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nsu DEVELOPMENT
MICROELECTRONICS ELEMENTARY PARTICLES
INNOVATIONS CATALYTIC MATERIALS
CATALYTIC MATERIALS
ASSEMBLY POINT DRUG DESIGN
SCIENTIFIC LABORATORY HYBRID MATERIALS
GEOPHYSICS ENGINEERING ENERGY CONSERVATION
BIOTECHNOLOGY GEOCHEMISTRY NANOTECHNOLOGY
HIGH ENERGIES SEMIOTICS SCIENCE COGNITIVE TECHNOLOGIES
MATHEMATICAL MODELING
IT DEEP LEARNING BRAIN STUDY ARCHEOLOGY
ASTROPHYSICS BIOINFORMATICS LASER PHYSICS KNOWLEDGE ECONOMY GEOLOGY

N* Novosibirsk State University
*THE REAL SCIENCE



BORESKOV INSTITUTE
OF CATALYSIS

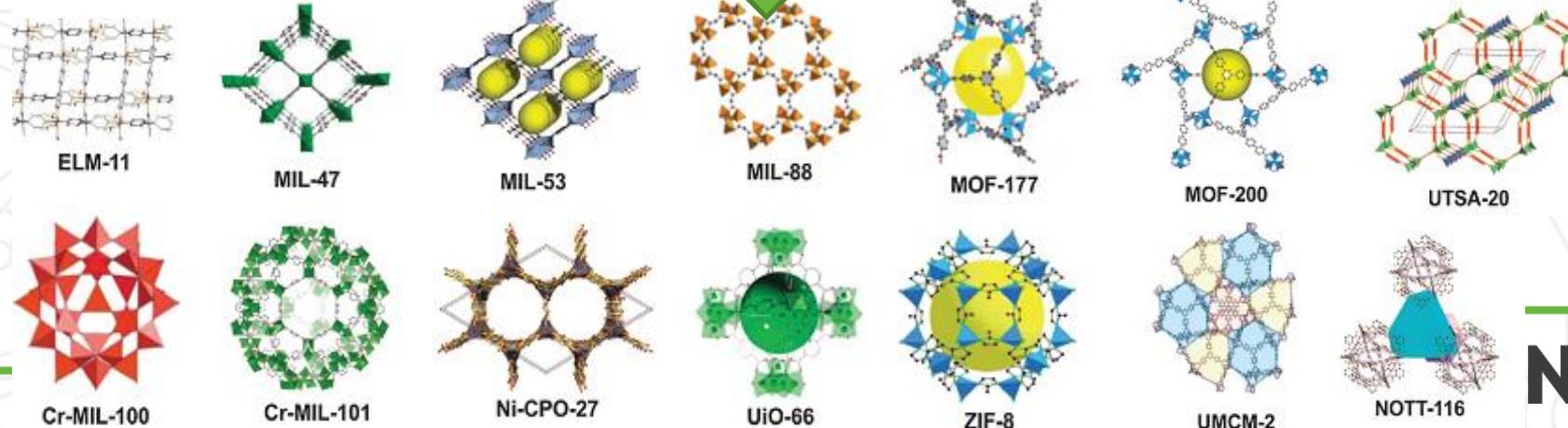


CaCl₂-MIL-101(Cr) composite as adsorbent for potable water extraction from the atmosphere

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* Metal-Organic Frameworks (MOFs)

MOFs – a family of crystalline solids with permanent porosity in which the metal ions or metal-oxygen clusters are bonded through bridging organic linkers.



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Metal-Organic Frameworks (MOFs)

Catalysis

Gas storage/
separation

Huge surface
area
 $S = 500\text{-}4500\text{m}^2/\text{g}$

Large
adsorption
capacity

APPLICATIONS

Adsorption
Water
Extraction from
Air (AWEA)

Water
purification

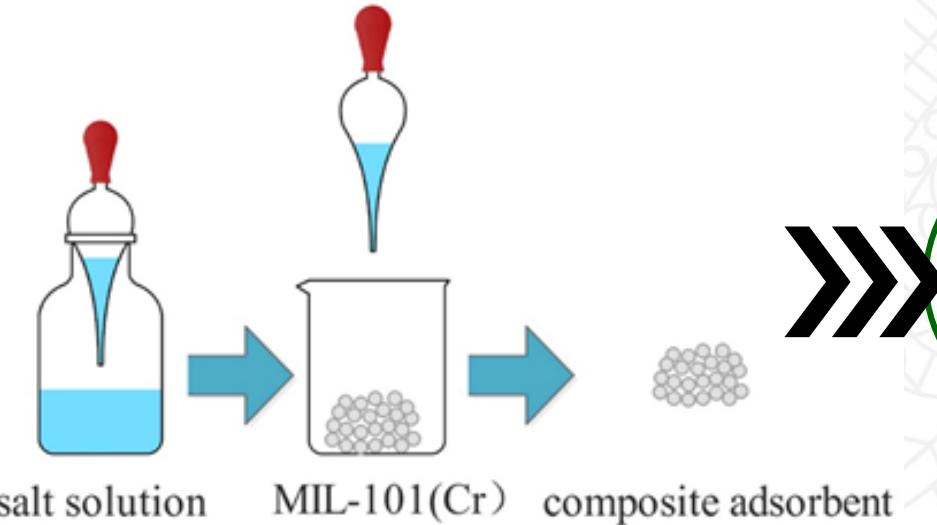
PROPERTIES

High porosity
(50-90%)

Tunable
adsorption
properties



*Composites “salt inside porous matrix” (CSPMs)



Growth
of the amount of
water adsorbed at low
relative pressure



*Tan B. et al. Composite salt in MIL-101 (Cr) with high water uptake and fast adsorption kinetics for adsorption heat pumps //Microporous and Mesoporous Materials. – 2019. – T. 286. – C. 141-148.



