

HotHybrids – project summary

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17/10/2024



Pioneering hybrid materials for CO₂ photoconversion

Acronym: HotHybrids

Financing institution: National Centre for Research and Development and Norwegian Funds

Funding amount: PLN 863,750.00

Project duration: 01.04.2022 - 30.04.2024

https://hothybrids.ug.edu.pl/

https://www.youtube.com/watch?v=vyrQsLgIm90&ab_channel=KatedraTechnologii%C5%9ArodowiskaWChUG



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"Pioneering hybrid materials for CO₂ photoconversion", no NOR/SGS/HotHybrids/0130/2020-00. Project financed by the Financial Mechanism of the European Economic Area (EEA) and the Norwegian Financial Mechanism 2014-2021.



People employed in the project:

Head of the project: prof. dr hab. inż. Adriana Zaleska-Medynska

Executor: dr inż. Anna Pancielejko

Executor: mgr inż. Hanna Zagórska

People supporting the project:

dr Magdalena Miodyńska-Melzer

dr inż. Anna Gołąbiewska

dr inż. Emilia Gontarek-Castro

mgr Mateusz Baluk

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The main goal of the HotHybrids project was to develop a class of hybrid materials consisting of new double perovskite nanocrystals (DPNs) and metal-organic frameworks (MOFs) with high activity and selectivity in the photoconversion of CO_2 to valuable hydrocarbons.

The detailed tasks concerned:

- correlation of synthesis methods with morphology, stability, and activity of DPNs;
- finding a method for effective encapsulation of DNPs in MOF structures;
- correlation of MOF composition (metal cations/organic ligand) and synthesis method of DPNs-MOFs hybrids with their morphology, stability and photoactivity;
- understanding the mechanism of CO₂ photoconversion of DPNs-MOFs hybrids;
- development of a synthesis method (laboratory and pilot scale) for the selected hybrid system.

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Problems in project implementation

- 1. Synthesis of double perovskites stable in aqueous solution.
- 2. Encapsulation of perovskites in a metal-organic framework structure.
- 3. Obtaining hybrids active in the CO_2 photoconversion reaction in aqueous solution.
- 4. Obtaining a scaled-up hybrid with proper morphology and high activity in the photocatalytic hydrogen generation reaction.



Project indicators

Publications:

- Pancielejko A. et al. Rational designing of TiO₂-X@Cs₃Bi₂X₉ nanocomposite for boosted hydrogen evolution, Catalysis Today (2024) 432, 114626.
- Pancielejko A. et al. CuGaS₂@NH₂-MIL-125(Ti) nanocomposite: Unveiling a promising catalyst for photocatalytic hydrogen generation, International Journal of Hydrogen Energy (2024) 79, 186-198.
- Głowienke H. et al. Novel room-temperature synthesis of pioneering CsPbX₃@(Ce)UiO-66-Y hybrid nanomaterials for boosted photocatalytic hydrogen evolution, Journal of Photochemistry and Photobiology A: Chemistry (2024), 454, 115731.
- Miodyńska M. et al. A comprehensive review of preparation methods, properties, and photocatalytic performance of diverse perovskite structures, Wiadomości Chemiczne (2024), 78, 3-4.
- Pancielejko A. et al. Cu-incorporated NH₂-MIL-125(Ti): A Versatile Visible-Light-Driven Platform for Enhanced Photocatalytic H₂ Generation and CO₂ Photoconversion, Materials Horizons, under review.

Patent application:

CuGaS₂@NH₂-MIL-125(Ti) nanocomposites, method of obtaining them and use of CuGaS₂@NH₂-MIL-125(Ti) nanocomposites as a photocatalytic material, P.448194.

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Catalysis Today 432 (2024) 114626



Contents lists available at ScienceDirect
Catalysis Today

journal homepage: www.elsevier.com/locate/cattod

Rational designing of TiO_2 -X@Cs₃Bi₂X₉ nanocomposite for boosted hydrogen evolution

Anna Pancielejko^{a,*}, Magdalena Miodyńska^a, Hanna Głowienke^a, Anna Gołąbiewska^a, Emilia Gontarek-Castro^a, Tomasz Klimczuk^b, Mirosław Krawczyk^c, Grzegorz Trykowski^d, Adriana Zaleska-Medynska^{a,*}

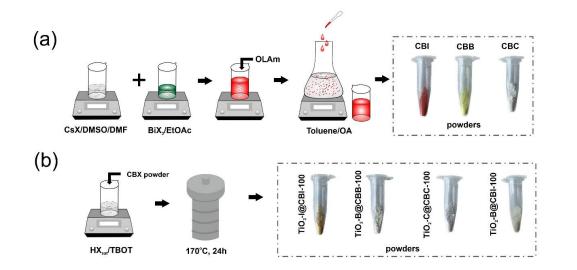


Fig. 1. Schematic diagram of the two-step preparation process of a) $Cs_3Bi_2X_9$ perovskites and b) TiO₂-X@CBX (X = I, Br, CI) nanocomposites.

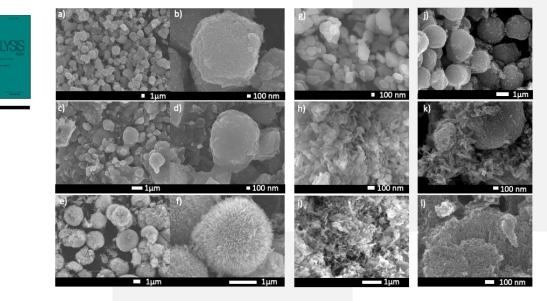


Fig. 2. SEM images of (a-b) TiO₂-I, (c-d) TiO₂-B, (e-f) TiO₂-C, (g) CBI, (h) CBB, (i) CBC, (j) TiO₂-I@CBI-100, (k) TiO₂-Br@CBB-100, (l) TiO₂-C@CBC-100.

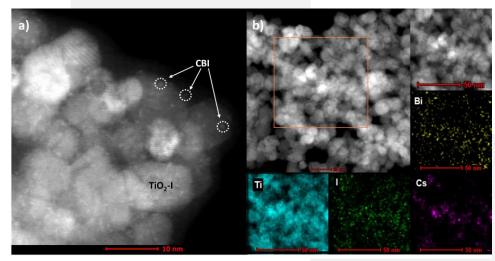


Fig. 3. STEM-EDS analysis of TiO₂-I@CBI-100 with elemental mapping (Bi, Ti, I and Cs).

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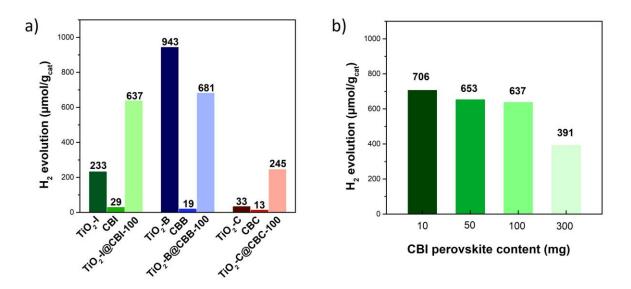
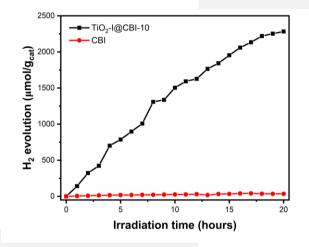
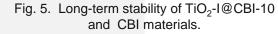


Fig. 4. Photocatalytic H₂ generation of a) TiO_2 -X, CBX, and TiO_2 -X@CBX-100 nanocomposites, and b) TiO_2 -I@CBI nanocomposites differ in CBI amount after 240 minutes of UV-Vis irradiation.





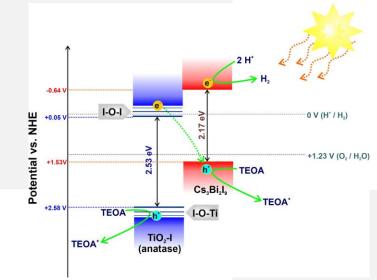


Fig. 6. Schematic separation and charge transfer diagram during photocatalytic hydrogen evolution in the TiO₂-I@CBI-10 photocatalyst.

