This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101017858

Exploring flexible nanoporous materials for energy-related applications

Yaroslav Grosu

Seminar at Sapienza Univeristy of Rome
16th June 2021

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MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

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> Expertise, experience and scientific interests

- **Positions:**
  - Group leader at CIC energiGUNE research center, Spain
  - Research professor at University of Silesia, Poland

- **Interests:**
  - Interfacial phenomena, wettability, capillarity, corrosion, porous media
  - Energy storage, conversion, dissipation

- **Expertise:**
  - Materials degradation
  - Wettability of complex topologies
  - Interfacial energy

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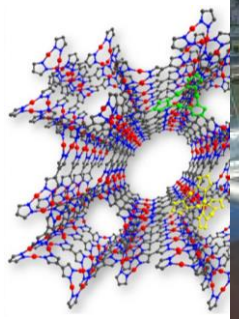

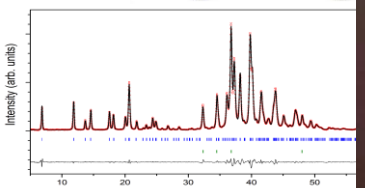

H2020 ORC-PLUS Project

200 kWh_t packed bed thermocline

~ 6.5 tons of storage material

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> Interfacial Phenomena, Colloids and Porous Media Group

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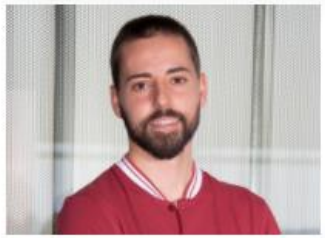
LUIS GONZALEZ FERNANDEZ
POSTDOCTORAL RESEARCHER

LUIS ANGEL BARTOLOME MARQUES
POSTDOCTORAL RESEARCHER

EDER AMAYUELAS LOPEZ
POSTDOCTORAL RESEARCHER



MIKEL INTXAURTIETA CARCEDO
LAB TECHNICIAN

MALENA NUÑEZ MARTINEZ
INTERNSHIP STUDENT

Application driven, but deep

Cross-disciplinary approach

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> Major activities of the group