* The aim of the work

**Study of CSPMs
 $\text{CaCl}_2\text{-MIL-101(Cr)}$
as adsorbents for
the process of
Adsorption Water
Extraction from the
Air (AWEA)**

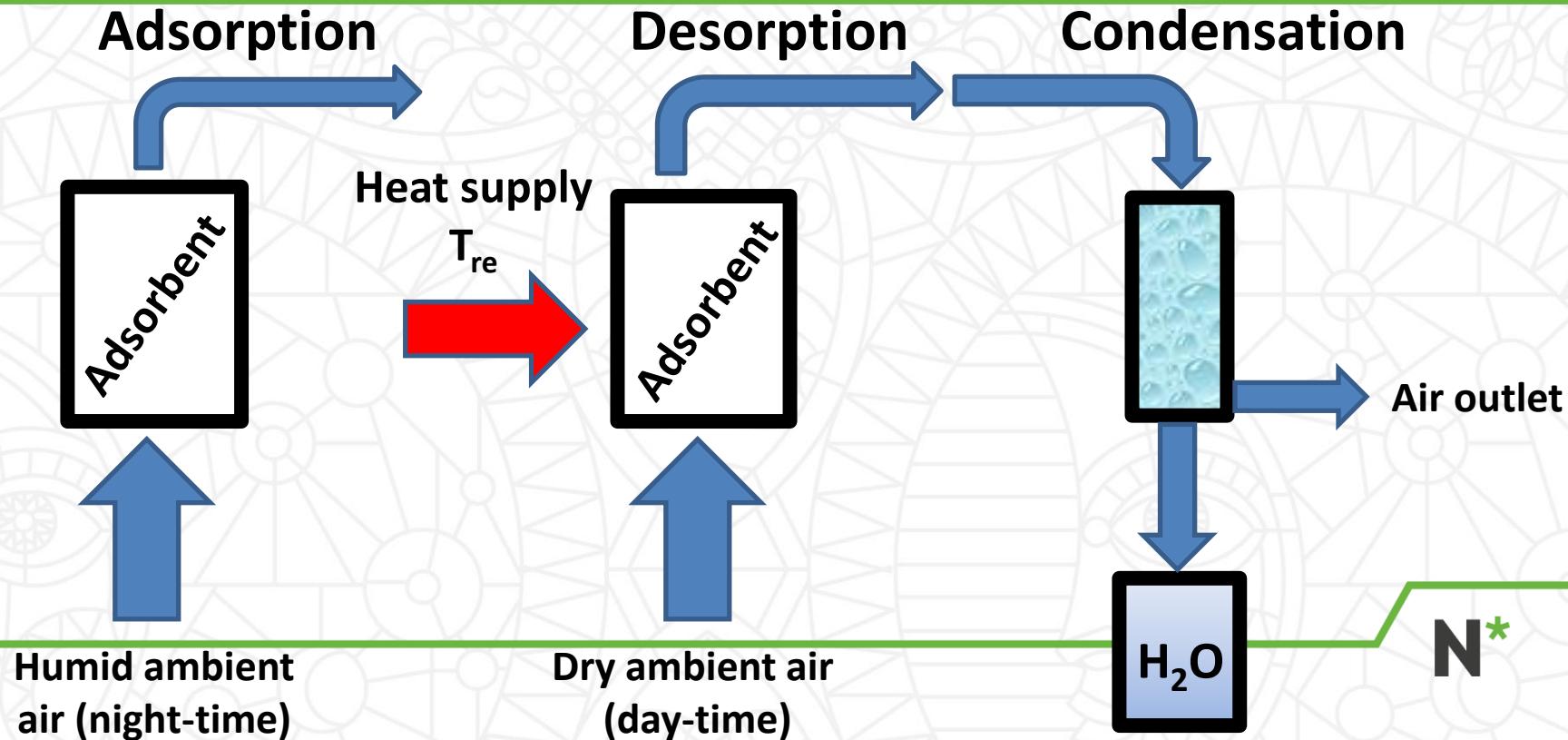
Synthesis of $\text{CaCl}_2\text{-MIL-101(Cr)}$ composites with different salt content in the composite

Study of textural and structural characteristics as well as the morphology of composites using low-temperature N_2 adsorption, PXRD, SEM