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International Journal of Hydrogen Energy 79 (2024) 186-198

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 $CuGaS_2@NH_2-MIL-125(Ti)$ nanocomposite: Unveiling a promising catalyst for photocatalytic hydrogen generation

Anna Pancielejko^{a,**}, Hanna Głowienke^a, Magdalena Miodyńska^a, Anna Gołąbiewska^a, Tomasz Klimczuk^b, Mirosław Krawczyk^c, Krzysztof Matus^d, Adriana Zaleska-Medynska^{a,*}

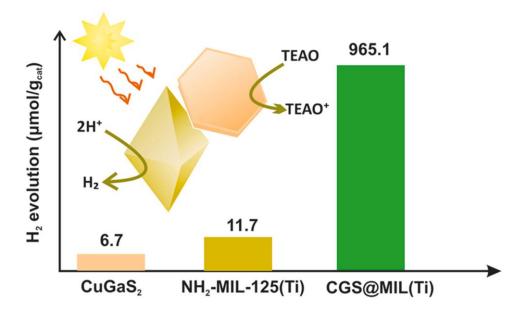


Fig. 7 Schematic diagram illustrating the concepts behind the work on the $CuGaS_2@NH_2-MIL-125(Ti)$ material.

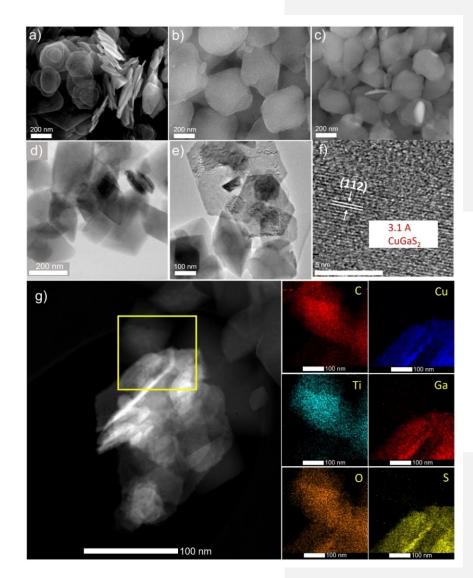


Fig. 8. SEM images of a) CuGaS₂, b) NH₂-MIL-125(Ti), c) CGS-30@MIL(Ti), and d) STEM, e) TEM, and f) HRTEM images with elemental mapping of CGS-30@MIL(Ti).

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International Journal of Hydrogen Energy 79 (2024) 186-198

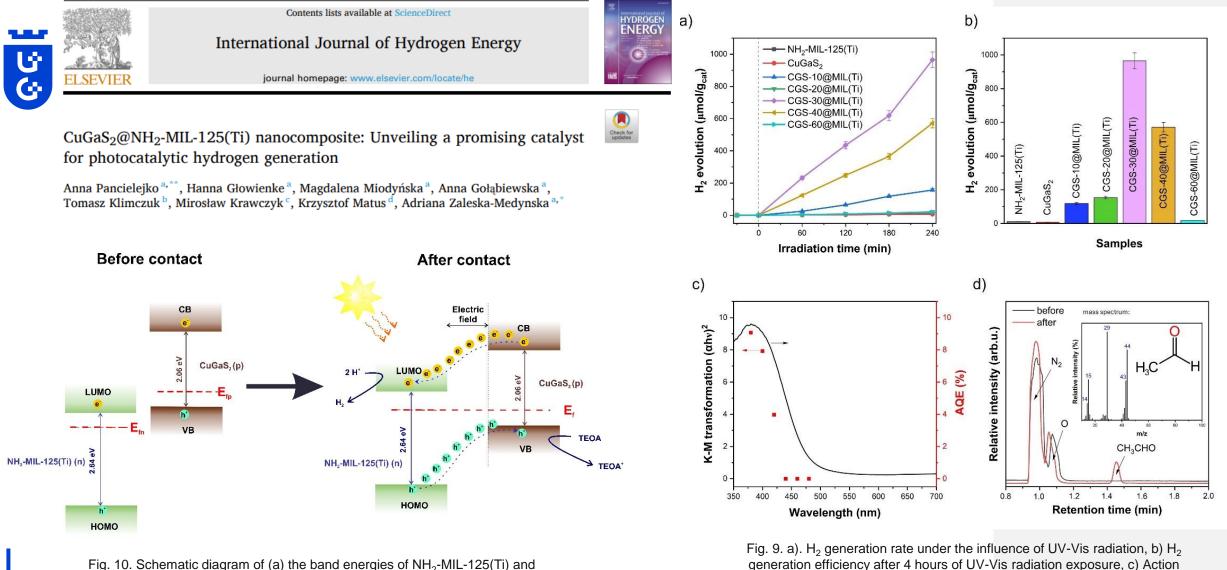


Fig. 10. Schematic diagram of (a) the band energies of NH_2 -MIL-125(Ti) and $CuGaS_2$ before (a) and after (b) composite formation and the proposed charge transfer and separation process of $CuGaS_2@NH_2$ -MIL-125(Ti) under UV-Vis radiation.

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Spectra measurement for the CGS-30@MIL(Ti) sample, and d) GC/MS spectra

of the electrolyte before and after the photocatalytic process in the presence of the CGS-30@MIL(Ti) sample.





Cu-incorporated NH2-MIL-125(Ti): A Versatile Visible-Light-**Driven Platform for Enhanced Photocatalytic H2 Generation** and CO2 Photoconversion

Anna Pancielejko a*, Mateusz A. Baluk a, Hanna Zagórska a, Magdalena Miodyńska-Melzer a,

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Krzysztof Matus^d Alicja Mikolajczyk^{f.g}, Henry P. Pinto^b, Aleksandra Pieczyńska^a, Joanna

Dołżonek^c, Adriana Zaleska-Medynska^{a*}

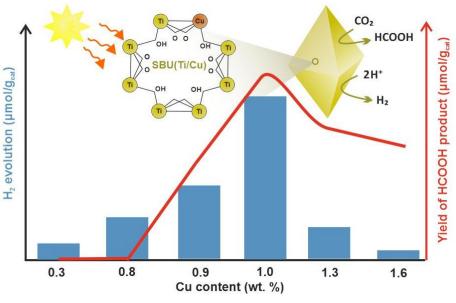
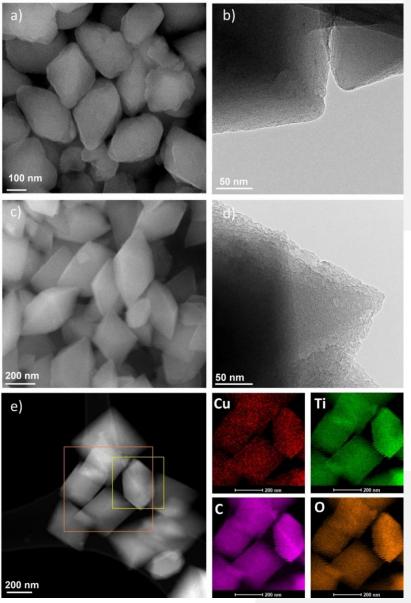


Fig. 11. Schematic diagram illustrating the work concepts for the Cu-NH₂-MIL-125(Ti) series.

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200 nm Fig. 12. (a) SEM and (b) TEM images of pristine NH₂- MIL-125(Ti). (c) SEM and (d) TEM images with elemental mapping (Cu, Ti, C, and O) of MIL(Cu/Ti)1.0 sample. "Pioneering hybrid materials for CO₂ photoconversion", no NOR/SGS/HotHybrids/0130/2020-00. Project financed by the Financial Mechanism of the European Economic Area (EEA) and the Norwegian Financial Mechanism 2014-2021.



