

Supporting Information

**A Cerium-Based MOF: Dual-Functional Catalyst
for Organic Pollutant Remediation**

1. Experimental section:

Ceric ammonium nitrate ($(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$) and terephthalic acid were procured from Sigma-Aldrich and used without any further purification. Distilled water was used as green solvent for synthesis. The synthesis of Ce-BDC was carried out following a previously reported method [1]. Initially, 0.274 g (0.5 mM) of Ceric(IV) ammonium nitrate in 5 mL distilled water (Solution 1) and 0.166 g (1 mM) of BDC in 5 mL DMF (Solution 2) stirred for 30 minutes. Then solution 1 was added slowly to Solution 2 under vigorous stirring. The resulting mixture was transferred to a Teflon lined autoclave and heated at 130°C for 6 hours. The resulted light-yellow particles were centrifuged, washed three times with DMF and water, refluxed in ethanol for 30 hours, and dried at 80 °C overnight to obtain the final product. The dried product was ground in to fine particles for characterization.

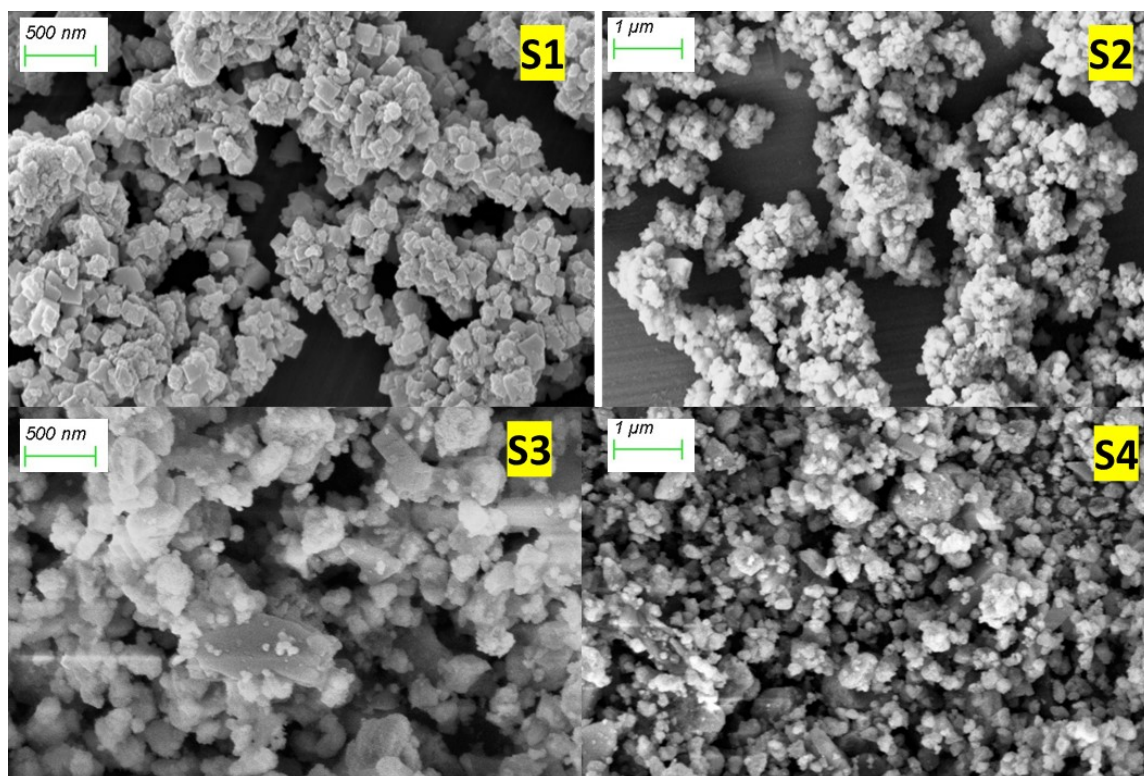
[1] M. Lammert, M. T. Wharmby, S. Smolders, B. Bueken, A. Lieb, K. A. Lomachenko, D. De Vos and N. Stock, *Chem. Commun.*, 2015, **51**, 12578–12581.