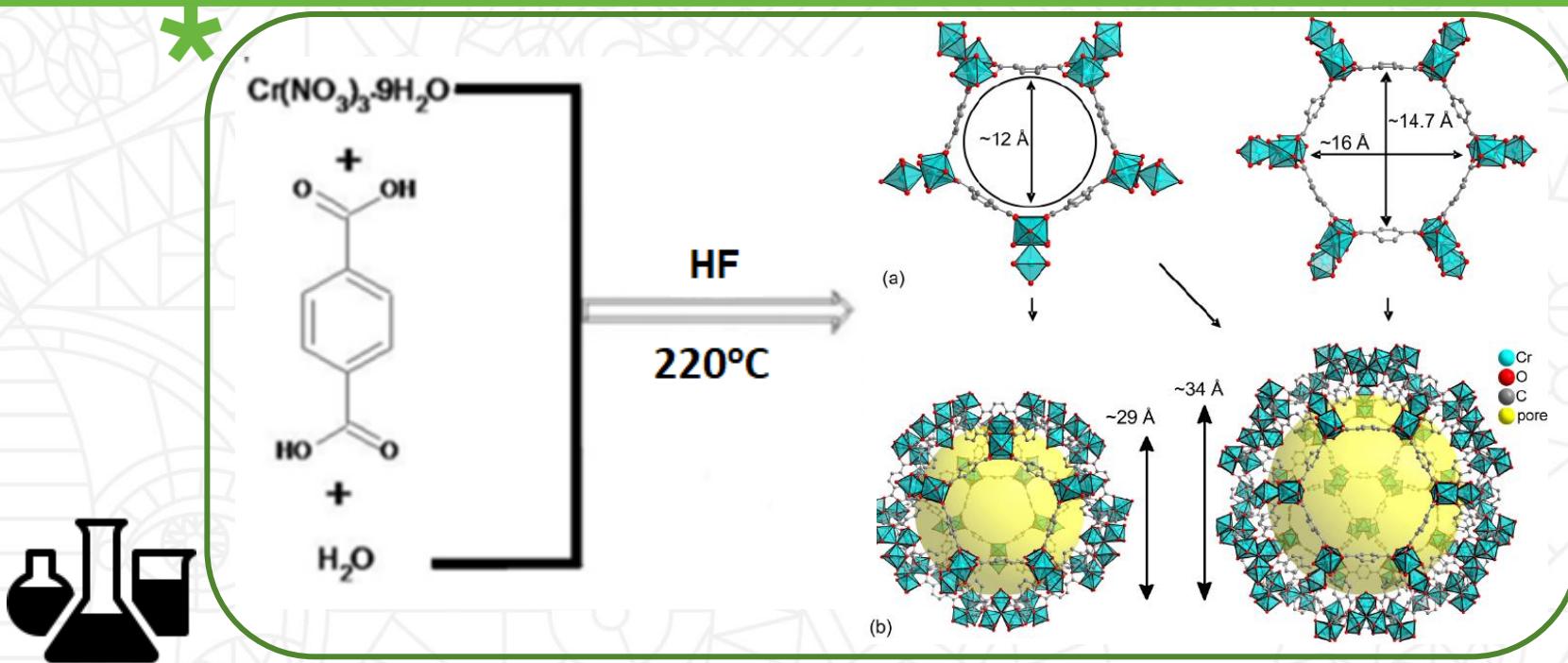
Study of water adsorption equilibrium on $\text{CaCl}_2\text{-MIL-101(Cr)}$ by thermogravimetric analysis (TG)

The efficiency estimation of the AWEA using $\text{CaCl}_2\text{-MIL-101(Cr)}$ composites as the adsorbents

* Adsorption Water Extraction from Air (AWEA)

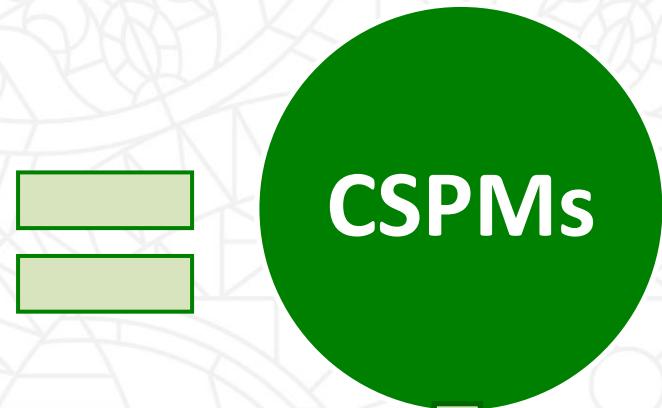
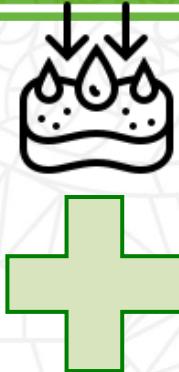
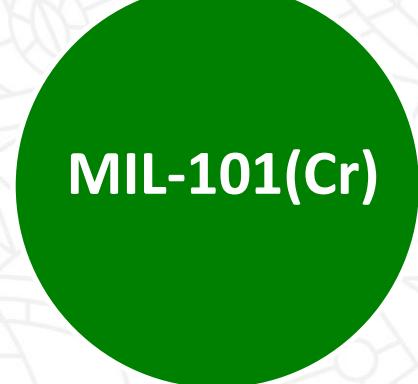


*Synthesis of MIL-101(Cr)

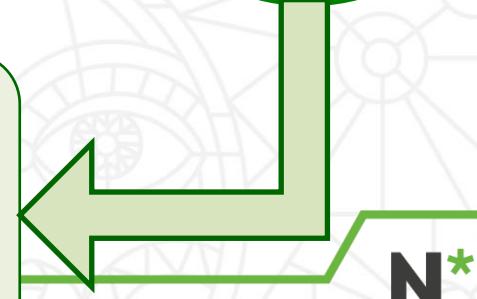


*G. Férey, C. Mellot-Draznieks, C. Serre, F. Millange, J. Dutour, S. Surblé, I. Margiolaki. *Science*. 309 (2005) 2040-2042.