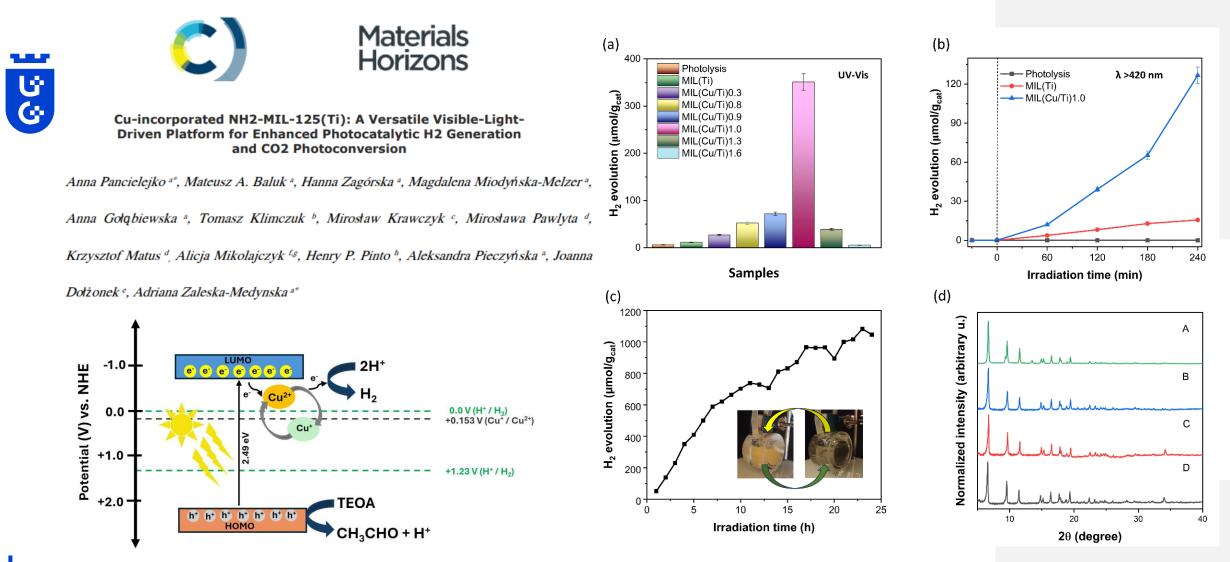


Fig. 14. Proposed mechanism of hydrogen generation in the presence of MIL(Cu/Ti)1.0 photocatalyst.

Fig. 13. Photocatalytic hydrogen generation after 4 hours of a) UV-Vis and b) visible irradiation.
c) Long-term stability of the most active sample under UV-Vis irradiation. d) XRD diffractograms of MIL(Cu/Ti)1.0 A – before irradiation, B – after 24 hours of UV-Vis radiation, C – after 4 hours of UV-Vis radiation, D - after 4 hours of Vis radiation.

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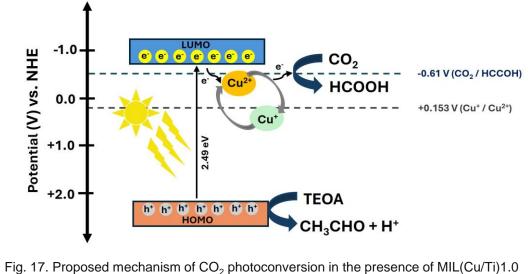
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g. 17. Proposed mechanism of CO₂ photoconversion in the presence of MIL(Cu/Ti)1.0 photocatalyst.

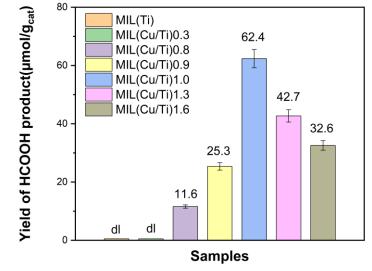


Fig. 15. Efficiency of photoconversion of CO_2 under visible irradiation (dl – detection limit).

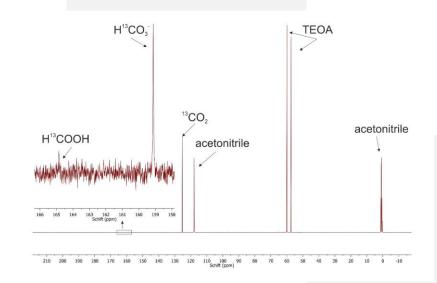


Fig. 16. ¹³C NMR spectra products detected during photoconversion of ¹³CO₂ in the presence of MIL(Cu/Ti)1.0 in visible range

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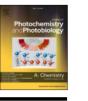
Journal of Photochemistry & Photobiology, A: Chemistry 454 (2024) 115731



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Novel room-temperature synthesis of pioneering CsPbX₃@(Ce)UiO-66-Y hybrid nanomaterials for boosted photocatalytic hydrogen evolution

Hanna Głowienke^a, Anna Pancielejko^{a,*}, Magdalena Miodyńska^a, Anna Gołąbiewska^a, Emilia Gontarek-Castro^a, Tomasz Klimczuk^b, Mirosław Krawczyk^c, Mirosława Pawlyta^d, Adriana Zaleska-Medynska^{a,*}

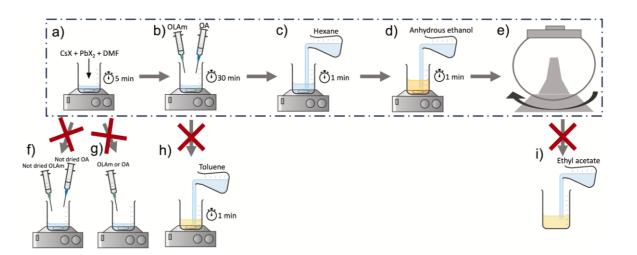


Fig. 18. (a-e) Schematic diagram of the successful synthesis route of $CsPbX_3$ (X = Br, I) perovskites along with (f-i) synthesis routes that did not allow obtaining the desired product.

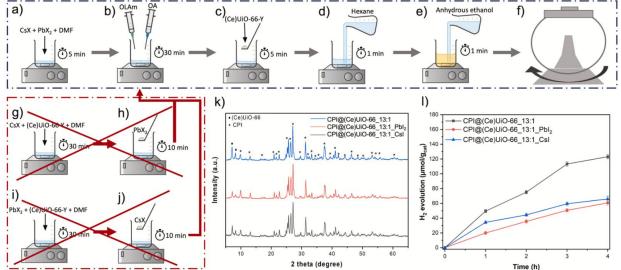


Fig. 19. (a-f) Schematic diagram of the successful synthesis route of $CsPbX_3@(Ce)UiO-66-Y$ (X = Br, I; Y = H, Br, NH₂) hybrids along with (g-j) problematic routes, k) XRD patterns for hybrids obtained with different order of reagent addition, I) efficiency of photocatalytic hydrogen evolution of hybrids obtained with different order of reagent addition.

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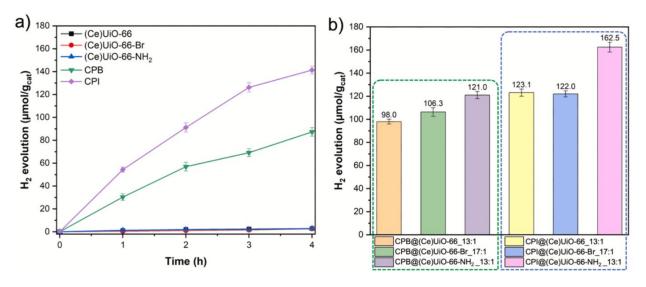


Fig. 20. a) Photocatalytic hydrogen generation efficiency of perovskites and MOFs and b) photocatalytic hydrogen generation after 4-h reaction using hybrids under UV-Vis radiation.

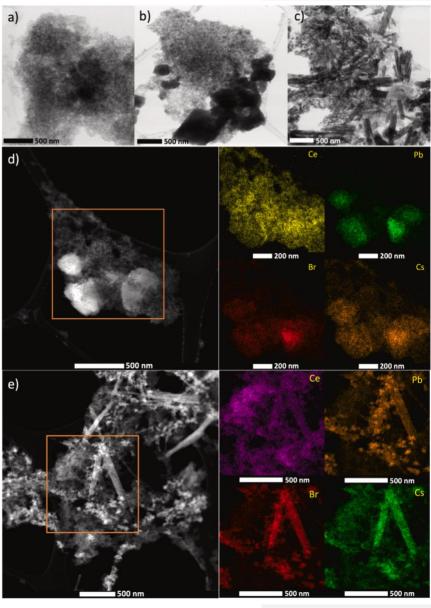


Fig. 21. TEM images a) (Ce)UiO-66-NH₂, b) CPB@(Ce)UiO-66-NH₂_13:1, b) CPI@(Ce)UiO-66-NH₂_13:1 and elemental mapping d) CPB@(Ce)UiO-66-NH₂_13:1 and e) CPI@(Ce)UiO-66-NH₂_13:1.

