Nature-Inspired α-$MnMoO_4$ Nanocubes from *Arachis hypogaea* for Next-Generation Wastewater Treatment and Organic Pollutant Catalysis

Aakash Venkatesan, [a] Aatika Nizam, [a*] Jeevitha Kallesh [a], Sumanth Hegde, [a] Sampath Chinnam, [b] Harini R, [c] Nagaraju G [d*]

[a] Department of Chemistry, Christ University, Bangalore-560029, India

[b] Department of Chemistry, M.S. Ramaiah Institute of Technology (Autonomous Institution, affiliated to Visvesvaraya Technological University, Belgaum), Bengaluru-560054, India.

[c] Department of Electronics and Communication Engineering, Govt. Polytechnic, Hiriyuru-577599, India.

[d] Energy Materials Research Laboratory, Department of Chemistry, Siddaganga Institute of Technology, Tumakuru-572103, India

Corresponding author

Email ID: aatika.nizam@christuniversity.in

Email ID: nagarajugn@gmail.com

3. Results and Discussions

3.2. Fourier Transform Infrared Spectroscopy (FTIR) Analysis

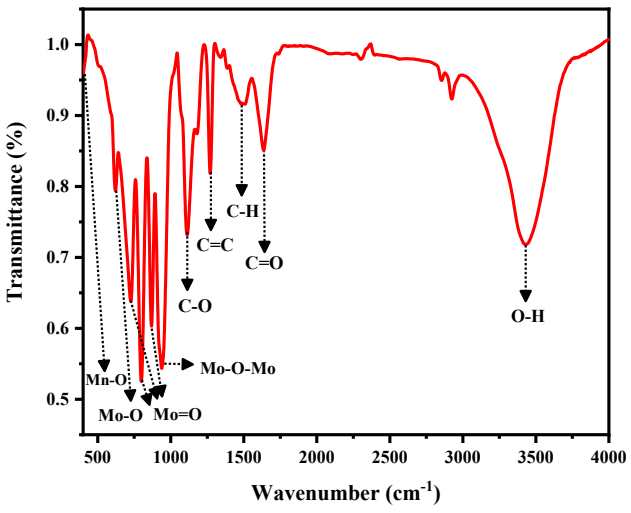


Figure S1: FTIR spectrum of $MnMoO_4$ NPs.

Table S1: Lattice parameters of $MnMoO_4$ NPs.

Lattice parameters	*Values*

a	11 ± 0.03 Å
b	10 ± 0.03 Å
c	7 ± 0.02 Å
β	105 ± 0.21°

Table S2: The FTIR absorption band values of $MnMoO_4$ NPs.

Type of Nanoparticle	***Absorption band***				
	v_1 (cm^{-1})	v_2 (cm^{-1})	v_3 (cm^{-1})	v_4 (cm^{-1})	v_5 (cm^{-1})
$MnZnO_3$ (1:0.5)	~	~727.94	~798.82	~869.82	~943.44
$MnZnO_3$ (1:1)	~618.66	~721.14	~797.08	~868.03	~943.05
$MnZnO_3$ (1:1.5)	~618.70	~728.75	~798.06	~869.64	~943.99

3.3. UV-VIS Spectral Analysis

Table S3: Optical band gap, valence band, and conduction band energies with respect to NPs

Type of Nanoparticle	***Optical band gap energy (eV)***	***Valence band energy (eV)***	***Conduction band energy (eV)***
$MnMoO_4$ (1:1.5)	4.71	3.775	-0.935
$MnMoO_4$ (1:1)	4.56	3.70	-0.86
$MnMoO_4$ (1:0.5)	4.62	3.73	-0.89