*Synthesis of $\text{CaCl}_2\text{-MIL-101(Cr)}$



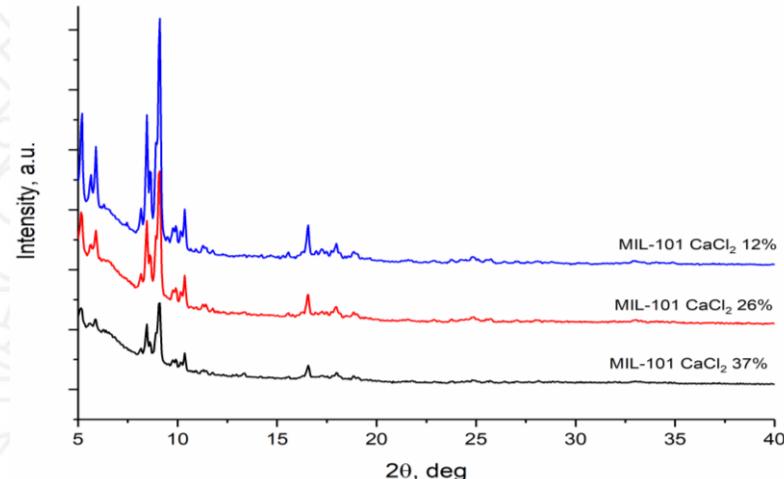
$\text{CaCl}_2(16\%)/\text{MIL-101} \leftrightarrow \text{CaCl}_2(16)$
 $\text{CaCl}_2(29\%)/\text{MIL-101} \leftrightarrow \text{CaCl}_2(29)$
 $\text{CaCl}_2(39\%)/\text{MIL-101} \leftrightarrow \text{CaCl}_2(39)$



* Structural and textural characteristics of $\text{CaCl}_2\text{-MIL-101(Cr)}$

Characteristics of porous structure $\text{CaCl}_2\text{-MIL-101(Cr)}$.

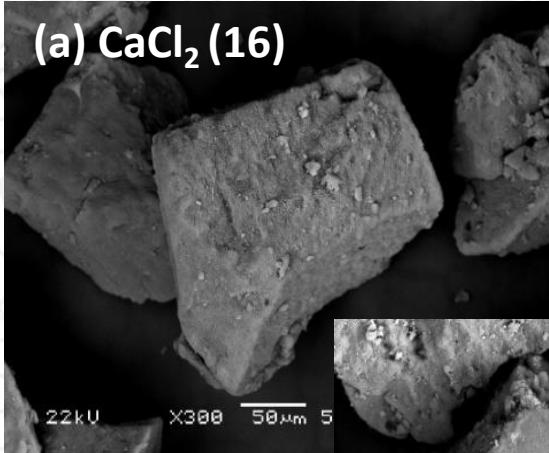
CaCl_2 content, wt%	S_{BET} , m^2/g	V_{pore} , cm^3/g
0	2040	2,00
16	1805	1,60
29	1075	1,30
39	555	1,00



PXRD patterns of the composite $\text{CaCl}_2\text{-MIL-101(Cr)}$ containing 12, 26, 37 wt% of CaCl_2

* Structural and textural characteristics of the studied CSPMs

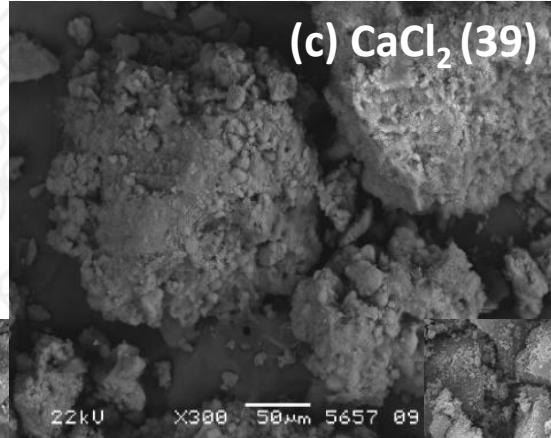
(a) CaCl_2 (16)



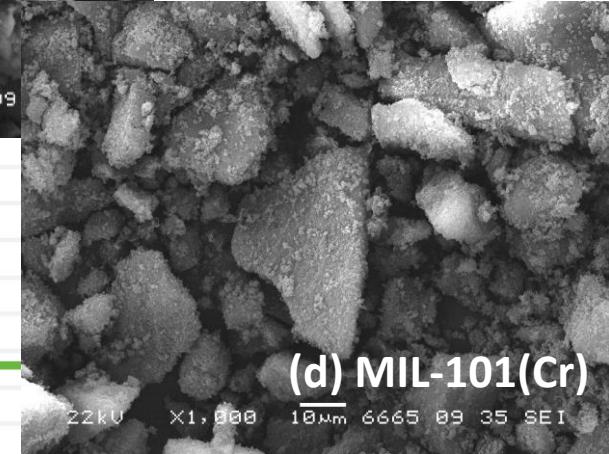
(b) CaCl_2 (29)



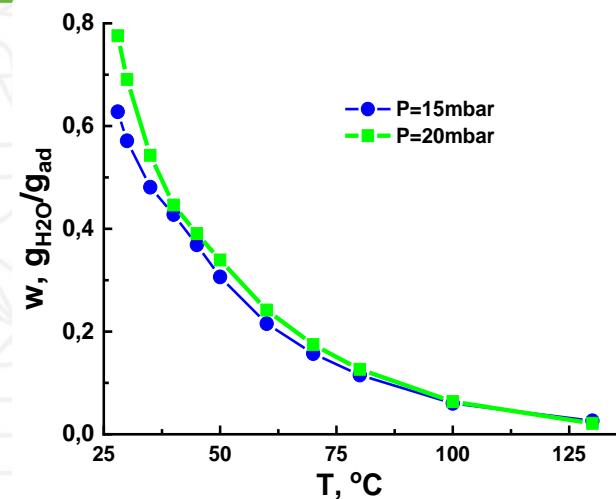
(c) CaCl_2 (39)