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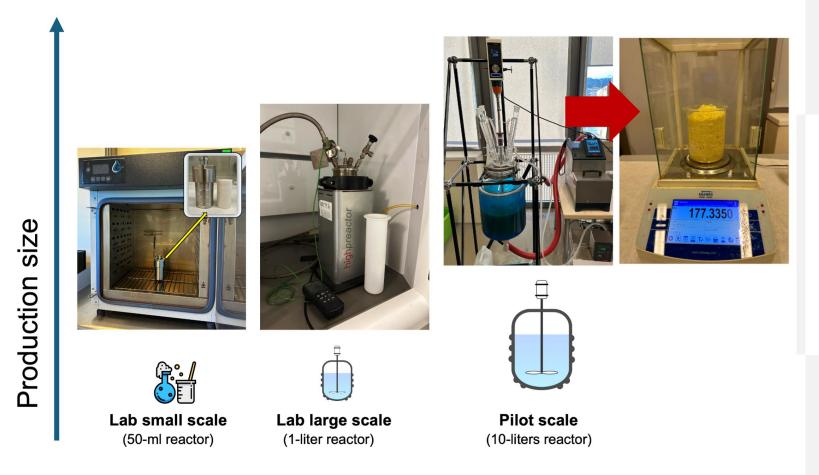


Fig. 22. Diagram showing the subsequent stages of the hybrid synthesis scale-up process.

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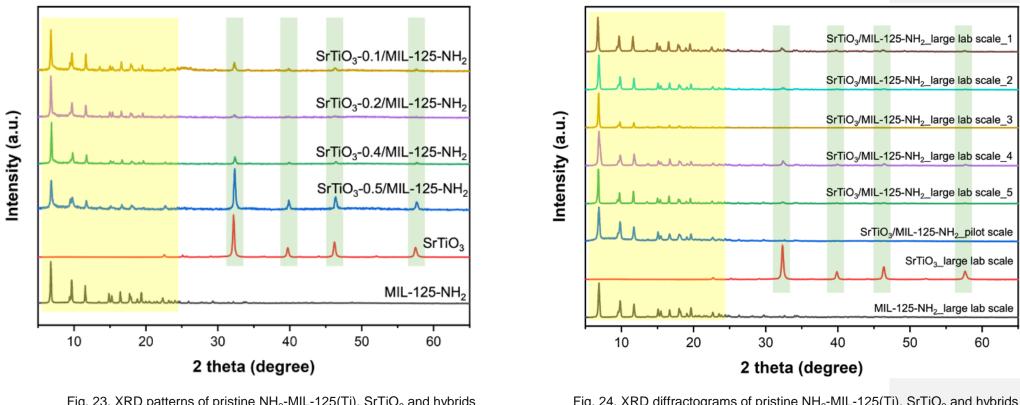


Fig. 23. XRD patterns of pristine NH_2 -MIL-125(Ti), SrTiO₃ and hybrids obtained on laboratory scale.

Fig. 24. XRD diffractograms of pristine NH₂-MIL-125(Ti), SrTiO₃ and hybrids obtained on large laboratory scale and pilot scale.

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Sample label	Amoun	t of H ₂ prod	H ₂ production rate		
Sample label	1 h	2 h	3 h	4 h	(µmol/h·g _{cat})
MIL-125-NH ₂	2.80	5.85	8.63	11.68	2.92
SrTiO ₃	5.22	10.40	20.55	23.89	5.97
SrTiO ₃ -0.1/MIL-125-NH ₂	118.78	161.10	201.83	217.20	54.30
SrTiO ₃ -0.2/MIL-125-NH ₂	32.11	60.91	113.81	160.67	40.17
SrTiO ₃ -0.4/MIL-125-NH ₂	1.89	3.79	6.30	6.65	1.66
SrTiO ₃ -0.5/MIL-125-NH ₂	2.02	4.63	7.14	9.71	2.43

Table 1. Results of the photocatalytic hydrogen generation reaction for samples obtained on a small laboratory scale after each hour of reaction.

Table 2. Photocatalytic hydrogen generation reaction results for large-scale laboratory and pilot-scale samples after each hour of reaction.

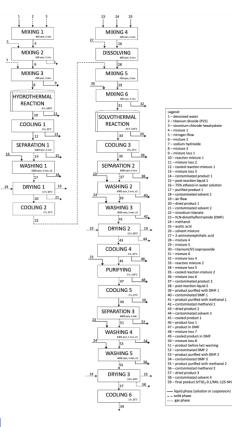
Sample label	Amou	Int of H ₂ pro	H ₂ production rate		
Sample laber	1h	2h	3h	4h	(µmol/h·g _{cat})
SrTiO ₃ /MIL-125-NH ₂ _large lab scale_1	3.30	7.90	14.34	19.14	4.79
SrTiO ₃ /MIL-125-NH ₂ _large lab scale_2	10.10	19.94	32.59	44.82	11.21
SrTiO ₃ /MIL-125-NH ₂ _large lab scale_3	3.35	9.22	17.47	26.34	6.59
SrTiO ₃ /MIL-125-NH ₂ _large lab scale_4	5.01	11.83	18.91	23.77	5.94
SrTiO ₃ /MIL-125-NH ₂ _large lab scale_5	2.23	5.98	8.42	10.25	2.56
SrTiO ₃ /MIL-125-NH ₂ _pilot scale	0.27	0.46	0.82	1.07	0.27
SrTiO ₃ large lab scale	139.16	239.16	307.43	354.30	88.58
MIL-125-NH ₂ large lab scale	22.46	48.08	65.73	82.36	20.59