3.4. Photoluminescence Analysis

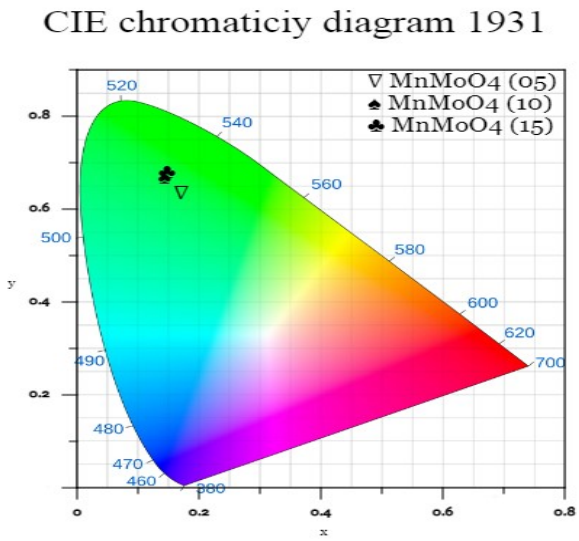


Figure S2: CIE diagram of $MnMoO_4$ NPs (1:0.5, 1:1, 1:1.5)

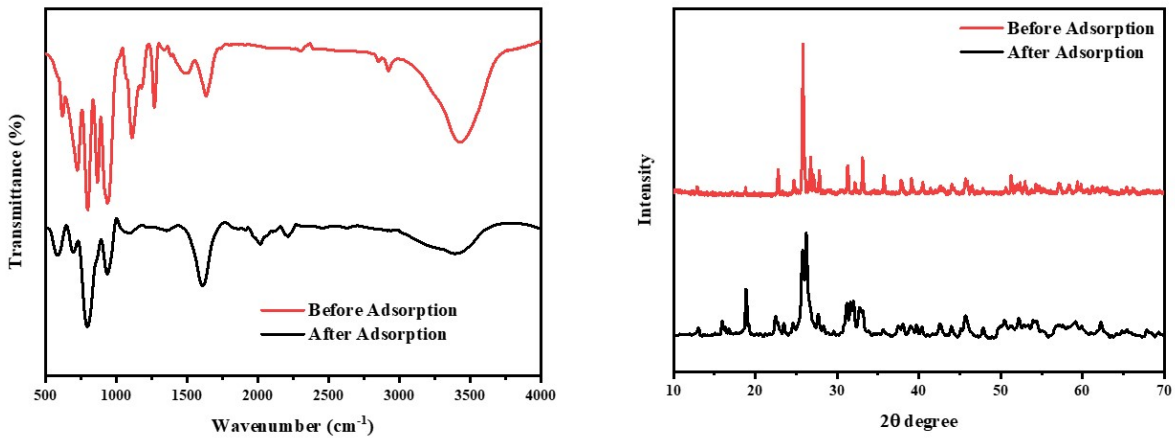


Figure S3: (a) FTIR spectrum of MMP before and after adsorption (b) XRD pattern of MMP before and after adsorption

3.8. Photocatalytic property

3.8.3. Kinetics of Photocatalytic property

Table S4: Rate constant values (k) for varying (a) Catalytic dosage (b) Dye concentration (c) pH Value

Catalytic dosage (mg)	5	10	15	20
k value (min^{-1})	8.28×10^{-3}	8.68×10^{-3}	7.79×10^{-3}	6.79×10^{-3}

Dye Concentration (mg)	5	10	15	20
k value (min^{-1})	8.68×10^{-3}	6.70×10^{-3}	4.06×10^{-3}	4.39×10^{-3}

pH Value	Basic	Neutral	Acidic
k value (min^{-1})	14.35×10^{-3}	8.68×10^{-3}	6.35×10^{-3}

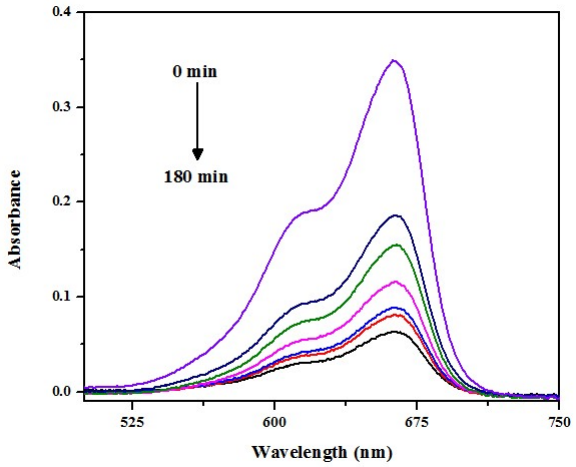


Figure S4: Absorption spectra of optimized photocatalytic degradation of MB dye by $MnMoO_4$ NPs

