Energy Materials

Supplementary Materials

Upcycling waste polyester into cobalt-molybdenum sulfide-decorated carbon foam for photothermal desalination and parametric optimization using Taguchi design of experiments (DOE)

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1. Calculation for average crystalline size

Debye–Scherrer Equation

$$D = \frac{0.9\lambda}{\beta \cos\theta} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

where

- D = crystallite size (nm)
- λ = X-ray wavelength = 0.15406 nm (Cu Kα radiation)
- K= 0.9
- β = FWHM (in radians)
- θ = Bragg angle = ½(2θ)

From XRD pattern, the strongest peak is

$$2\theta \approx 28.8^{\circ}$$

Therefore,

$$\theta = \frac{28.8}{2} = 14.4^{\circ}$$

Convert FWHM into radians

peak crosses the half-maximum line

- Left intersection = 28.35°
- Right intersection = 29.00°

β= 29.00° −28.35° = 0.65

Convert degrees to radians:

$$\beta = 0.65 \times \frac{\pi}{180}$$

$$\beta = 0.01134 \text{ radians}$$

Calculate cosθ

$$\cos(14.4^{\circ}) = 0.969$$

Substitute into the Scherrer equation (1)

$$D = \frac{0.9 \times 0.15406}{0.01134 \times 0.969}$$

Numerator

$$0.9 \times 0.15406 = 0.13865$$

Denominator

$$0.01134 \times 0.969 = 0.01099$$

Finally,

$$D = \frac{0.13865}{0.01099}$$

$$D = 12.6 \text{ nm}$$

Normally, crystallite size is calculated for each major diffraction peak separately and then averaged.

Peak (2θ)	**θ (°)**	**β (°)**	**Size (nm)**
17.5	8.75	0.74	11.0
25.7	12.85	0.65	12.5
28.8	14.4	0.60	13.6
47.8	23.9	0.48	17.0
56.6	28.3	0.53	14.0

Average:

$$\frac{11.0 + 12.5 + 13.6 + 17.0 + 14.0}{5} = 13.6 \text{ nm}$$

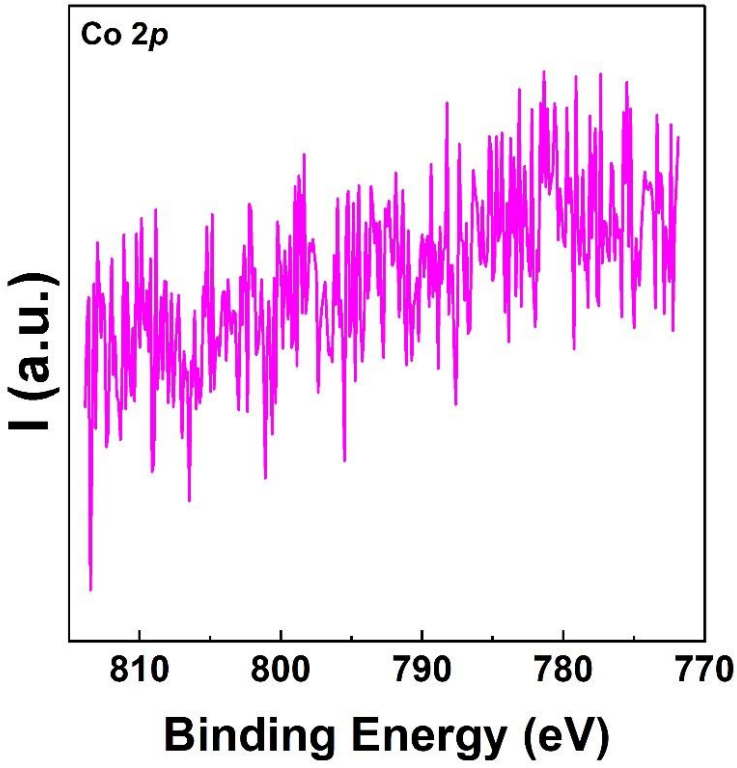
Supplementary Table 1. Scientific literature study for upcycling of waste PET bottles for desalination