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Flow chart



Mass balance

1	Process unit		INPUT	A.L		OU	TPUT
		Stream Delonized water	Mass (g)	Calculations	Stream	Mass (g)	Calculations
		Titanéum dicolde	0.502		Moture 1	52,112	m = 49,940 o + 0.502 o + 1.670 o = 52,112 o
1	Mixing 1	Strontium chloride hexalrychole	1.670				
		SUM	62.112		5UM	62.112	
2	Mixing 2	Mixture 1	52.112		Mixture 2	52.112	
-	-	Mistare 2	52.112		Modure 3	52.937	m = 52.112 g + 2.031 g = 54.143 g
3	Mixing 3	Sodium hydroxide Clim	2.031		Mixture loss 1	1.206	Millione tree 1 = 54.143 g - 52.937 g = 1.206 g
-			54.543		Reaction mixture 1	54.143	
4	Hydrothermal reaction	Mixture 3	52.937		Mixture loss 2	0.092	Present tot 2 = 52.937 g - 52.845 g = 0.2921 g
_	reactions	SUM	52.937		SuM Cooled reaction mixture 1	52.837 52.600	
s	Cooling 1	Reaction minture 1	52.845			0.245	- ffmater tes) = 52.845 g - 52.600 g = 0.245 g
·		SUM	52.845		505	52.845	
	Separation 1	Cooled reaction misture 1	52.600		Contaminated product 1 Post-reaction liquid 1	2.608	- Internetionant = 52,600 g - 2,608 g = 49,992 g
	Coperation 1	SUM	52.600		SUM	52.600	
		Contaminated product 1	2.008		Purified product 1	2.378	After 1st washing: 2,529 g After 2nd washing: 2,414 g After 3nd washing: 2,378-g
7	Washing 1	75% ethanol in water	100.719	1st washing: 33.621 g 2nd washing: 33.509 g 3nd washing: 33.589 g Summary: 100.719 g	Conteminated aslvent 1	100.949	$m_{Output = 2.078}$ g) = 100.949 g
-			103.327		SUM Dried product 1	103.327	
•	Drying 1	Purified product 1	2.378			1.210	**************************************
_			2.378		SUM	2.378	
9	Cooling 2	Dried product 1 SUM	1.168		Strontium Stanate	1,168	
		N.N-Sinethyllomeanide	1.582				Manutman = 16.941 g + 1.582 g + 2.013 g =
10	Mixing 4	Methanol Acetic acid	1.582		Solvent mixture	20.536	20.536 g
_			20.536		SUM	20.536	
	-	Solver4 midure	20.536 0.543		Mixture 4	21.079	master 4 = 20.536 g = 0.543 g = 21.079 g
11	Dissolving	2-aminoterephthalic acid SUM	0.543		5.00	21.079	
_		Mixture 4	21.079		Mixture 5	21.104	menue + 21.079 g = 0.025 g = 21.104 g
12	Mixing 5	Strontium titanate KLIM	0.025			21.104	
_		Mature 5	21.954		Mixture 6	21.005	
13	Mixing 6	Titerkum(Tv') isoproposide	0.553		Mixture loss 4	0.069	#mature test t = 21.104 g - 21.005 g = 0.099 g
-	Columbury 1	Minture 6	21.005		Reaction mixture 2	20,755	
14	Solvothermal reaction			-	Mixture loss 5	0.270	Minuter Inst = 21.005 g - 20.735 g = 0.270 g
-		SUM	21.005		Sum Cooled reaction minture 2	21.005	
15	Cooling 3	Reaction mixture 2	20.735	-	Modure less 6	0.256	minutes tes t = 20.735 g - 20.439 g = 0.296 g
_		SUM	20.735		SUM	20.735	
16	Separation 2	Cooled reaction mixture 2	20.439		Conteminated product 2 Post-reaction liquid 2	1.923	Minut median light (* 20.433 g - 1.923 g = 18.516 g
		SUM	20.439			20.439	
		Contaminated product 2	1.923		Product purified with DMF 1	1.696	After 1st washing: 1.703 g After 2nd washing: 1.699 g After 3nd washing: 1.699 g
17	Washing 2	N/N-dimethy/formamide	81.748	1st washing: 27.329 g 2nd washing: 27.154 g 3nd washing: 27.265 g Summary: 81.748 g	Contaminated DMF 1	01.973	тоничения т = 01.748 g + (1.923 g - 1.666 g) 81.973 g
		SUM	83.671		SUM	83.671	
					Product purified with methanol 1	1.342	After 1st washing: 1.497 g After 2nd washing: 1.401 g After 3nd washing: 1.342 g
		Product purified with DMF 1	1.098		Product particula with instruction of		
18	Weshing 3	Methanol	67.995	- fist washing: 22.597 g 2nd washing: 22.768 g 3nd washing: 22.632 g Summary, 67.995 g	Contaminated methanol 1	68.251	Новительно и 67.005 g + (1.606 g = 1.342 g) = 68.351 g
18	Washing 3	Methanol	67.995	- 1st washing: 22,597 g 2nd washing: 22,768 g 3nd washing: 22,432 g Summary: 67,995 g	Contaminated methanol 1	69.693	ET 105 a 1 /1 808 a - 1 347
18		Methanol SUM Product purfled with	67.995	2nd washing: 22,766 g 3nd washing: 22,632 a	Contaminated methanol 1 SUM		$\begin{array}{l} eq:massessessessessessessessessessessessesse$
	Washing 3 Drying 2	Methanol	67.995	2nd washing: 22,766 g 3nd washing: 22,632 a	Contentinated methanol 1 Dried product 2 SUM Contentinuted solvert 3 SUM	69.693 0.318 1.004 1.342	ET 105 a 1 /1 808 a - 1 347
19	Drying 2	Methanol SUM Product partied with methanol 1	67.995 69.993 1.342	2nd washing: 22,766 g 3nd washing: 22,632 a	Conteminated methanol 1 Sulli Dried product 2 Conteminated extent 3 Sulli Cooled product 1	69.693 0.318 1.004 1.342 0.317	Microsof Americanian (* 67.096 g + (1.696 g - 1.542 g) + 68.001 g ;
19		Methanol Sum Product putfied with methanol 1 Sum	67.995 69.993 1.342 1.342 0.318	2nd washing: 22,766 g 3nd washing: 22,632 a	Contentinated methanol 1 Dried product 2 Contentinated solvent 3 Cooled product 1 Product loss 1 Sum Sum	69.693 0.318 1.004 1.342 0.317 0.001	$\begin{array}{l} eq:massessessessessessessessessessessessesse$
19	Drying 2 Cooling 4	Methanol Finduct perfled with methanol 1 South Dried product 2 South Cooled product 1	67.995 69.993 1.342 1.342 0.318 0.318 0.317	2nd washing: 22,766 g 3nd washing: 22,632 a	Contentinated methanol 1 Drived product 2 Contentinated asheret 3 Contentinated asheret 3 Freduct loss 1 Preduct loss 1 Preduc	69.683 0.318 1.004 1.342 0.317 0.001 0.318 36.563	$\begin{array}{l} & Minormation of the set of the set$
19	Drying 2	Methanol Sum Product purfled with methanol 1 Sum Dried product 2 SUM	67.985 69.993 1.342 1.342 0.318 0.318 0.317 36.613	2nd washing: 22,766 g 3nd washing: 22,632 a	Contentinated methanol 1 Dried product 2 Contentinated solvent 3 Cooled product 1 Product loss 1 Sum Sum	69.693 0.318 1.604 1.342 0.317 0.001 0.318 36.560 0.337	Microsof Americanian (* 67.096 g + (1.696 g - 1.542 g) + 68.001 g ;
19	Drying 2 Cooling 4	Methanol Finduct perfled with methanol 1 South Dried product 2 South Cooled product 1	67.995 69.993 1.342 1.342 0.318 0.318 0.317	2nd washing: 22,766 g 3nd washing: 22,632 a	Contentinated methanol 1 Divid product 2 Solid Contentiated soliced 3 Solid Product iso Product iso 1 Briefwirt lass 7 Solid S	69.893 0.318 1.004 1.304 0.317 0.001 0.318 30.590 0.337 36.800	Microsovensovenske (* 67.365 g + (1.606 g - 1.342 g)) - - - - Microsovensovenske (* 67.365 g - 0.316 g - 1.024 g) - - - - Microsovensovenske (* 63.316 g - 0.316 g - 0.316 g - 0.316 g - 0.317 g - 0.001 g) - - - - - - - - - - - - - - - - - - -
19 20 21	Drying 2 Cooling 4 Paritying	Nethanol State methanol 1 State Dried product 2 Socied product 1 N.V-dimethyfformanide	67.985 69.993 1.342 1.342 0.318 0.318 0.317 36.613	2nd washing: 22,766 g 3nd washing: 22,632 a	Conteminated methanol 1 Conteminated methanol 1 Evid product 2 Contempode 1 Contempode 1 Product 1 Product in CMF Mature lass 7 Cooried product in CMF Cooried product in CMF	69.893 0.315 1.004 1.342 0.317 0.001 0.318 39.563 0.337 36.800 0.337 36.800 0.307	$\begin{array}{l} \begin{array}{l} \begin{array}{l} \text{There exists a result of 2.056 g + (1.056$ g - 1.342$ g + 6.351$ g \\ \text{9 + 63.351$ g \\ \end{array}} \\ \begin{array}{l} \begin{array}{l} \text{1 - 1.342$ g - 0.316$ g = 1.342$ g \\ \end{array}} \\ \begin{array}{l} \text{2 - 0.316$ g - 0.316$ g = 1.342$ g \\ \end{array}} \\ \begin{array}{l} \text{2 - 0.316$ g - 0.317$ g - 0.001$ g \\ \end{array}} \\ \begin{array}{l} \begin{array}{l} \text{2 - 0.316$ g = 1.342$ g \\ \end{array}} \\ \begin{array}{l} \text{2 - 0.316$ g = 1.342$ g \\ \end{array}} \\ \begin{array}{l} \text{2 - 0.316$ g = 0.317$ g \\ \end{array}} \\ \begin{array}{l} \text{2 - 0.316$ g \\ \end{array}} \end{array} \\ \begin{array}{l} \text{2 - 0.316$ g \\ \end{array}} \\ \begin{array}{l} \text{2 - 0.316$ g \\ \end{array}} \\ \begin{array}{l} \text{2 - 0.316$ g \\ \end{array}} \end{array} \\ \begin{array}{l} \text{2 - 0.316$ g \\ \end{array}} \\ \begin{array}{l} \text{2 - 0.316$ g \\ \end{array}} \end{array} $
	Drying 2 Cooling 4	Methanol SuM Product purified with methanol 1 SuM Dried product 2 SuM Cooled product 1 N/4-dereity/formatile SUM	67.995 99.993 1.342 1.342 0.318 0.318 0.317 36.613 36.939	2nd washing: 22,766 g 3nd washing: 22,632 a	Contaminated methanol 1 Contaminated methanol 1 Drivit product 2 Solid Contaminated solved 3 Solid Contaminated solved 1 Product loss 7 Noture loss 7 Contaminated to DMF Modure loss 7 Solid Contaminated to DMF	69.693 0.318 1.204 1.342 0.317 0.301 0.318 39.593 0.337 36.890 35.694 0.305 36.694 0.305 36.694	Microsovensovenske (* 67.365 g + (1.606 g - 1.342 g)) - - - - Microsovensovenske (* 67.365 g - 0.316 g - 1.024 g) - - - - Microsovensovenske (* 63.316 g - 0.316 g - 0.316 g - 0.316 g - 0.317 g - 0.001 g) - - - - - - - - - - - - - - - - - - -
19 20 21 22	Drying 2 Cooling 4 Puritying Cooling 5	Methanol Product perflect with methanol 1 Dried product 2 Gooled product 1 N.N. dissethytformanside BOM Product in DMF	67.995 69.993 1.342 1.342 0.318 0.318 0.317 36.613 36.939 36.993	2nd washing: 22,766 g 3nd washing: 22,632 a	Contentinuited methanol 1 Dried prestant 2 Government a submit 3 Dried prestant 3 Dried methanis a submit 3 Dried methanis 4	69.693 0.315 1.224 1.342 0.317 0.317 0.317 0.318 30.593 0.337 36.694 0.337 36.694 0.159 38.899 36.694 0.159	Minimum (1978) 9 (1989) 9 (198
19 20 21 22	Drying 2 Cooling 4 Paritying	Methanol Product purified with methanol 1 SUM Dried product 2 SUM Cooled product 1 SUM No-disentity/formanice No-disentity/formanice SUM Product in DMF	67.995 99.993 1.342 1.342 0.318 0.318 0.319 0.317 34.939 36.913 34.939 36.913 34.939 35.935	2nd washing: 22,766 g 3nd washing: 22,632 a	Contaminated methanol 1 Contaminated methanol 1 Drivit product 2 Solid Contaminated solved 3 Solid Contaminated solved 1 Product loss 7 Noture loss 7 Contaminated NUM Contamina	69.693 0.318 1.204 1.342 0.317 0.301 0.318 39.593 0.337 36.890 35.694 0.305 36.694 0.305 36.694	Barrensmann AF 2006 g + 1,040 g - 1,342 g -1,042 g