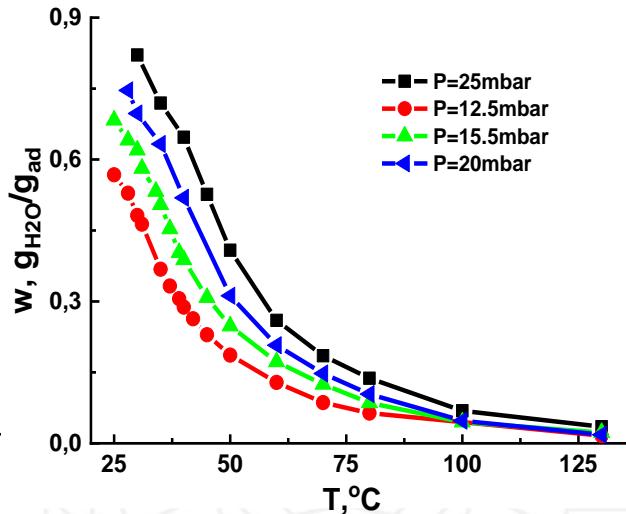
(d) MIL-101(Cr)



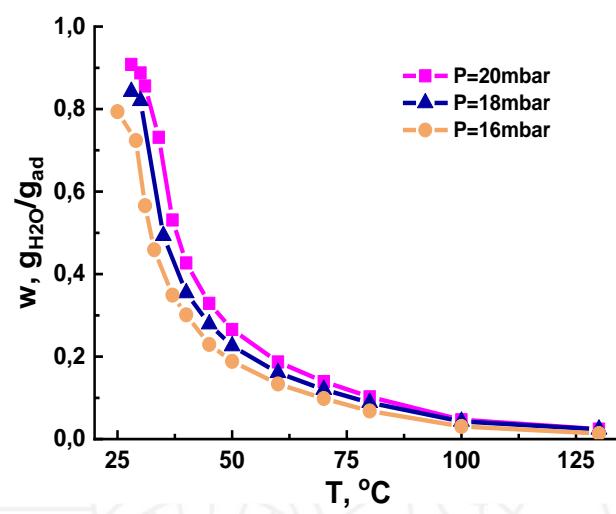
* Water adsorption equilibrium on $\text{CaCl}_2\text{-MIL-1O1(Cr)}$



Isobar of water adsorption on
 CaCl_2 (39)

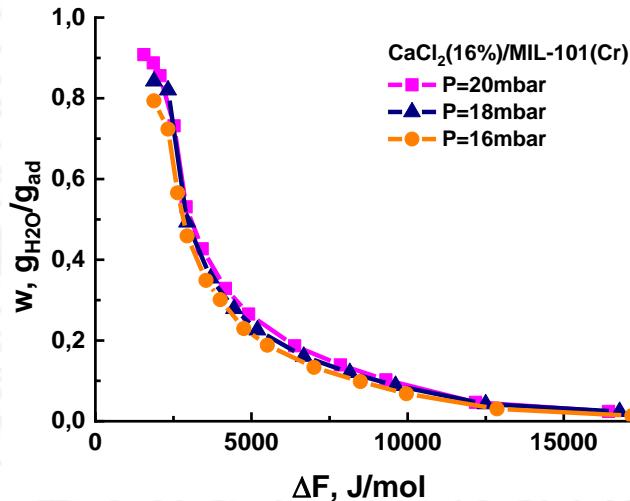
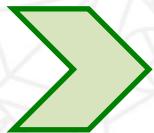
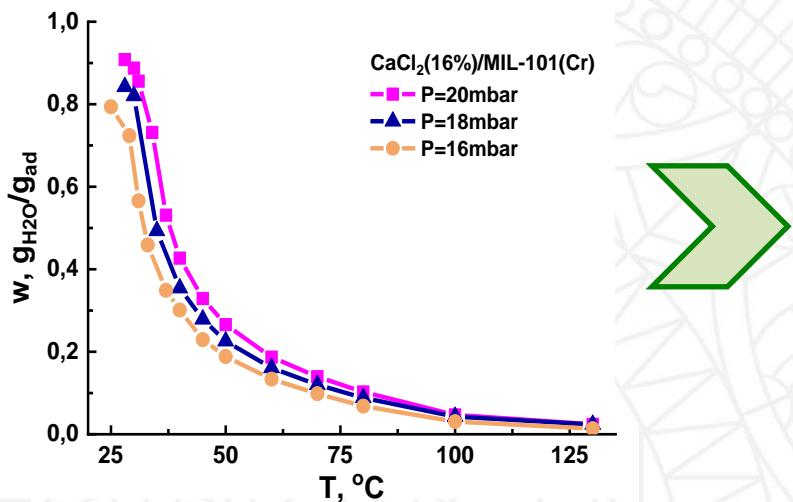


Isobar of water adsorption on
 CaCl_2 (29)



Isobar of water adsorption on
 CaCl_2 (16)