Sr No.	Material	Carbonization Temperature (°C)	Evaporation rate (kg m^{-2} h^{-1})	Efficiency (%)	Reference
1	PET+$ZnCl_2$/NaCl	550	1.68	97%	[1]
2	PET+sodium lignosulfonate(SLS) + ZnO	550	1.51	83.4%	[2]
3	PET+melamine+ $ZnCl_2$/NaCl	340	2.4	98-99%	[3]
4	PET+ZnO (coated on wood)	550	2.38	-	[4]
5	PET+NaCl,	550	0.99	63.5%	[5]
6	PET+$CaCl_2$+DMF/H_2O (solovothermal method)	700-900	2.49	90.8%	[6]
7	PET+melamine+ $ZnCl_2$/NaCl Carbonization followed by soaking in $Fe(NO_3)_3$ solution then calcination at 300°C	340	2.5	87.2%	[7]
8	$MnCl_2$+waste PET bottles in DMF and H_2 (one pot solvothermal	400-700	2.38	98.4%	[8]

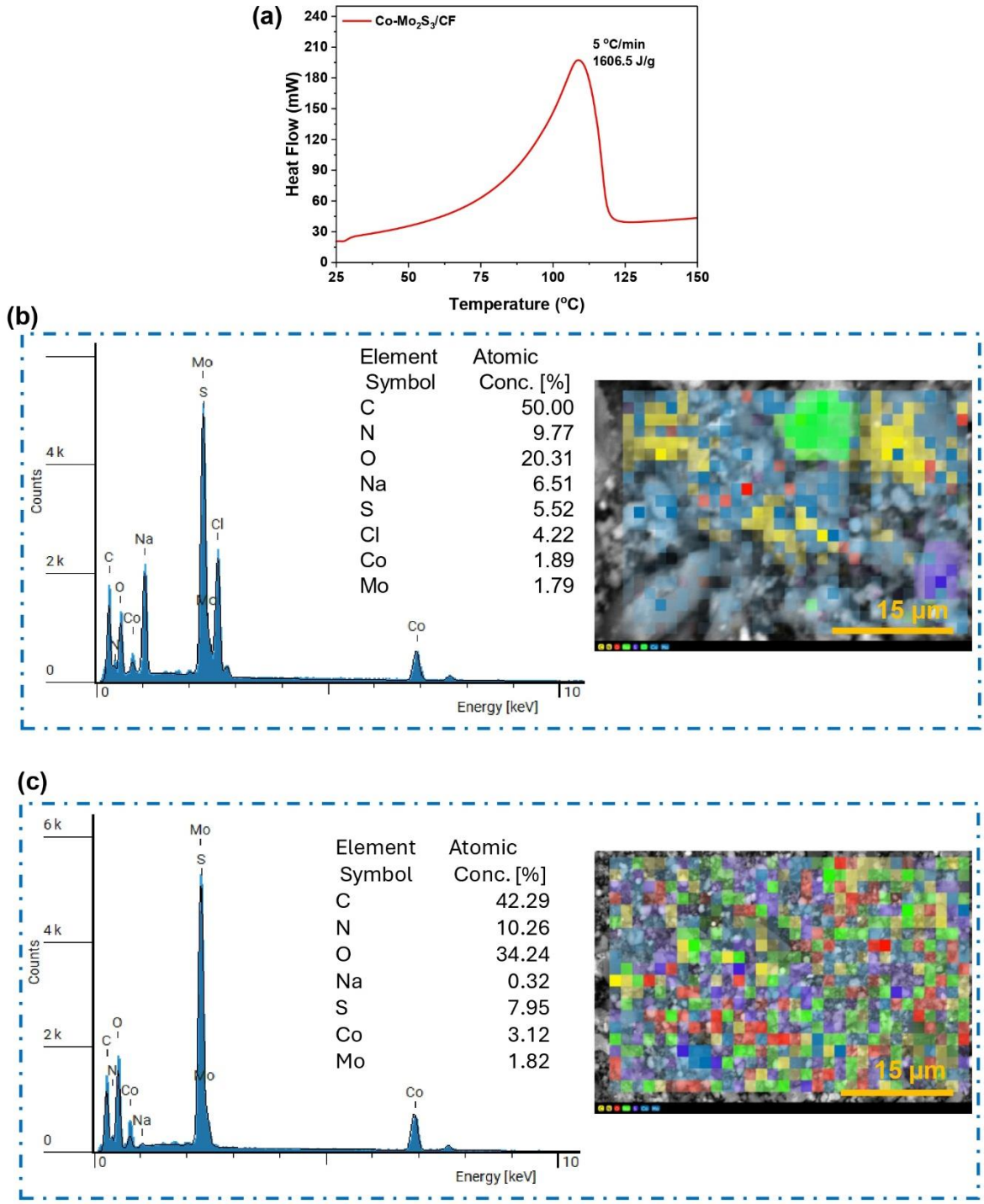
	method)				
9	Waste PET bottles+ $Co(NO_3)_2 \cdot 6H_2O$ in DMF and water (one pot solvothermal method)	180	2.25	89.1%	[9]
10	PET+carbon black(trifluoroacetic acid was used as solvent)	-	1.457	93.91%	[10]

