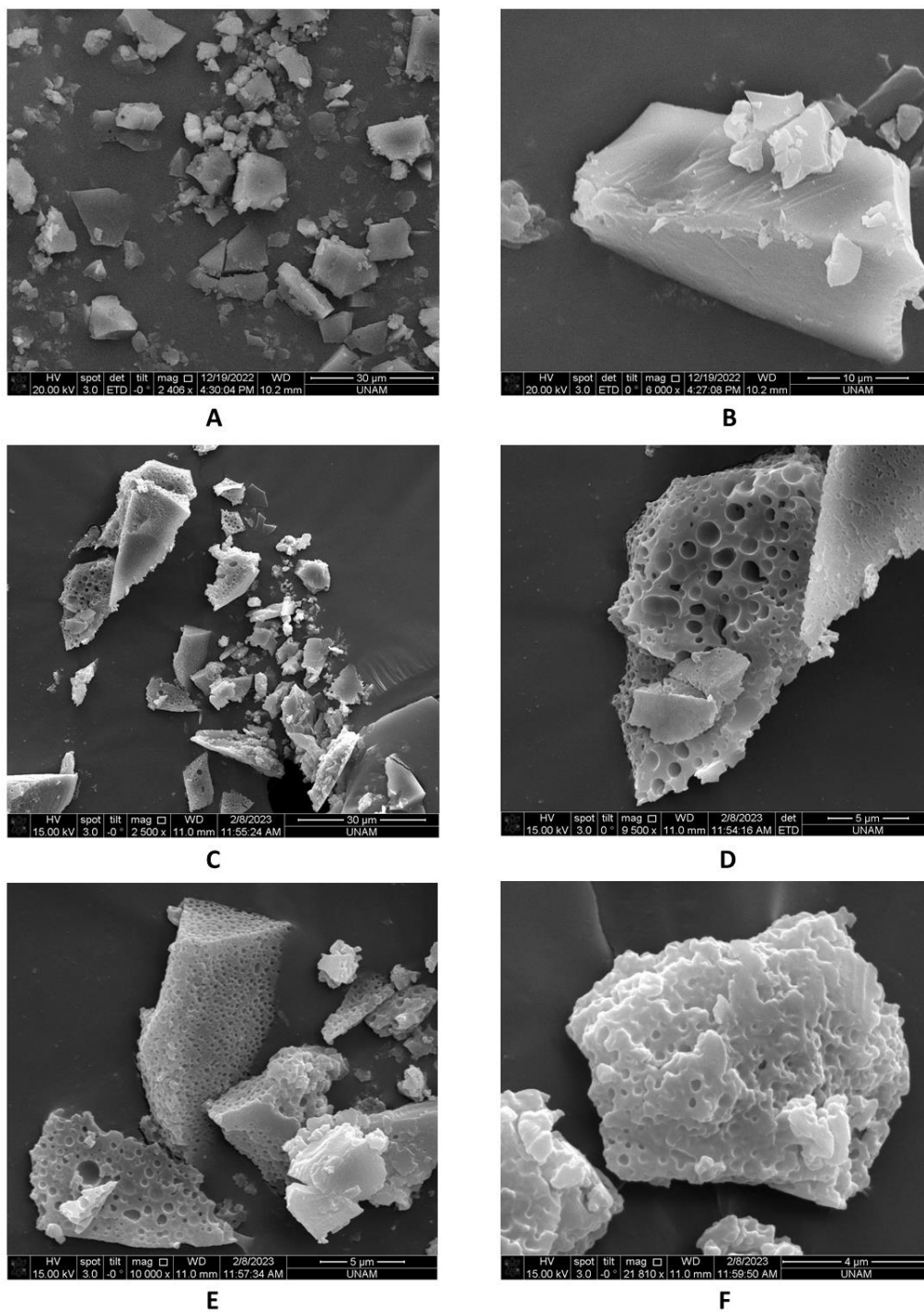
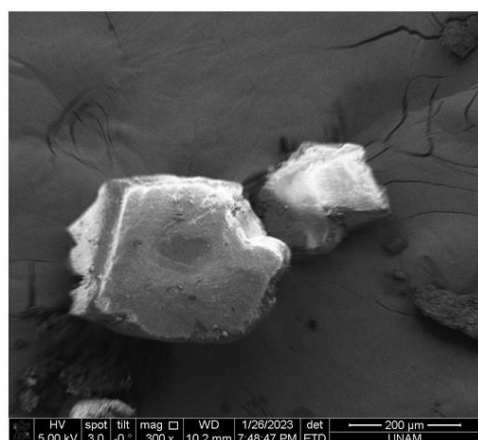
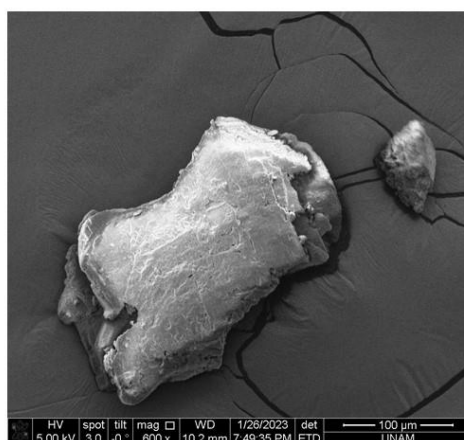