19 20 21 22 23	Drying 2 Cooling 4 Paritying Cooling 5 Separation 3	Methanol Product purified with restloand 1 SUM Dried product 2 SUM Coded product 1 SUM Nu-dimetry/tomacrise SUM Coded product in DMF SUM Coded product in DMF	67.985 49.993 1.342 0.318 0.318 0.377 31.613 34.939 35.939 35.434	2nd washing: 22,766 g 3nd washing: 22,632 a	Contentinated methanel 1 Contentinated methanel 1 Oried predent 2 Content ended to level 3 Content ended to level 3 Content of the set of	69.663 0.318 1.404 0.317 0.001 0.317 0.001 0.318 30.550 0.337 36.650 0.337 36.650 0.337 36.650 0.555 36.656 36.656 36.656	Minimum (1973) 9 9 1 1 202 9 - 1 202 9 1 1 202 9 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
19 20 21 22 23	Drying 2 Cooling 4 Puritying Cooling 5	Methanol Seal motivate perified with motivation 1 Seal Dried product 2 Seal Coded product 1 Seal Product in CMF Seal Seal Coded product in CMF Seal Coded product in CMF	67.995 99.993 1.342 1.342 0.318 0.318 0.319 0.317 34.939 36.913 34.939 36.913 34.939 35.934	204 washing 22.768 g di washing 27.682 g Seremary 87.995 g	Contentinuited methanol 1 Dried prestant 2 Government a submit 3 Dried prestant 3 Dried methanis a submit 3 Dried methanis 4	69.693 0.318 1.204 1.342 0.317 0.001 0.318 30.595 0.337 36.694 0.307 36.694 0.109 36.694 0.109 36.694 0.109 36.694 0.109	$\begin{split} & \text{Restructures and } (7.200 \text{ g} + 1.000 \text{ g} - 1.302 \text{ g} \\ & + 0.201 \text{ g} \\ & \text{Restructures and } + 1.302 \text{ g} - 0.214 \text{ g} + 1.024 \text{ g} \\ & \text{Restructures } + 3.014 \text{ g} - 0.214 \text{ g} + 0.024 \text{ g} \\ & \text{Restructures } + 3.014 \text{ g} - 0.214 \text{ g} - 0.024 \text{ g} \\ & \text{Restructures } + 3.042 \text{ g} + 0.217 \text{ g} - 0.024 \text{ g} \\ & \text{Restructures } + 3.042 \text{ g} - 1.324 \text{ g} + 0.223 \text{ g} \\ & \text{Restructures } + 3.042 \text{ g} - 1.214 \text{ g} - 3.029 \text{ g} \\ & \text{Restructures } + 3.042 \text{ g} - 1.2143 \text{ g} - 3.1042 \text{ g} \\ & \text{Restructures } + 3.044 \text{ g} - 1.214 \text{ g} - 3.1042 \text{ g} \\ & \text{Restructures } + 3.044 \text{ g} - 1.214 \text{ g} - 3.1042 \text{ g} \\ & \text{Restructures } + 3.044 \text{ g} - 1.214 \text{ g} \\ & \text{Restructures } + 3.044 \text{ g} \\ & $
19 20 21 22	Drying 2 Cooling 4 Paritying Cooling 5 Separation 3	Nathand Product purfield with exclusional 1 5000 Cried product 3 5000 Cried product 1 5000 Product in DAF Product in DAF Product in DAF Product before last weaking N.NGreetly/Jorrumski	67.985 68.993 1.342 0.318 4.334 0.318 4.334 0.317 36.933 36.939 35.434 36.939 35.444 1.618 81.773	20 de westing 22 76 g de westing 27 84 g Serenary 87 994 g - - - - - -	Contentinated methanel 1 Contentinated methanel 3 Content contential attention 3 Content content of 3 Content content of 3 Content content of 3 Content content of 3 Products to Mar. Products for SMP Products for SMP Product for SMP Product attential Content of 3 Product attentia	69,893 0,315 1,424 0,317 0,261 0,317 0,261 0,317 0,261 0,317 0,317 0,317 0,317 0,317 0,317 0,317 0,317 0,317 0,316 0,318 0,418 0,119 0,110	$\begin{split} & & \text{Reservations} \rightarrow 67.206 \text{ g} + (1.406 \text{ g} - 1.342 \text{ g}) \\ & & \text{Reservations} + 1.342 \text{ g} - 0.314 \text{ g} + 1.024 \text{ g}) \\ & & \text{Reservations} + 1.344 \text{ g} - 0.314 \text{ g} = 1.024 \text{ g}) \\ & & \text{Reservations} + 2.344 \text{ g} - 0.317 \text{ g} - 0.304 \text{ g}) \\ & & \text{Reservations} + 2.344 \text{ g} - 1.024 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.347 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.344 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} - 1.024 \text{ g} + 2.844 \text{ g} + 2.844 \text{ g}) \\ & & \text{Reservations} + 2.844 \text{ g} + 2.8$
19 20 21 22 23	Drying 2 Cooling 4 Paritying Cooling 5 Separation 3	Nathand Product purfield with exclusional 1 5000 Cried product 3 5000 Cried product 1 5000 Product in DAF Product in DAF Product in DAF Product before last weaking N.NGreetly/Jorrumski	67.945 93.993 1.342 1.342 0.318 0.358 0.357 0.577 36.613 34.939 35.943 34.939 35.943 34.944 1.618	204 washing 22.768 g di washing 27.682 g Seremary 87.995 g	Contentinated methanel 1 Contentinated methanel 3 Content contential attention 3 Content content of 3 Content content of 3 Content content of 3 Content content of 3 Products to Mar. Products for SMP Products for SMP Product for SMP Product attential Content of 3 Product attentia	69,663 0,315 1,524 1,524 1,525 0,317 0,551 0,337 36,555 0,337 36,656 0,337 36,656 0,359 36,664 0,559 34,859 34,859 34,859 34,859 34,859 1,615	Bigs of the second se
19 20 21 22 23	Drying 2 Cooling 4 Paritying Cooling 5 Separation 3	Nerhand Product putfort sith Annual Constant Constant Constant Product 2 Constant product 1 Solid Constant product 1 Solid Constant product 10 Solid Product to Konst Solid Product to Konst Solid Product to Konst Solid Nuk densethyliotreamide Solid	67.995 69.993 1.342 5.342 0.318 0.318 0.317 34.939 34.939 35.903 34.939 35.933 34.944 1.418 81.773 83.394	20 de westing 22 76 g de westing 27 84 g Serenary 87 994 g - - - - - -	Containing in exchange 1 Des product 2 Des p	69,890 0.315 1.604 0.315 1.604 0.317 0.001 0.317 0.001 0.337 0.601 0.337 0.601 0.337 0.601 0.337 0.601 0.339 0.406 0.359 0.406 0.359 0.406 0.359 0.406 0.359 0.400 0.400000000	Barray All P. 201 a. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
19 20 21 22 23	Drying 2 Cooling 4 Paritying Cooling 5 Separation 3	Nathand Product purfield with exclusional 1 5000 Cried product 3 5000 Cried product 1 5000 Product in DAF Product in DAF Product in DAF Product before last weaking N.NGreetly/Jorrumski	67.985 68.993 1.342 0.318 4.334 0.318 4.334 0.317 36.933 36.939 35.434 36.939 35.444 1.618 81.773	20-4 watring 22 746 g 3-mmar, 27 295 g 3-mmar, 27 295 g - - - - - - - - - - - - -	Contentinated methanel 1 Contentinated methanel 3 Content contential attention 3 Content content of 3 Content content of 3 Content content of 3 Content content of 3 Products to Mar. Products for SMP Products for SMP Product for SMP Product attential Content of 3 Product attentia	69,893 0,315 1,424 0,317 0,261 0,317 0,261 0,317 0,261 0,317 0,317 0,317 0,317 0,317 0,317 0,317 0,317 0,317 0,316 0,318 0,318 0,317 0,316 0,318 0,418 0,119 0,110	Bigs of the second se
19 20 21 22 23	Drying 2 Cooling 4 Paritying Cooling 5 Separation 3	Nerhand Product putfort sith Annual Constant Constant Constant Product 2 Constant product 1 Solid Constant product 1 Solid Constant product 10 Solid Product to Konst Solid Product to Konst Solid Product to Konst Solid Nuk densethyliotreamide Solid	67.995 69.993 1.342 5.342 0.318 0.318 0.317 34.939 34.939 35.903 34.939 35.933 34.939 35.454 1.418 81.773 83.394	2014 washing 22 768 g 3.mmark 27 295 g 3.mmark 27 295 g - - - - - - - - - - - - -	Containing in exchange 1 Des product 2 Des p	69,890 0.315 1.604 0.315 1.604 0.317 0.001 0.317 0.001 0.337 0.406 0.339 0.337 0.406 0.359 0.359 0.466 0.359 0.45900000000000000000000000000000000000	Barray 41,000 p.
19 20 21 22 23 24	Drying 2 Cooling 4 Purthying Cooling 5 Separation 3 Washing 4	Nerband Product performance Product performance Deter products 2 Both Product to DOM Record product in DOM Record performance Record perfo	67.985 99.993 1.342 1.342 1.342 0.318 8.358 0.317 36.993 36.995	204 watering 22.768 g 34 watering 27.768 g 34 watering 27.768 g - - - - - - - - - - - - -	Contentated methanel 1	69.663 0.518 1.629 1.629 0.347 0.347 0.347 0.347 0.347 0.347 0.347 0.347 0.347 0.348 0.3450 0.350 0.460	Barray All P. 2014 (* 1000 B) P. 2014 (* 1000
19 20 21 22 23 24	Drying 2 Cooling 4 Purifying Cooling 5 Separation 3 Washing 4	Nerband Protect perfort AN Protect perfort AN Dried protect 2 Coded protect in DAP Protect in DAP Protect in DAP Protect protect in DAP Protect perfort in DAP	67.985 93.993 1.342 0.318 0.318 0.318 0.327 34.939 34.939 34.943 34.943 34.943 34.944 1.618 81.773 83.775 83.775 63.384	2014 washing 22 768 g 3.mmark 27 295 g 3.mmark 27 295 g - - - - - - - - - - - - -	Contentated methods 1 Description of the second status 2 Description of the second status 3 Description of the second sta	69,6853 0.318 1.324 0.317 0.501 0.347 0.501 0.318 30,550 0.337 34,830 36,650 36,484 1.460 34,839 34,650 34,450 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 34,650 35,651 34,652 35,651 34,652 35,651 35,651 35,651 35,651 35,651 35,651 35,651 35,651 35,651 <td>The second second</td>	The second
19 20 21 22 23 24	Drying 2 Cooling 4 Purthying Cooling 5 Separation 3 Washing 4	Nerband Franket terford (M) Product profest 2 Dried product 2 Body Product in DAP Product in DAP Product in DAP Product before last watering SAR Product public watering SAR Product pub	67.985 69.992 1.342 1.342 0.318 8.398 0.327 36.693 36.993 35.993 35.993 35.993 35.993 35.993 35.993 35.494 35.494 35.494 35.494 1.418 67.875 69.399 1.200	2014 washing 22 768 g 3.mmark 27 295 g 3.mmark 27 295 g - - - - - - - - - - - - -	Contentated methanel 1 Deter provide 1 Deter p	69 850 0.335 1.342 0.347 0.347 0.261 0.347 0.261 0.348 0.261 0.337 34.899 36.464 0.350 38.889 34.859 34.4566 33.4556 38.4544 1.4460 1.460 81.911 1.209 63.150 99.359 0.2627 0.2627	Barray All Fill Stag + 1 (100 g + 1 (200 g + 1 (
19 20 21 22 23 24	Drying 2 Cooling 4 Purifying Cooling 5 Separation 3 Washing 4	Nerband Protect perfort AN Protect perfort AN Dried protect 2 Coded protect in DAP Protect in DAP Protect in DAP Protect protect in DAP Protect perfort in DAP	67.985 93.993 1.342 0.318 0.318 0.318 0.327 34.939 34.939 34.943 34.943 34.943 34.944 1.618 81.773 83.775 83.775 63.384	2014 washing 22 768 g 3 membra 27 768 g 3 membra 27 768 g - - - - - - - - - - - - -	Contentated methods 1 Description of the second status 2 Description of the second status 3 Description of the second sta	69,6853 0.318 0.318 1.3624 0.317 0.561 0.338 0.561 0.338 0.550 0.337 34.839 34.636 36.644 1.440 34.655 34.655 34.654 34.655 34.654 34.655 34.654 34.655 34.654 34.655 34.654 34.655 34.654 34.655 35.654 34.655 35.654 34.655 35.654 34.655 35.654 34.655 35.654 34.655 35.654 34.655 35.654 34.655 35.654 34.655 35.654 34.655 35.654 35.655 35.656 35.656 35.656 35.657 35.656 35.658 35.656 35.658 35.656 35.656 35.656 35.657 <t< td=""><td>The second second</td></t<>	The second