3.8.4. Mechanism of photo degradation

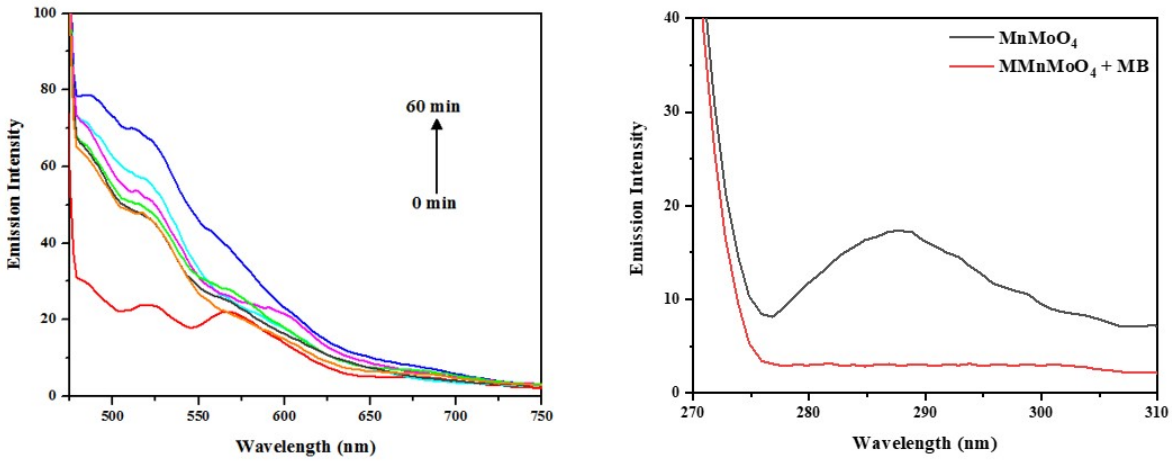


Figure S5: (a) Detection of ȮH radicals under UV light radiation (b) Emission spectra of MMP with and without MB

3.9. Catalytic property of $MnMoO_4$ NPs

Spectral data of benzimidazole compounds

Compound 3c: Brown powder, ^{1}H-NMR: δ, ppm (DMSO-d6): 7.28 (d, 2H), 7.59 (d, 2H), 8.43 (m, 4H), 13.30 (s, 1H).

Compound 3d: Dark brown powder, ^{1}H-NMR: δ, ppm (DMSO-d6): 3.00 (s, 6H), 6.85–6.83 (d, 2H), 7.15–7.13 (d, 2H), 7.57–7.46 (m, 2H), 8.01 (d, 2H), 12.57 (s, 1H).

Compound 3h: Pale Beige powder, ^{1}H-NMR: δ, ppm (DMSO-d6): 7.00-7.057 (m, 2H) 7.29-7.28 (d, 2H), 7.37-7.41 (m, 1H), 7.66 (s, 2H), 8.072-8.053 (d, 1H), 13.18 (s, 2H).

Compound 3i: Beige powder, ^{1}H-NMR: δ, ppm (DMSO-d6): 6.94-7.042 (m, 1H), 7.31 (s, 2H), 7.45-8.93 (m, 4H), 13.28 (s, 2H).

Compound 3j: Light beige powder, ^{1}H-NMR: δ, ppm (DMSO-d6): 3.84 (s, 3H), 6.96-7.09 (d, 2H), 7.29 (s, 2H), 7.63-7.73 (d, 3H), 13.27 (s, 2H).