Figure S8. SEM images of H₂L (A,B) and H₂L(MOF) at 70 min (C-F)

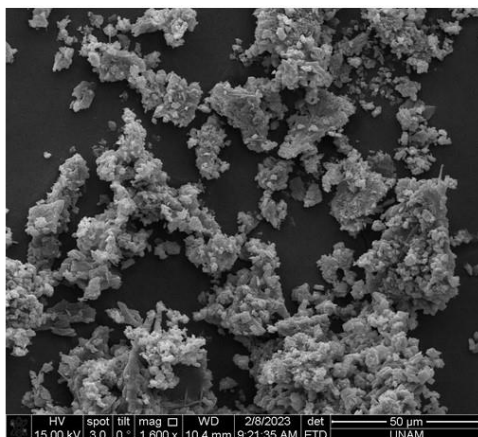
When the SEM images of H₂L(MOF) are examined, it is seen that the perforated structures with layers are formed.



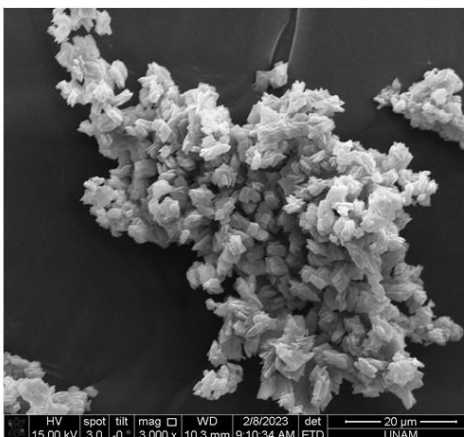
A



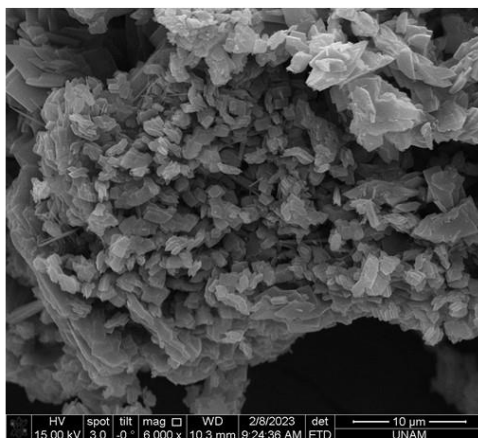
B



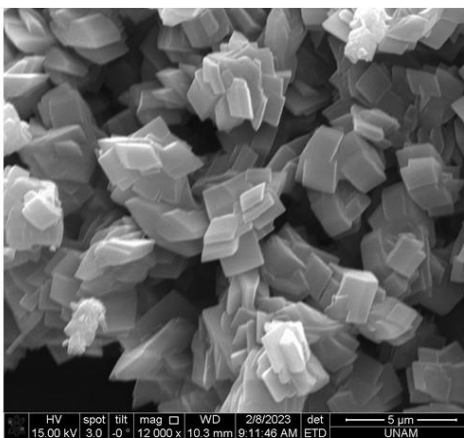
C



D



E



F

Figure S9. SEM images of bpe (A,B) and bpe(MOF) at 70 min (C-F)