*The adsorption potential ΔF



$$\Delta w = f(\Delta F)$$

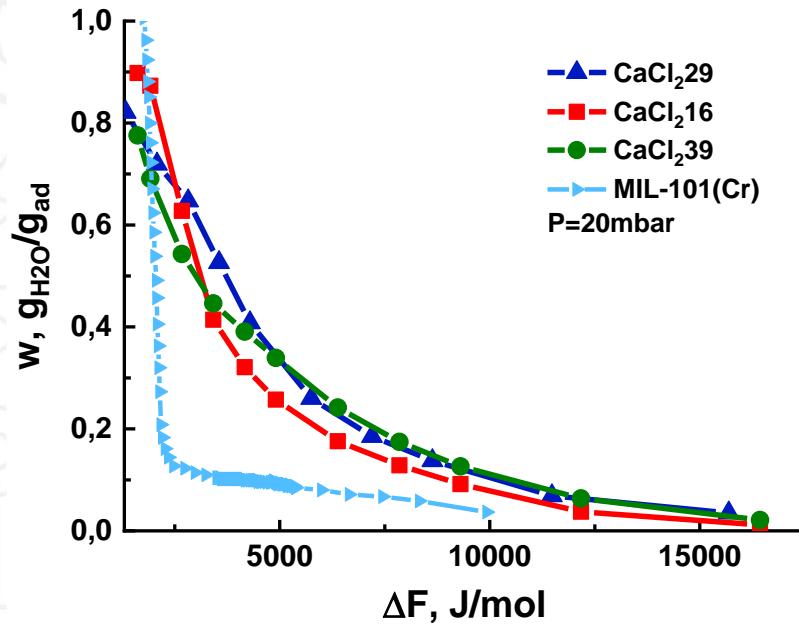
The adsorption potential $\Delta F = -RT\ln(P/P_0)$

P - the vapor pressure,

P_0 - the saturation vapor pressure at temperature T

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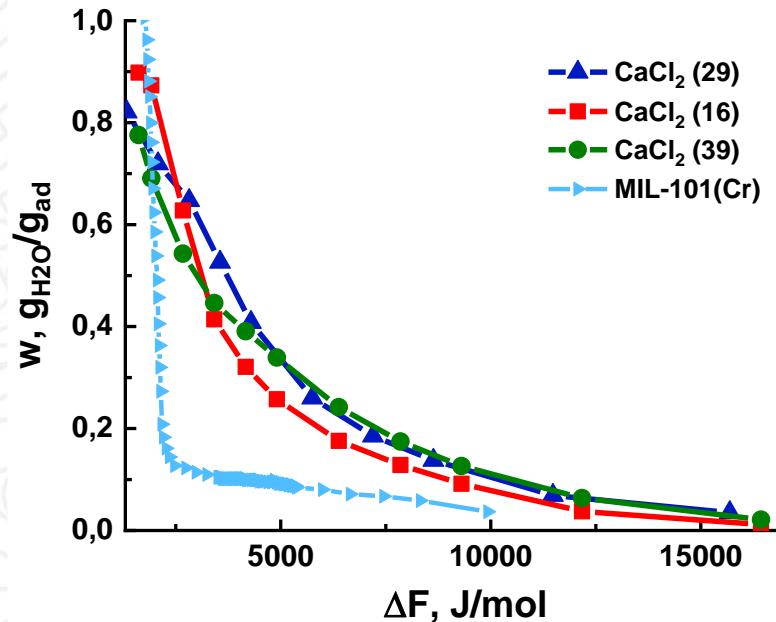
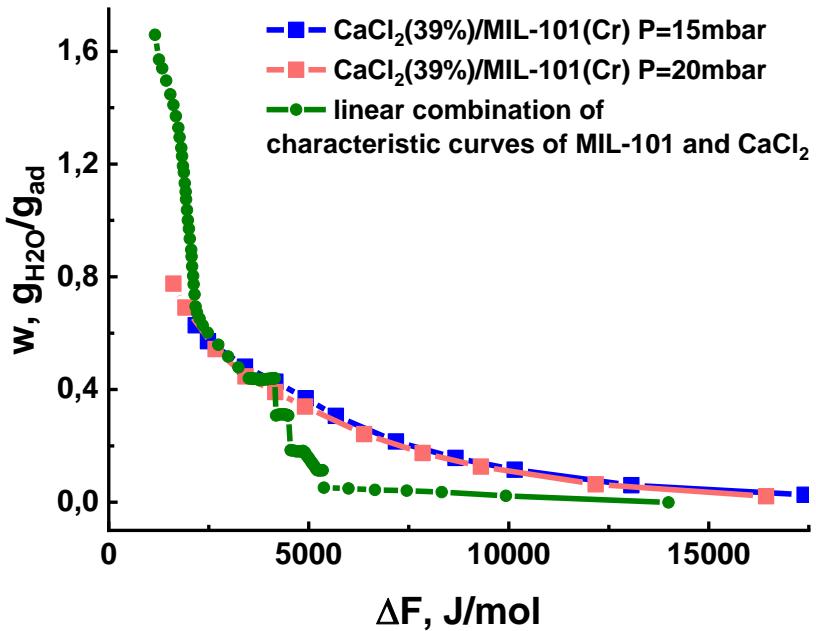
*The adsorption potential ΔF



Characteristic curves for
CaCl₂-MIL-101(Cr) and MIL-101(Cr)

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* Water adsorption equilibrium on CaCl₂-MIL-101(Cr)



* Climatic data of Saudi Arabia (SA) and Sahara Desert (SD)