Supplementary Table 2. Taguchi $L_9(3^4)$ OA

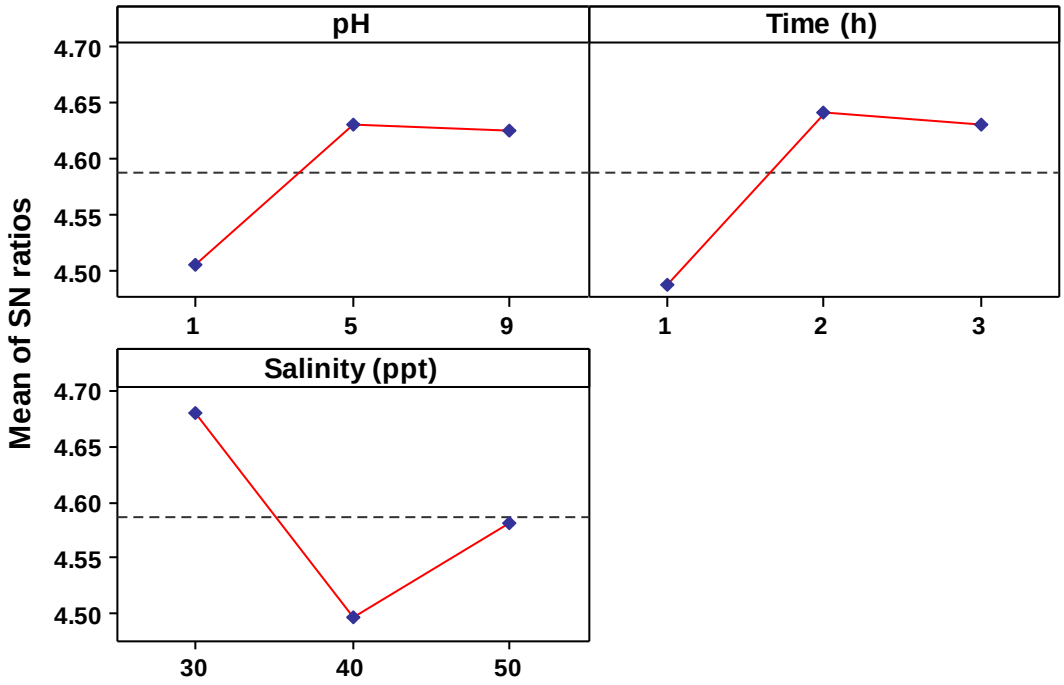
Run	**Operating Parameters**		
	pH	**Time (hrs.)**	**Salinity (gL^{-1})**
1	1	1	30
2	1	2	40
3	1	3	50
4	5	1	40
5	5	2	50
6	5	3	30
7	9	1	50
8	9	2	30
9	9	3	40