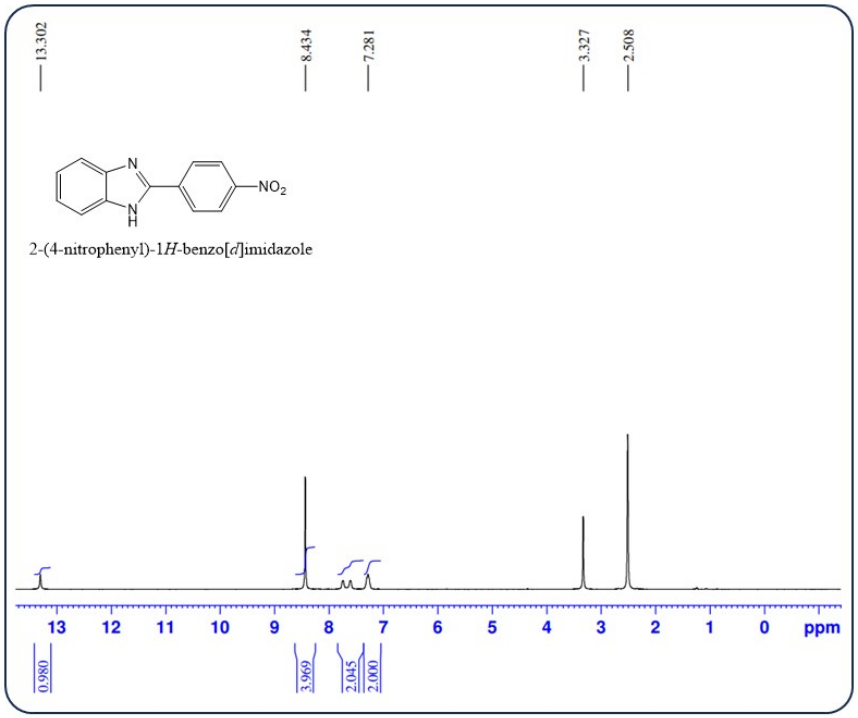


Figure S6: ^{1}H NMR spectrum of 2-(4-mitrophenyl)-1-H-benzo[d]imidazole (Compound 3c)

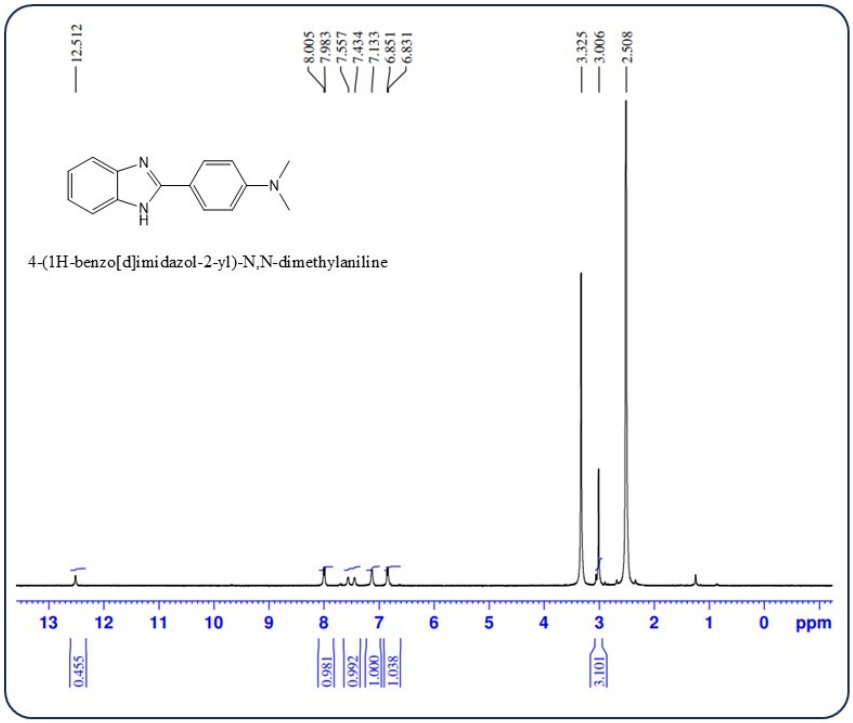


Figure S7: ^{1}H NMR spectrum of 4-(1H-benzo[d]imidazol-2-yl)-N,N-dimethylaniline (Compound 3d)