PROCESS UNIT	INPUT	OUTPUT		
	Calculations/assumptions	Enthalpy (kJ)	Calculations/assumptions	Enthalpy (kJ)
Mixing 1	$\begin{array}{l} \Delta H_{reactants} = \Delta H_{H_{2}O} + \Delta H_{SYCI_2 \times SH_2O} + \Delta H_{TiO_2} \\ = (-792.321 \ kJ) + (-4.973 \ kJ) + (-5.668 \ kJ) \\ = -802.962 \ kJ \end{array}$	-802.962	ΔH of the dissolution process of $SrCl_2\cdot 6H_2O$ in water $(-0.347\ kJ)$	-0.347
Mixing 3	ΔH of Mixing 1 process (-0.347 kJ) + ΔH of the NaOH (-21.722 kJ) = -22.069 kJ	-22.069	ΔH of the exothermic process (1.992 kJ) + ΔH of the dissolution process of NaOH in water (-2.264 kJ) = -0.272 kJ	-0.272
Hydrothermal reaction	ΔH of Mixing 3 process (-0.272 kJ)	-0.272	ΔH of the hydrothermal reaction with change of temperature from 25°C to 180°C (-0.785 k/) + energy losses (7176.686 k/) = 7175.901 k/	7175.901
Cooling 1	ΔH of the hydrothermal reaction with change of temperature from 25°C to 180°C (-0.785 kJ)	-0.785	ΔH associated with temperature change from 180°C to 25°C (-34.251 kJ)	-34.251
Drying 1	$\Delta H_{reactants} = \Delta H_{srtio_3} + \Delta H_{geon} + \Delta H_{water}$ = (-10.531 kJ) + (-5.358 kJ) + (-4.800 kJ) = -20.689 kJ	ΔH associated with solvents vaporization in 60°C (1.529 kJ)		3242.609
Cooling 2	ΔH of Drying 1 process (1.529 kJ)	1.529	ΔH associated with temperature change from 60°C to 25°C (-0.221 kl)	-0.221
Dissolving	$\begin{array}{l} \Delta H_{reactants} = \Delta H_{DMF} + \Delta H_{HeOH} + \Delta H_{acctlc acid} \\ & + \Delta H_{2-antinoterrphithalic acid} \\ & = (-55.448 kJ) + (-11.682 kJ) + (-16.440 kJ) \\ & + (-2.449 kI) = -86.019 kJ \end{array}$	-86.019	ΔH for the dissolution process of 2-aminoterephthalic acid in DMF (-0.399 k/)	-0.399
Mixing 6	ΔH of the dissolution process of 2-aminoterephthalic acid in DMF (-0.399 k/) + ΔH of the titanium(IV) isopropoxide (-3.337k/) + ΔH of the strontium titanate (-0.165 k]) = -3.928 k/	-3.928	ΔH for the dissolution process of titanium(IV) isopropoxide DMF (38.058 k/)	
Solvothermal reaction	ΔH of the dissolution process of titanium(IV) isopropoxide in DMF (38.058 kJ)	38.058	ΔH of the solvothermal reaction with change of temperature from 25°C to 150°C (2.557k/) + energy losses (23 150.621 k/) = 23 153.178 k/	23 153.178
Cooling 3	ΔH of the solvothermal reaction with change of temperature from 25°C to 150°C (2.557kJ)	2.557	ΔH associated with temperature change from 60°C to 25°C (-5.353 kJ)	-5.353
Drying 2	$\Delta H_{reactants} = \Delta H_{srTiO_{\chi} \rightarrow 0.1/MIL-125-NH_{\chi}} + \Delta H_{MeOH}$ = (-0.501 kl) + (-7.629 kl) = -8.13 kl	-8.13	ΔH associated with methanol vaporization in 60°C (1.139 kJ) + energy losses (3 241.080 kJ) = 3242.219 kJ	3242.219
Cooling 4	ΔH associated with methanol vaporization in 60°C (1.139 kJ)	1.139	ΔH associated with temperature change from 60°C to 25°C (-0.012 k/	-0.012
Purifying	$\Delta H_{reactants} = \Delta H_{STI0_2-0.1/MIL-12S-NH_2} + \Delta H_{DMF}$ = (-0.499 kJ) + (-119.739 kJ) = -120.238 kJ	-120.238	ΔH associated with temperature change from 25°C to 150°C (-9.444 kJ) + energy losses (51 006.375 kJ) = 50996.931 kJ	50996.931
Cooling 5	ΔH associated with purifying process (-9.444 kJ)	-9.444	ΔH associated with temperature change from 60°C to 25°C (-9.425 kJ)	-9.425
Drying 3	$\Delta H_{reactants} = \Delta H_{SrTiO_2-0.1/MIL-12S-NH_2} + \Delta H_{McOH}$ = (-0.452 kJ) + (-6.914 kJ) = -7.366 kJ	-7.366	ΔH associated with methanol vaporization in 60°C (1.032 kJ) + energy losses (3 241.080 kJ) = 3242.112 kJ	3242.112
Cooling 6	ΔH associated with methanol vaporization in 60°C (1.032 kJ)	1.032	ΔH associated with temperature change from 60°C to 25°C (-0.010 kl)	-0.010