2. Characterization Techniques

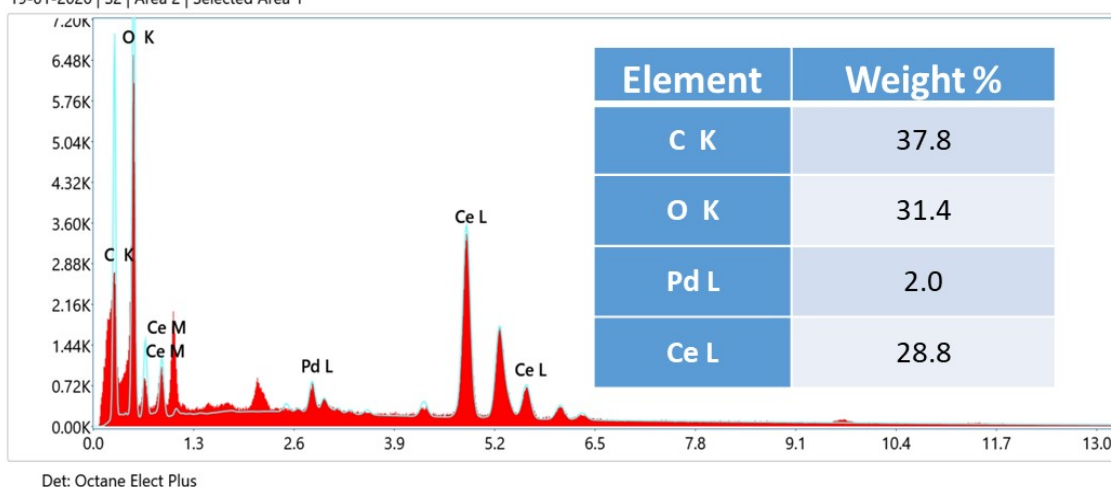
The crystalline structure and lattice parameters were analyzed by Powder X-ray Diffraction (PXRD) using a Bruker D8 Advance diffractometer equipped with Cu-K α radiation ($\lambda = 0.15406$ nm). Functional groups were identified using Fourier-transform infrared (FT-IR) spectroscopy (Thermo Scientific Nicolet iS5). Raman spectroscopy, conducted on a Renishaw Invia Raman microscope with a 632 nm laser and 10 s exposure time, provided insights into molecular vibrations. Optical absorption properties were assessed through UV-Visible diffuse reflectance spectroscopy (UV-Vis DRS) using a Jasco V-770 spectrophotometer. Surface morphology was investigated via field emission scanning electron microscopy (FE-SEM) using a Gemini SEM 450 equipped with Tungsten and LaB $_6$ filament sources. Nitrogen adsorption-desorption isotherms were recorded at 77 K with a Quantachrome analyzer to estimate surface area, pore size, and volume distribution. Elemental composition and oxidation states were examined by X-ray photoelectron spectroscopy (XPS) using Thermo Scientific Escalab 250Xi with Al K α radiation. Electrochemical behaviour and redox properties were evaluated through cyclic voltammetry (CV) using a BioLogic electrochemical workstation configured with a three-electrode system: Ag/AgCl (reference), platinum gauze (counter), and graphite (working) electrodes.

3. Field emission scanning microscopy (FESEM):

Fig. S1, S2. Field emission scanning microscopy (FESEM) images of Ce-BDC. **Fig. S3, S4.** Field emission scanning microscopy (FESEM) images of Pd@Ce-BDC. Scale bars are included in each paragraph.