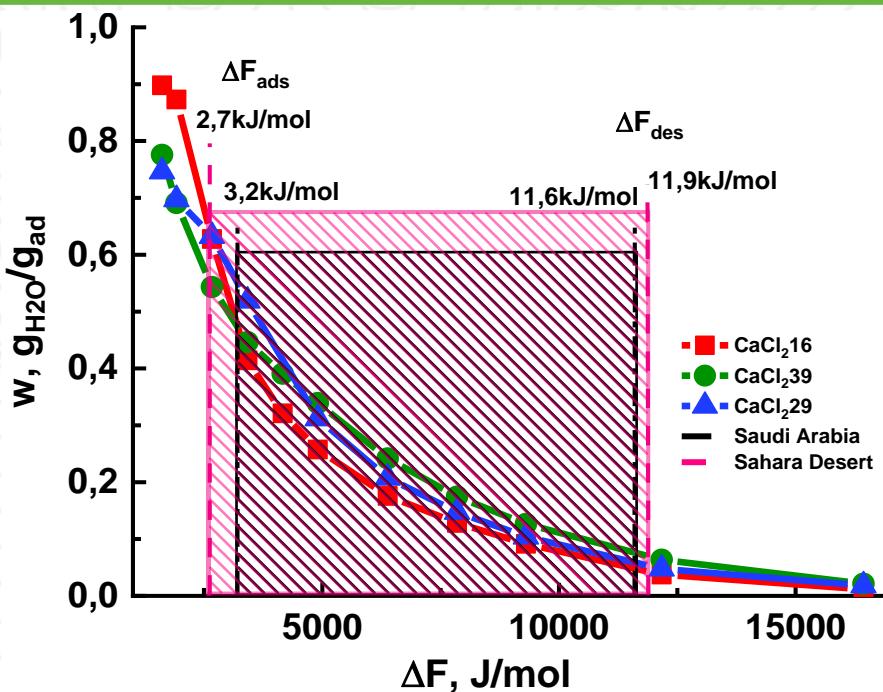
Climatic data of Saudi Arabia (SA) and Sahara Desert (SD)

Region	$T_n, ^\circ\text{C}$	$\text{RH}_n, \%$	$T_d, ^\circ\text{C}$	$\text{RH}_d, \%$	P_{am}
January (wet season)					
SA	12,5	55,9	16,3	45,1	8,3
SD	11,1	33,0	14,9	27,2	4,5
July (dry season)					
SA	32,6	20,2	36,7	16,5	10,1
SD	26,9	25,8	30,4	21,2	9,3



Database "Meteonorm"

* Water adsorption equilibrium on $\text{CaCl}_2\text{-MIL-1O1(Cr)}$



Characteristic curves for composites $\text{CaCl}_2\text{-16}$, $\text{CaCl}_2\text{-29}$ and $\text{CaCl}_2\text{-39}$ ($P = 20\text{mbar}$).
The values ΔF_{ads} and ΔF_{des} for the operating conditions adsorption and regeneration stages in the SA and SD regions.

* Efficiency of AWEA

Amount of adsorbed/desorbed water

$$\Delta W = W_{\text{ads}} - W_{\text{des}}$$

Specific Water Production

$$SWP = \Delta W \cdot \delta_{\text{col}}$$

Efficiency of AWEA

Fraction of water extracted

$$\delta_{\text{ex}} = 1 - \frac{P_{\text{out.ad}}}{P_{\text{am}}}$$

Fraction of water collected

$$\delta_{\text{col}} = 1 - \frac{P_0(T_d)}{P_{\text{out.re}}}$$

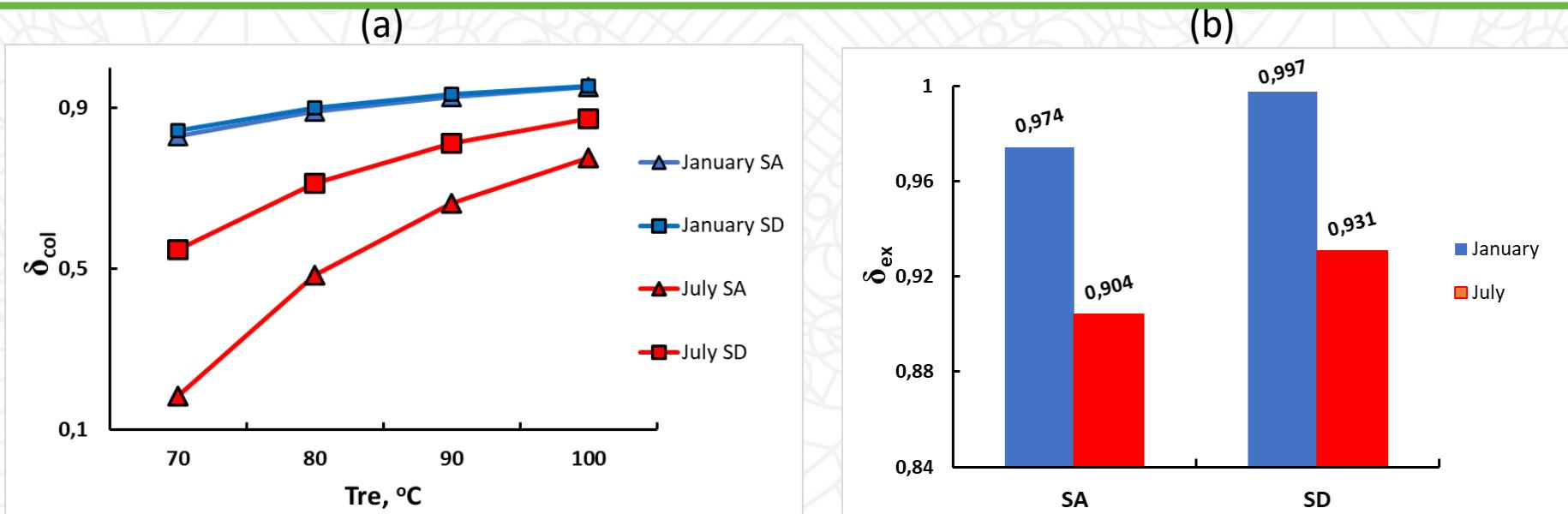
$P_{\text{out.ad}}$ – vapor pressure at the adsorption stage

