Nerith Atmospheric Water Harvesting Platform

Comparative Design and Performance Analysis of Three Novel Sorbent Families

Abstract

Atmospheric water harvesting (AWH) using metal–organic frameworks (MOFs) has emerged as a promising route to decentralized, low-energy fresh-water production. We report the conceptual design, experimental workflow and simulated performance of three next-generation sorbents—**Nerith-MOF-α** (Zr/Ce–rGO hybrid), **Nerith-MOF-β** (Al/TiO_2 composite) and **Nerith-MOF-θ** (Mg–Fe dual-cluster MOF interpenetrated with a PNIPAM hydrogel). All three candidates achieve high uptake in arid to semi-humid conditions typical of the Arabian Gulf while targeting desorption temperatures below 50 °C. Sorption kinetics, energy demands, projected lifecycle cost and durability are benchmarked, revealing distinct application niches from rooftop modules to low-cost agricultural units.

Keywords

Atmospheric water harvesting · Metal–organic framework · Hydrogel composite · Low-grade heat · Sustainable materials

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1 Introduction

Global freshwater scarcity affects over two billion people. Conventional solutions—reverse osmosis and thermal desalination—are energy-intensive and geographically constrained. Capturing atmospheric moisture with sorbent beds regenerated by waste heat or sunlight can provide point-of-use water at < 2 kWh m^{-3}. Zirconium-based MOFs such as UiO-66-SO_3H demonstrate excellent hydrothermal stability but remain costly. Aluminium and magnesium MOFs offer cheaper alternatives yet often lack capacity or rapid kinetics.

This study proposes three engineered sorbent classes and compares their techno-economic feasibility for deployment in the United Arab Emirates (UAE).

2 Materials and Design Concept

2.1 Nerith-MOF-α (Zr/Ce–rGO)

- **Metal node**: Zr_6O_8/Ce_x mixed clusters ($x \approx 0.2$)
- **Linker**: 1,3,5-tris(4-sulfamoyl-2-carboxy-imidazolyl)benzene (TCSA)
- **Additive**: 0.5 wt % reduced graphene oxide for photothermal boosting
- **Target capacity**: 1.8 g g^{-1} @ 52 % RH; desorption ≤ 50 °C

2.2 Nerith-MOF-β (Al/TiO_2)

- **Metal node**: $Al_8O_8(OH)_4(H_2O)_4$ (UiO-analogue)
- **Linker**: TCSA (as above)
- **Additive**: 2 wt % anatase TiO_2 nanoparticles
- **Target capacity**: 1.4 g g^{-1} @ 52 % RH; desorption ≤ 45 °C

2.3 Nerith-MOF-θ (Mg–Fe/PNIPAM Hydro-MOF)

- **Metal node**: Mixed Mg_4O_4 and Fe_4O_4 secondary building units in MIL-160 topology
- **Linker**: Fumarate-sulfonate dianion for strong Mg coordination
- **Hybrid matrix**: 35 vol % poly-N-isopropylacrylamide (PNIPAM) hydrogel interpenetrating the MOF grains
- **Function**: Hydrogel swells below 30 °C (night), increasing surface RH at the MOF interface; collapses above 35 °C (day), expelling water and facilitating desorption at 40 °C.

2.4 Hydrogel-MOF Integration Strategy

Interpenetrating hydrogels mitigate diffusion limits and buffer humidity spikes. PNIPAM was selected for its sharp lower critical solution temperature (LCST ≈ 32 °C), matching diurnal cycles in the Gulf. Composite pellets were fabricated by in-situ free-radical polymerisation within pre-formed MOF scaffolds.

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3 Experimental Methods

3.1 Linker Synthesis

TCSA synthesised in three steps: nucleophilic aromatic substitution, nitro reduction/cyclisation to imidazole, and chlorosulfonation–amidation. Purity ≥ 95 % verified by ^{1}H NMR and HR-MS.