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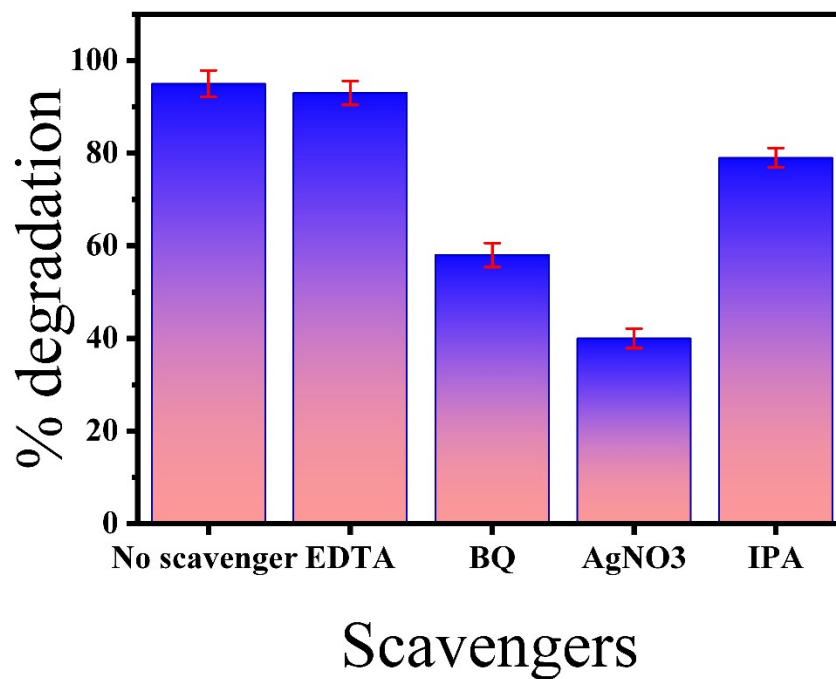
FESEM analysis of Ce-BDC (Fig. S1 and S2) revealed the presence of irregularly shaped, intergrown nanoparticles with a tendency to form aggregated clusters. The particles displayed rough surfaces and heterogeneous morphology matches with the literature [2].

References for FESEM:

[2] J. He, C. Pei, Y. Yang, B. Lai, Y. Sun and L. Yang, *J. Clean. Prod.*, 2021, **321**, 128778.

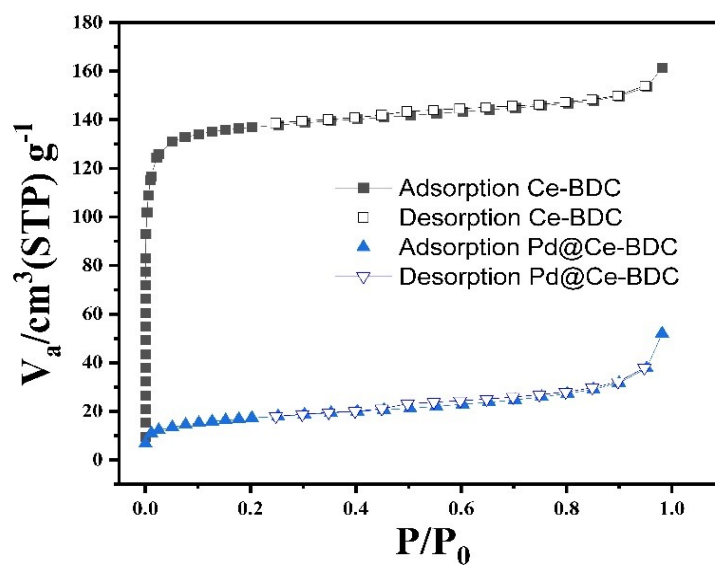
4. Scavenger Experiment

Fig. S5. Effect of various trapping agents in the presence of Pd@Ce-BDC for the degradation of Cr(VI)



