Supporting Information

Highly Stable Indium Based Metal Organic Framework for Efficient Arsenic Removal from Water

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Crystallographic data and structural refinement summary for 1	
Compound	1
Empirical formula	$C_{14}H_8InN_2O_8$
Formula weight	447.04
Crystal system	Tetragonal
Space group	P42/ncm
a/ Å	12.5808(3)
b/ Å	12.5808(3)
c/ Å	12.9625(3)
V/A^3	2051.66(11)
T/K	147(2)
$Dc/Mg m^{-3}$	1.447
Z	4
m(Mo-Ka)/mm ⁻¹	9.561
No. unique data (<i>R</i> int)	988 (0.1002)
No. total reflns	40927
Final <i>R</i> indices $[I > 2s(I)]^a$	$R_1 = 0.0477, wR_2 = 0.1186$
<i>R</i> indices (all data)	$R_1 = 0.0685, wR_2 = 0.1320$

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Figure S1. Crystal structure of In-MOF with pts topology.



Figure S2. HRSEM images of AUBM-1 after dispersion in solutions of pH 2 (A and B) and pH 8(C and D).



Figure S3. (A) IR spectra of the as synthesized MOF, 2-methylimidazole and 1,2,4,5 benzenetetracarboxylic acid, (B) N_2 isotherm of the MOF at 77 K. (C) N_2 isotherm of the MOF after treatment with acid (pH = 2) (D) N_2 isotherm of the MOF after treatment with basic solution (pH = 8).



Figure S4. SEM EDX of washed In-MOF



Figure S5. SEM-EDX of activated In-MOF



FigureS6. TGA curves of the washed In-MOF and activated one (A), FTIR spectra recorded for the produced species (ammonia) from the combustion of the washed sample between 560 to 706 °C (max appeared at 635°C) and for activated sample between 485 - 755 °C (max appeared at 647 °C); For the washed In-MOF NH3 gas was detected.



14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 f1(ppm)









Figure S7. ¹H NMR of the digested In-MOF in TFA/DMSO-d6 (A), 1,2,4,5-Benzenetetracarboxylic acid (B), 2-Methylimidazole (C) and the comparison of all three spectra (D) showing the existence of both organic species within the framework.



Figure S8. Zeta potential measurement at different pHs values showing negatively charge surface between pH = 3 and pH = 9.



Figure S9. Intraparticle diffusion kinetic plot for arsenic adsorption onto the activated MOF



Figure S10. Effect of temperature on the As removal by the MOF



Figure S11. IR spectrum of Na₂HAsO₄.H₂O (green), activated MOF plus As (red), and activated MOF (black)



Figure S12. TGA curve as synthesized MOF (red), activated MOF plus As (blue), and Assynthesized MOF (black).



Figure S13. As adsorption by AUBM-1 in the presence of anions. $m_{AUBM-1} = 10 \text{ mg}$; [As]₀ = 40 mg/L, contact time =12 h. the control experiment was performed in the absence of anions.



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Figure S14. Arsenic removal in the presence of Pb^{2+} (A). SEM-EDX of the collected sample after the adsorption test showing the adsorption of both As and Pb on the surface of the MOF crystals (B). [As]₀ = [Pb]₀ = 25 ppm m_{AUBM-1} = 10 mg.

Α



Figure S15. Effect of the mass of AUBM-1 on the removal efficiency of low concentration (40 ppb) and high concentration (40 ppm) As solution.



Figure S16. PXRD of the recycled AUBM-1 (Black) compared to the simulated pattern (Red).