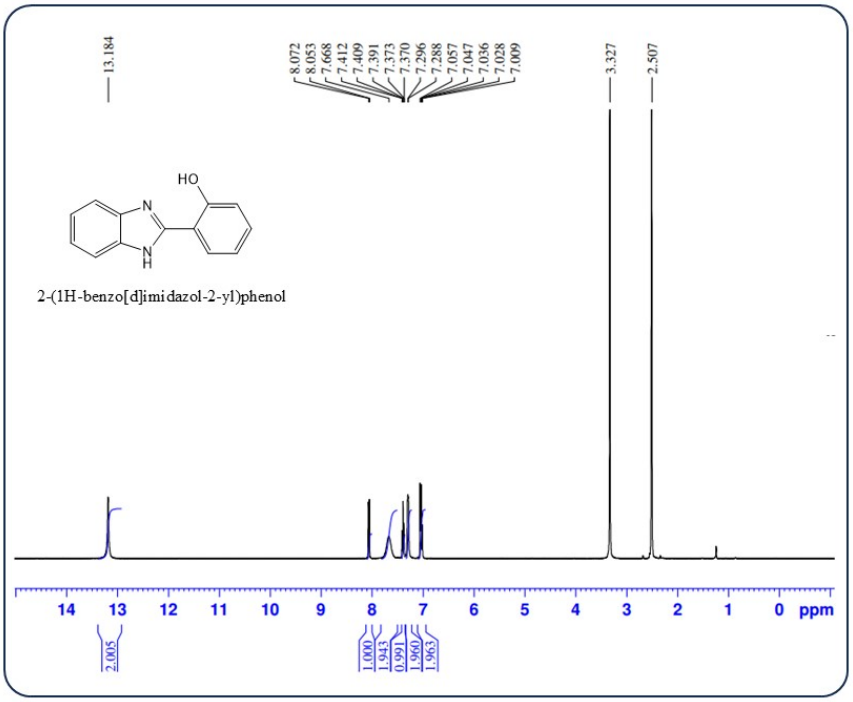


Figure S8: ^{1}H NMR spectrum of 2-(1H-benzo[d]imidazol-2-yl) phenol (Compound 3h)

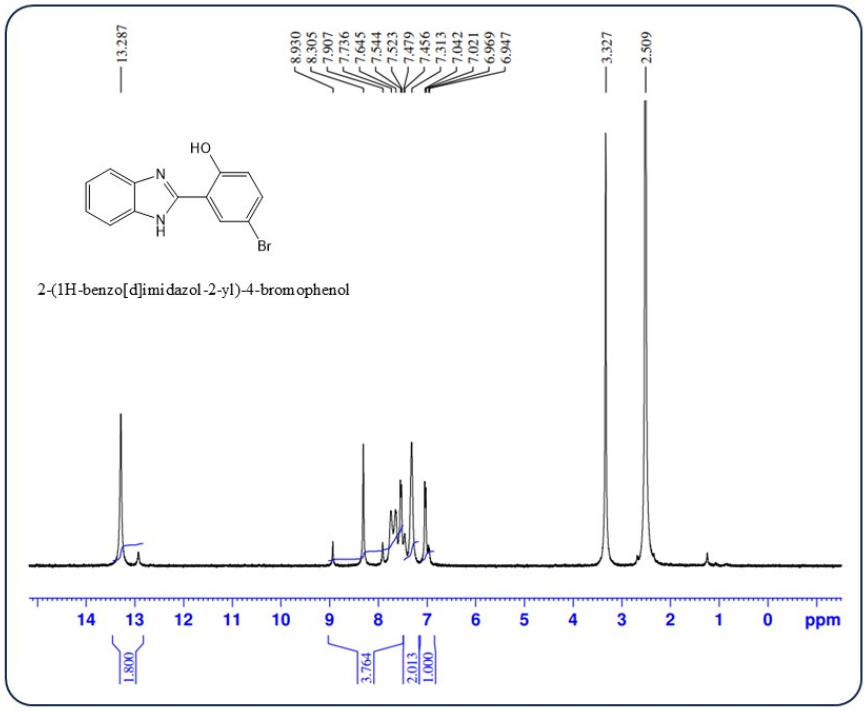


Figure S9: [1]H NMR spectrum of 2-(1H-benzo[d]imidazol-2-yl)-4-bromophenol (Compound 3i)