P_{am} – partial water vapor pressure of ambient air

$P_{\text{out.re}}$ – vapor pressure at the desorption stage

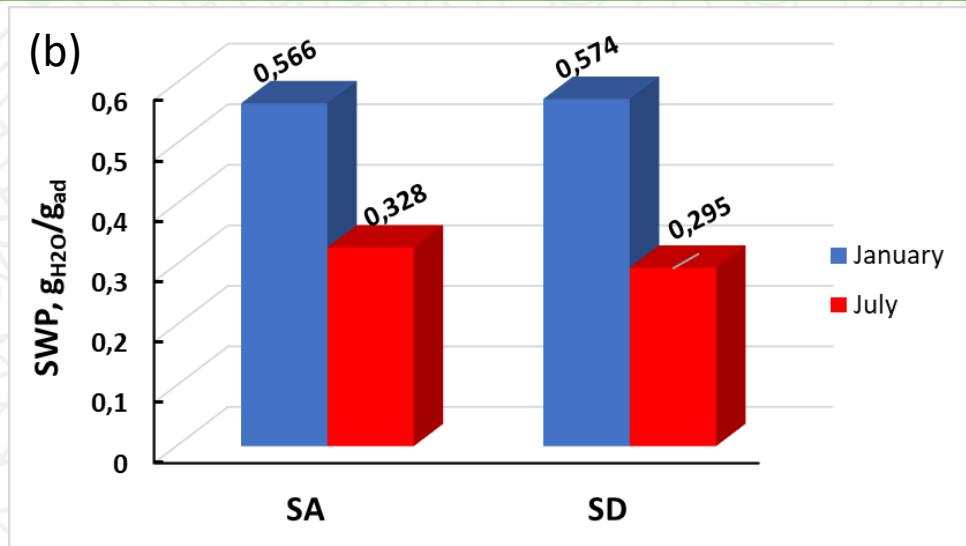
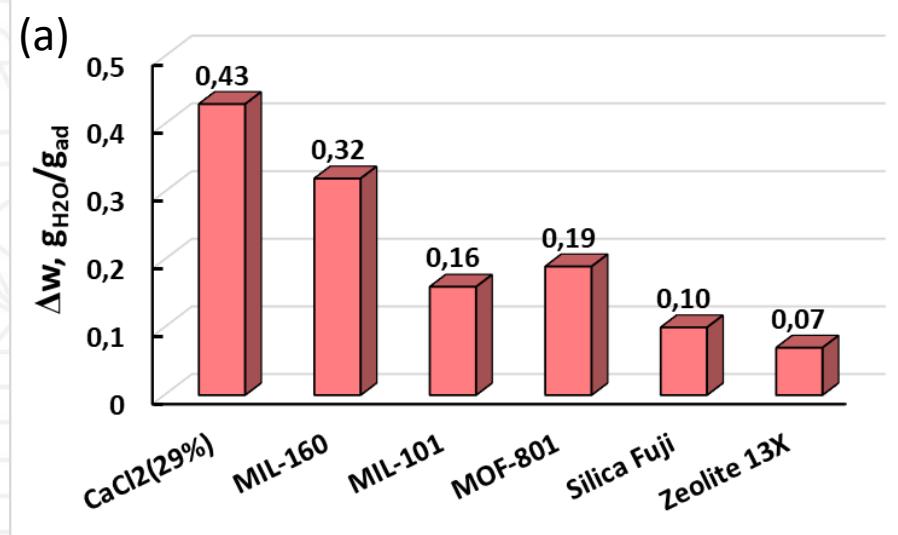
$P_0(T_d)$ – the saturation vapor pressure at temperature T_d

* Efficiency estimation of the AWEA employing CaCl_2 (29) as adsorbent



δ_{col} (a) and δ_{ex} (b) values for CaCl_2 (29)
under climatic conditions of SA and SD regions

* Efficiency estimation of the AWEA employing CaCl_2 (29) as adsorbent



(a): Δw values for different adsorbents under climatic conditions of SA (dry season) region; (b): SWP values of AWEA



*Conclusions

CSPMs $\text{CaCl}_2\text{-MIL-101(Cr)}$ with different salt content (16, 29, 39 wt%) were synthesized

Textural and structural characteristics as well as particle morphology were studied

The synergistic effect of salt and porous matrix in the process of water adsorption was revealed

*Conclusions

Saudi Arabia:

$$\delta_{\text{col}} = 0,83-0,95; \delta_{\text{ex}} = 0,97 - \text{January}$$

$$\delta_{\text{col}} = 0,18-0,77; \delta_{\text{ex}} = 0,90 - \text{July}$$

Sahara Desert:

$$\delta_{\text{col}} = 0,84-0,96; \delta_{\text{ex}} = 0,99 - \text{January}$$

$$\delta_{\text{col}} = 0,55-0,87; \delta_{\text{ex}} = 0,93 - \text{July}$$

Potential of the composite CaCl_2 (29) as an adsorbent in the AWEA process was estimated

**THANK YOU
FOR YOUR ATTENTION!**