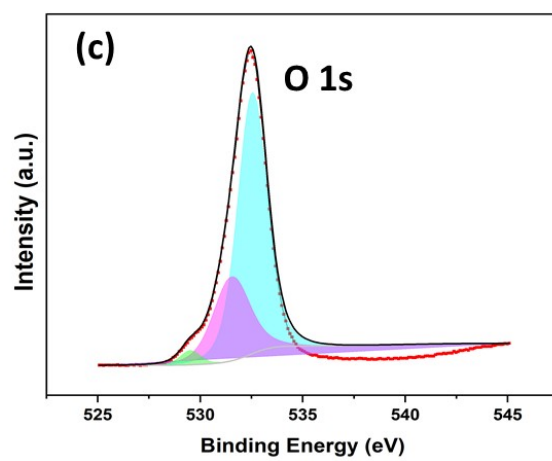
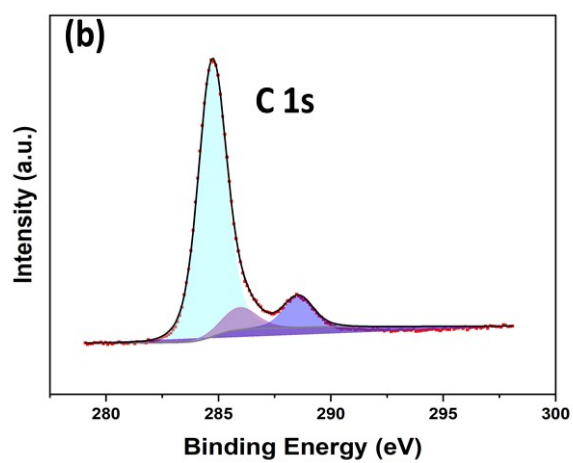
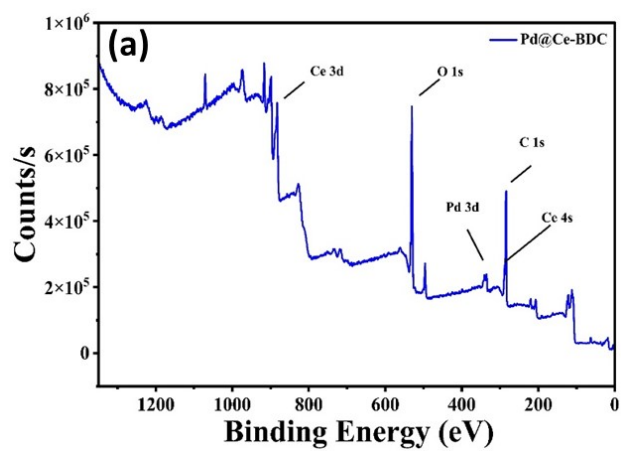
5. BET surface area

Fig. S6. N₂ adsorption/desorption isotherm of Pd@Ce-BDC at 77 K.