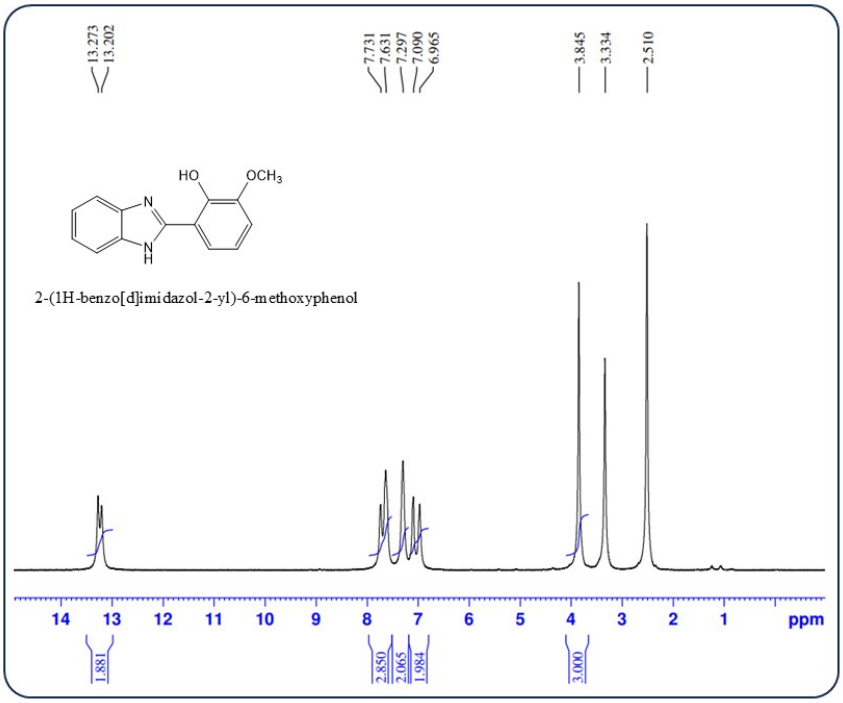
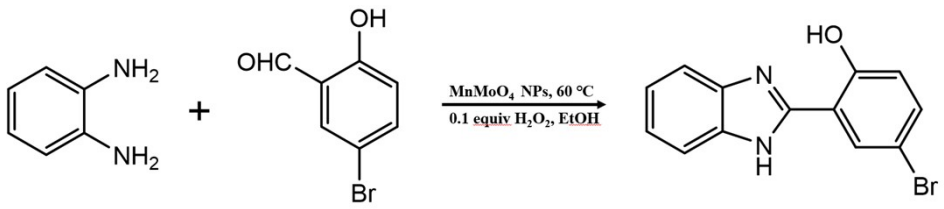


Figure S10: [1]H NMR spectrum of 2-(1H-benzo[d]imidazol-2-yl)-6-methoxyphenol (Compound 3j)

3.9.2. Green Chemistry Parameters



0.108 g **0.201 g** **0.230 g**

Catalyst Mass = 0.020 g

Reaction Solvent Mass = 3.945 g

By-products: 2 H_2O

Yield: 85 %

Atom Economy (AE): $\frac{288.25\ g/mol}{(108.14\ +201.02)\ g/mol} \times 100 =\ 93.28$ %

Generalized reaction mass efficiency (gRME): $\frac{0.230\ g}{(0.108\ +0.201)\ g} \times 100 =\ 74.43$ %

E-factor: $\frac{0.079\ g}{0.230\ g} = 0.34$

Eco-scale: 81

3.9.3. Reusability of $MnMoO_4$ Nano-catalyst

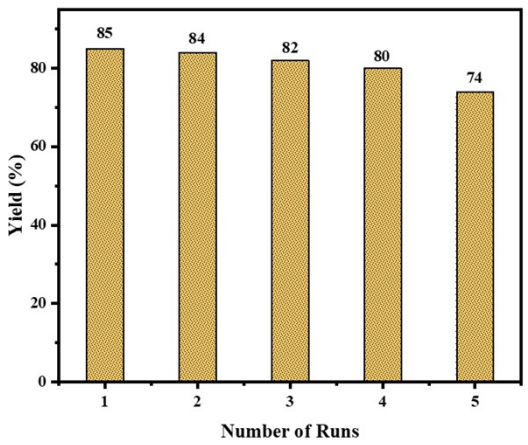


Figure S11: Reusability of $MnMoO_4$ catalyst for the model reaction under the same reaction conditions.