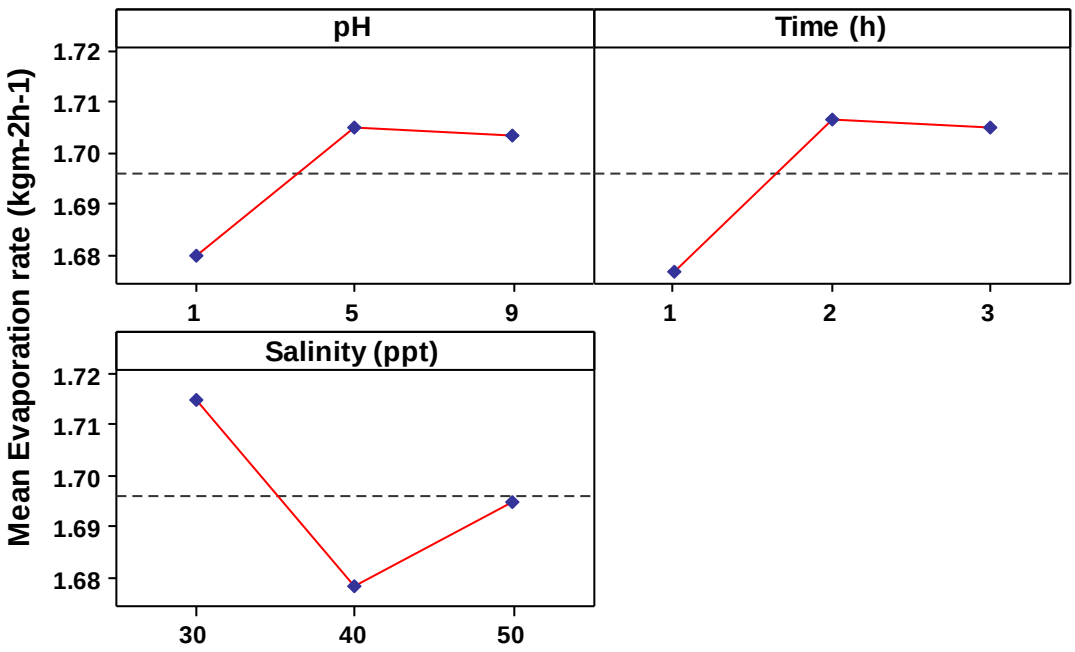
Supplementary Figure 1. XPS high resolution of Co2*p*.



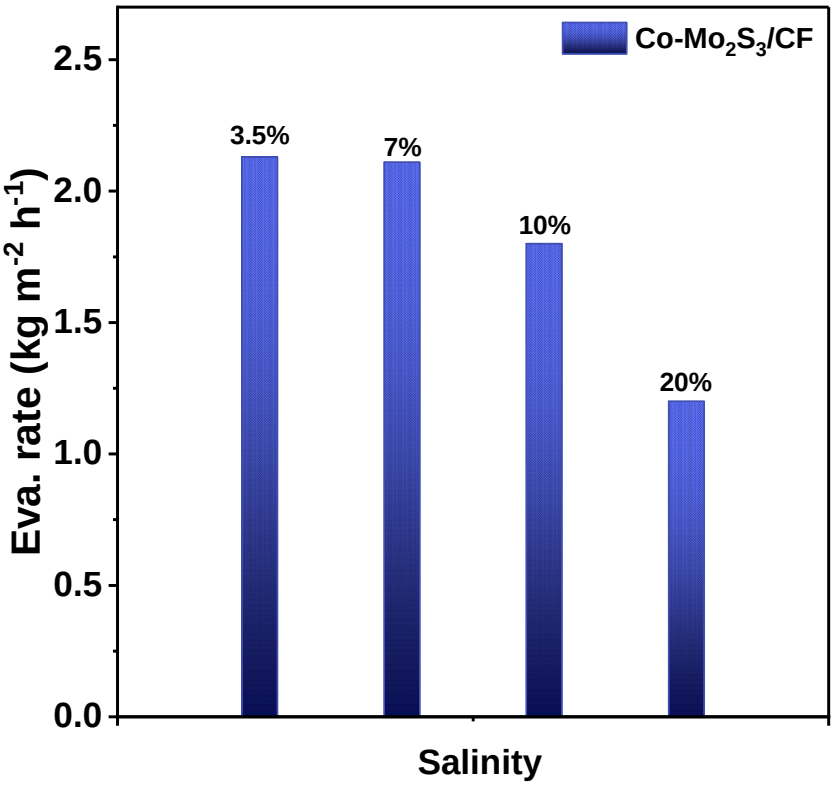
Supplementary Figure 2. (a) DSC analysis of Co-Mo_2S_3/CF, (b) EDS analysis of solar evaporator after three cycles of stability test, and (c) EDS analysis after 5 hours of self-cleaning of Co-Mo_2S_3/CF solar evaporator.



Supplementary Figure 3. Effect of each factor on SN ratio



Supplementary Figure 4. Effect of each factor on mean evaporation rate



Supplementary Figure 5. Effect of salt concentration on the evaporation rate of Co-Mo_2S_3/CF solar evaporator.

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