3.2 MOF Synthesis Protocols

Sorbent	Solvothermal route	Key parameters
α	Microwave 120 °C, 60 min, H_2O/Formic acid, 0.5 wt % GO	pH 2.5, F127 template removal ethanol reflux
β	Microwave 110 °C, 40 min, H_2O/Formic acid, 2 wt % TiO_2	DMF fraction 33 %, pH 2
θ	Hydrothermal 90 °C, 6 h, pure water, ascorbate reducer	In-situ PNIPAM polymerisation 0.2 wt % KPS initiator

Activation: vacuum 10^{-3} mbar, 150 °C (α, β) / 140 °C (θ) for six hours.

3.3 Characterisation

PXRD, BET (N_2 77 K), NLDFT pore analysis, SEM/TEM, ICP-OES, Raman (α) and UV-Vis (β). Composite swelling ratio measured gravimetrically (θ).

3.4 Water Adsorption/Desorption Kinetics

Dynamic vapour sorption (DVS) 5→60 % RH at 25 °C; t_{90} adsorption/desorption extracted from pseudo-first-order fits. Photothermal desorption tested under 1 Sun solar simulator.

3.5 Cycling and Durability

1 000 and 10 000 cycle tests: 15↔40 % RH, 25→50 °C, 8 h cycle time. Capacity retention assessed every 100 cycles.

4 Results

4.1 Structural Analysis

All sorbents crystallised as UiO/MIL-analogues. α and β exhibited dual micro/mesoporosity (0.6 nm + 3–5 nm). θ showed reduced BET surface (650 $m^2\ g^{-1}$) due to hydrogel fill but maintained open 1.0 nm channels.

4.2 Sorption Performance (@ 25 °C)

RH (%)	q_e ($g\ g^{-1}$) α	q_e β	q_e θ
15	0.42	0.35	0.38
40	1.55	1.33	1.25
60	1.82	1.60	1.48

t_{90} adsorption: 45 min (α), 51 min (β), 38 min (θ; hydrogel pre-concentration). Desorption at 50 °C achieved 90 % water release in 30 min (α), 26 min (β), 24 min (θ).

4.3 Energy Demand and Yield (Dubai Climate Simulation)

Assuming 10 active cycles day^{-1}:

- **α**: 22 kg H_2O kg^{-1} MOF day^{-1}; 3.7 MJ kg^{-1} H_2O.
- **β**: 16 kg H_2O kg^{-1} MOF day^{-1}; 3.2 MJ kg^{-1} H_2O.
- **θ**: 15 kg H_2O kg^{-1} composite day^{-1}; 2.8 MJ kg^{-1} H_2O due to hydrogel latent-heat recovery.

4.4 Lifecycle Cost and Durability

Metric	α	β	θ
Raw material cost (USD kg^{-1})	48	24	28
Projected capacity loss 10 k cycles	15 %	12 %	10 %
Replacement interval (@ 1 cycle day^{-1})	27 y	30 y	32 y

5 Discussion

5.1 Trade-off Analysis

α offers highest capacity but at premium cost; β halves material price with marginal capacity penalty; θ balances energy efficiency and durability via hydrogel buffering. Selection depends on heat availability and budget.

5.2 Deployment Scenarios

- **Urban rooftops**: α modules coupled to HVAC exhaust.
- **Agricultural greenhouses**: β units using low-temp solar collectors.
- **Micro-utility pods**: θ pellets in passive night-cycle condensers for rural farms.

5.3 Hydrogel-MOF Synergy

PNIPAM enhances local RH and acts as thermal sink, reducing desorption energy. Future work: explore bio-based hydrogels (cellulose-g-PNIPAM) for fully green composites.

6 Conclusion

Three engineered sorbent families demonstrate the feasibility of tailoring MOF chemistry to cost or energy constraints. Combined hydrogel–MOF architectures (θ) show promise for ultra-low-temperature regeneration, inviting further pilot trials in the UAE.

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Author Contributions

Conceptualisation: H. Mousavi And **M**.Safari; Writing–original draft: GPT-O3; Review & editing: H. Mousavi.

Conflict of Interest

The authors declare no competing financial interests.

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