Energy balance

Costs of synthesis

No.	Reagent	Producer	Mass/volume	Gross price (PLN)
1	Titanium(IV) oxide, Aeroxide® (P25)	Acros Organics	1 kg	1173.53
2	Strontium chloride hexahydrate	Thermo Scientific	100 g	136.83
3	Sodium hydroxide (NaOH)	STANLAB	1 kg	20
4	Ethyl alcohol, 96%	POCH	1L	147.48
5	N,n-dimethylformamide (DMF)	POCH	1L	34.44
6	Acetic acid, 99.5-99.9%	POCH	1 L	25.34
7	Methanol	STANLAB	1L	14.76
8	2-aminoterephthalic acid, 99%	Thermo Scientific (Acros)	100 g	1684.12

	Sr1iO ₃ (1.11	g of product from 1 synth	nesis)
No.	Reagent	Amount used	Gross price (PLN)
1	Titanium(IV) oxide, Aeroxide® (P25)	0.5 g	0.59
2	Strontium chloride hexahydrate	1.67 g	2.29
3	Sodium hydroxide (NaOH)	2 g	0.04
4	Ethyl alcohol, 96%	30 ml	4.42
			In total: 7.34 PLN
			6.61 PLN per g of product
			6 612.61 PLN per kg of product
	SrTiO ₃ large lab sc	ale (12.46 g of product from	n 1 synthesis)
No.	Reagent	Amount used	Gross price (PLN)
1	Titanium(IV) oxide, Aeroxide® (P25)	5.5 g	6.49
2	Strontium chloride hexahydrate	18.37 g	25.19

1	Titanium(IV) oxide, Aeroxide® (P25)	5.5 g	6.49
2	Strontium chloride hexahydrate	18.37 g	25.19
3	Sodium hydroxide (NaOH)	22 g	0.44
4	Ethyl alcohol, 96%	90 ml	13.27
			In total: 45.39 PLN
			3.64 PLN per g of product
			3 642.86 PLN per kg of product

No.	Reagent	Amount used	Gross price (PLN)
1	SrTiO ₃ (synthesized in I step)	25 mg	0.09
2	DMF	238 ml	8.20
3	Acetic acid	2 ml	0.05
4	Methanol	182 ml	2.69
5	2-aminoterephthalic acid	0.543 g	9.14
6	Titanium(IV) isopropoxide	0.6 ml	0.53
	SrTiO ₃ /MIL-125-NH2_large lab scale_3	72 125.	In total: 20.7 PLI 2.13 PLN per g of product 44 PLN per kg of product
No.	Reagent	Amount used	Gross price (PLN)
1	SrTiO ₃ (synthesized in I step)	600 mg	3.97
2	DME	2.132 L	73.43
3	Acetic acid	48 ml	1.22
4	Methanol	1.248 L	18.42
5	2-aminoterephthalic acid	13.032 g	219.36
6	Titanium(IV) isopropoxide	14.4 ml	12.72
		28 711.	In total: 329.12PL 71 PLN per g of products 51 PLN per kg of products
No.	SrTiO ₃ /MIL-125-NH ₂ pilot scale (17)	Amount used	
	Reagent		Gross price (PLN) 39.66
2	SrTiO ₃ (synthesized in I step) DMF	6 g 12.32 L	424.37
3	Acetic acid	12.32 L 480 ml	424.37
4	Methanol	480 mi 6.48 L	95.64
			2193.6
5	2-aminoterephthalic acid Titanium(IV) isopropoxide	130.32 g	2193.6
0	i itanium(iv) isopropoxide	144 mi	127.2 In total: 2892.67 PL
		16	3.31 PLN per g of produc

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WP1: Development of single and double perovskite synthesis methods

Efforts to introduce double perovskites into MOF synthesis demonstrated their instability, as they degraded in the solvents required for MOF formation and under elevated temperatures. Ultimately, several single perovskites were selected for further investigation, including CsPbX₃ (X = Br, I), Cs₃Bi₂X₉ (X = I, Br, CI), and SrTiO₃.

WP2: Synthesis of MOFs and their composites suitable for heterogeneous photocatalysis

The goal was to synthesize MOFs that are both theoretically attractive for photocatalytic applications and stable in aqueous solutions for hybrid material development. While various combinations were explored (e.g., CsPbX₃@UiO-66, CsPbX₃@ZIF-67, CsPbB₃/SiO₂@In-MIL-68, Cs₂AgBiBr@UiO-66-NH₂, CsAgBiBr₆@ZIF-68), only a few showed significant photocatalytic activity. These included: (i) CsPbX₃@UiO-66-Y (X = Br, I; Y = H, NH₂, Br), (ii) SrTiO₃@NH₂-MIL-125(Ti), (iii) TiO₂-X@Cs₃BiX₉ (X = Cl, Br, I), (iv) CuGaS₂@NH₂-MIL-125(Ti), and (v) Cu-NH₂-MIL-125(Ti).

WP3: Photocatalytic activity analysis

The photocatalytic performance of the hybrids was assessed in H_2 generation and CO_2 photoconversion reactions. All hybrid systems exhibited activity in H_2 generation, while only Cu-NH₂-MIL-125(Ti) demonstrated activity in CO_2 photoconversion.

WP4: Scaling up SrTiO₃@NH₂-MIL-125(Ti) hybrid synthesis

A scalable synthesis method for SrTiO₃@NH₂-MIL-125(Ti) was developed using a 10-liter batch reactor, yielding over 170 grams per batch. A detailed process flow diagram was created, accompanied by mass and energy balances and an economic analysis.

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