6. Full XPS spectrum

Fig. S7. Full XPS survey of (a) Pd@Ce-BDC (b) C 1s & (c) O 1s



7. Recyclability of Pd@Ce-BDC

Fig. S8 (a). Recyclability after reduction of 4-NP using Pd@Ce-BDC

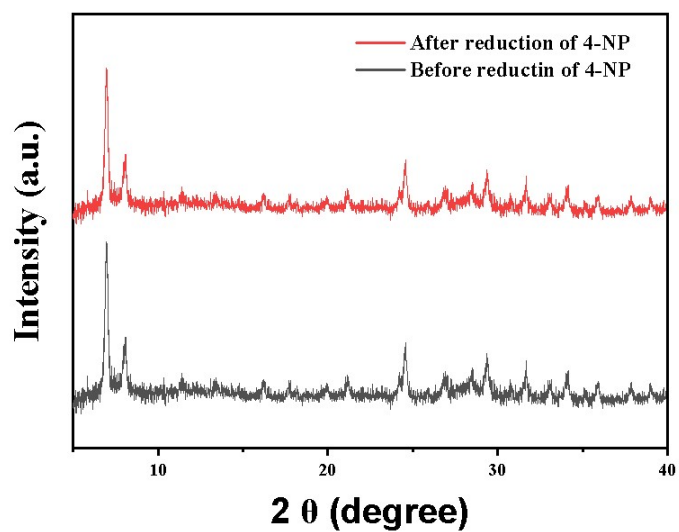


Fig. S8 (b). Recyclability after reduction of Cr(VI) using Pd@Ce-BDC

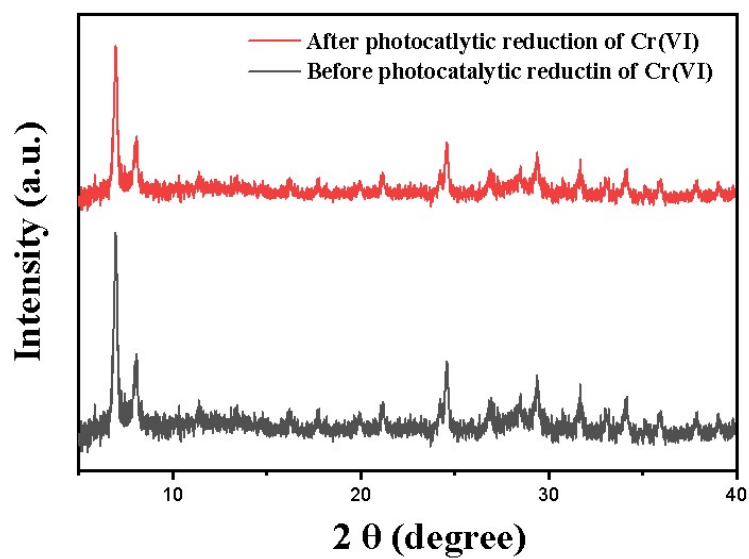


Table S1. Comparison of 4-NP & Cr(III) reduction using other MOF/NPs and present work.

Catalyst	Target pollutant	Time taken (min)	Efficiency (%)	Rate constant	References
Ag-CeO ₂	NP	10	-	0.656 min ⁻¹	[8]
CeO ₂ /Ni MOF	NP	-	97.6%	1.102	[9]
Au-Pd/Ce-MOF-808	NP	18	92	0.141	[10]
Ce-BDC/PVDF composite film	Cr(VI)	120	95.9%	0.02 min ⁻¹	[11]
CAU-1/Ce-BDC-NH ₂	Cr(VI)	75	40.3%	-	[12]
g-C ₃ N ₄ /Ce-BDC	Cr(VI)	90	98	-	[13]
Pd@Ce BDC	NP	-	95%	0.253 min ⁻¹	This work
Pd@Ce BDC	Cr(VI)	25	94%	0.206 min ⁻¹	This work

References for Table S1:

[8] Ismail A, Alsouz MA, Almashhadani HA, Khan MF, Zahid M. An efficient Ag decorated CeO₂ synergetic catalyst for improved catalytic reduction of lethal 4-nitrophenol. *Chemical Physics Impact*. 2023 Jun 1;6:100173.

[9] Zhao, H., Pang, X., Huang, Y., Ma, C., Bai, H., & Fan, W. (2022). CeO₂/Ni-MOF with Synergistic Function of Enrichment and Activation: Efficient Reduction of 4-Nitrophenol Pollutant to 4-Aminophenol. *Inorganic Chemistry*, 61(49), 19806-19816.

[10] Hassan, H. M., Alruwaili, H. A., Alhumaimess, M. S., Alanazi, A. H., El-Aassar, M. R., Alshammari, M. S., ... & Alsohaimi, I. H. (2025). Sustainable nitrophenol reduction using Ce-mof-808-supported bimetallic nanoparticles optimized by response surface methodology. *Environmental Research*, 264, 120340.

[11] Valizadeh, Z., Hosseini, S. M., Cheraghi, R., & Safarifard, V. (2025). Polyvinylidene fluoride supported Ce-BDC thin film towards Cr (VI) photoreduction. *Materials Research Bulletin*, 185, 113304.

[12] Goudarzi, M. D., Khosroshahi, N., & Safarifard, V. (2022). Exploring novel heterojunctions based on the cerium metal–organic framework family and CAU-1, as dissimilar structures, for the sake of photocatalytic activity enhancement. *RSC advances*, 12(50), 32237-32248.

[13] Maged, S., El-Borady, O. M., El-Hosainy, H., & El-Kemary, M. (2023). Efficient photocatalytic reduction of p-nitrophenol under visible light irradiation based on Ag NPs loaded brown 2D g-C₃N₄/g-C₃N₄ QDs nanocomposite. *Environmental Science and Pollution Research*, 30(55), 117909-117922.