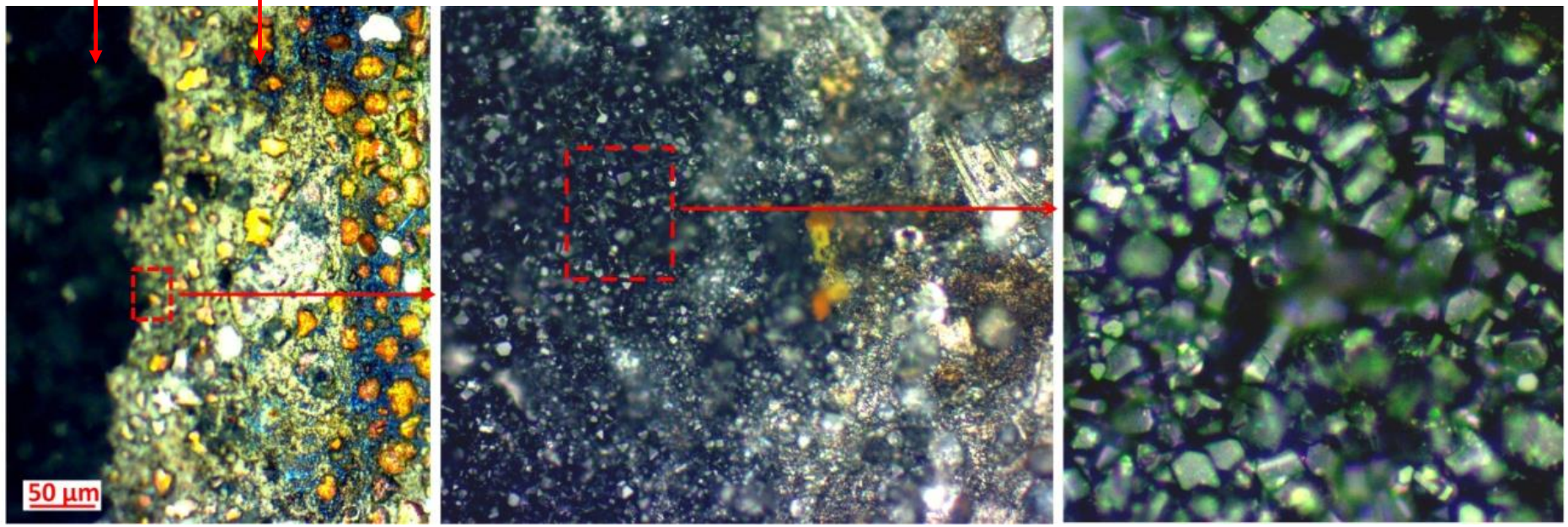
CORROSION

Degradation and protection at 300 – 800ºC for

- Molten salts
- Oils
- Gases

+

- Metallic alloys
- Plastic crystals
- Ceramics



https://www.nature.com/articles/s41529-018-0055-0

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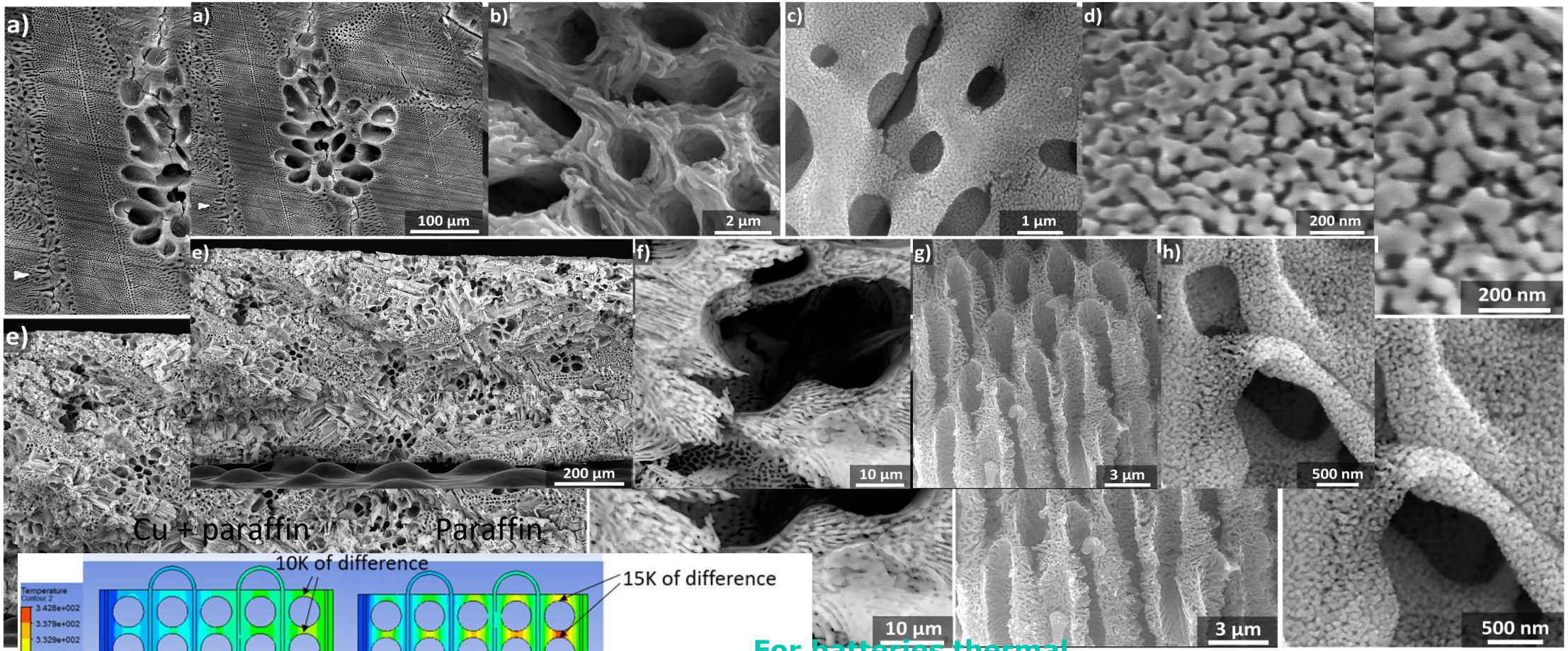
> Major activities of the group

HIERARCHICAL POROUS MATERIALS FOR THERMAL ENERGY STORAGE

Trimodal hierarchical macro-nanoporous copper + paraffin composite



For batteries thermal management

Applied Surf Sci 2019
Applied Surf Sci 2020
Applied Energy 2020

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Flexible nanoporous materials for energy applications

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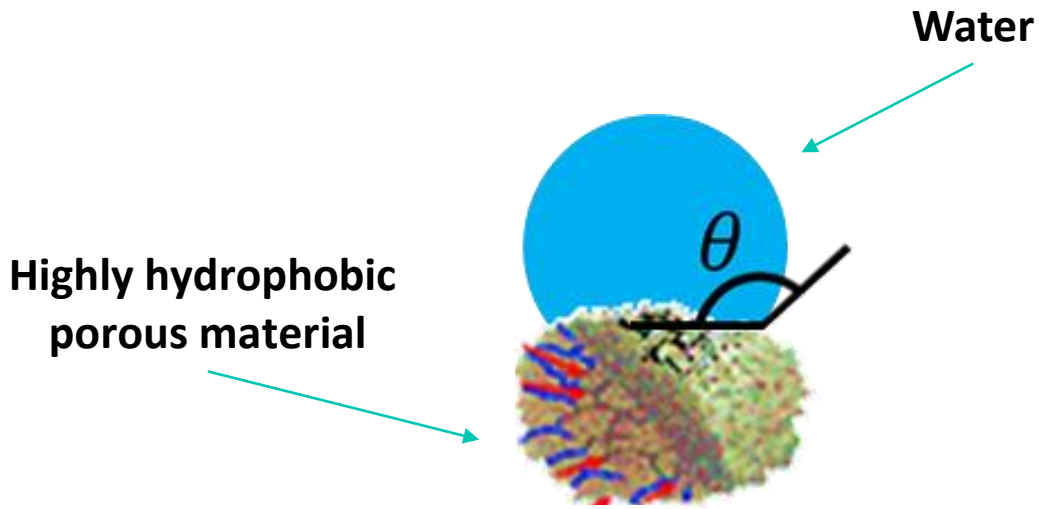
> Intrusion-extrusion for energy applications

ENERGY BALANCE



$$\textbf{Non} - \textbf{wetting: } \boldsymbol{\theta} > 90°$$

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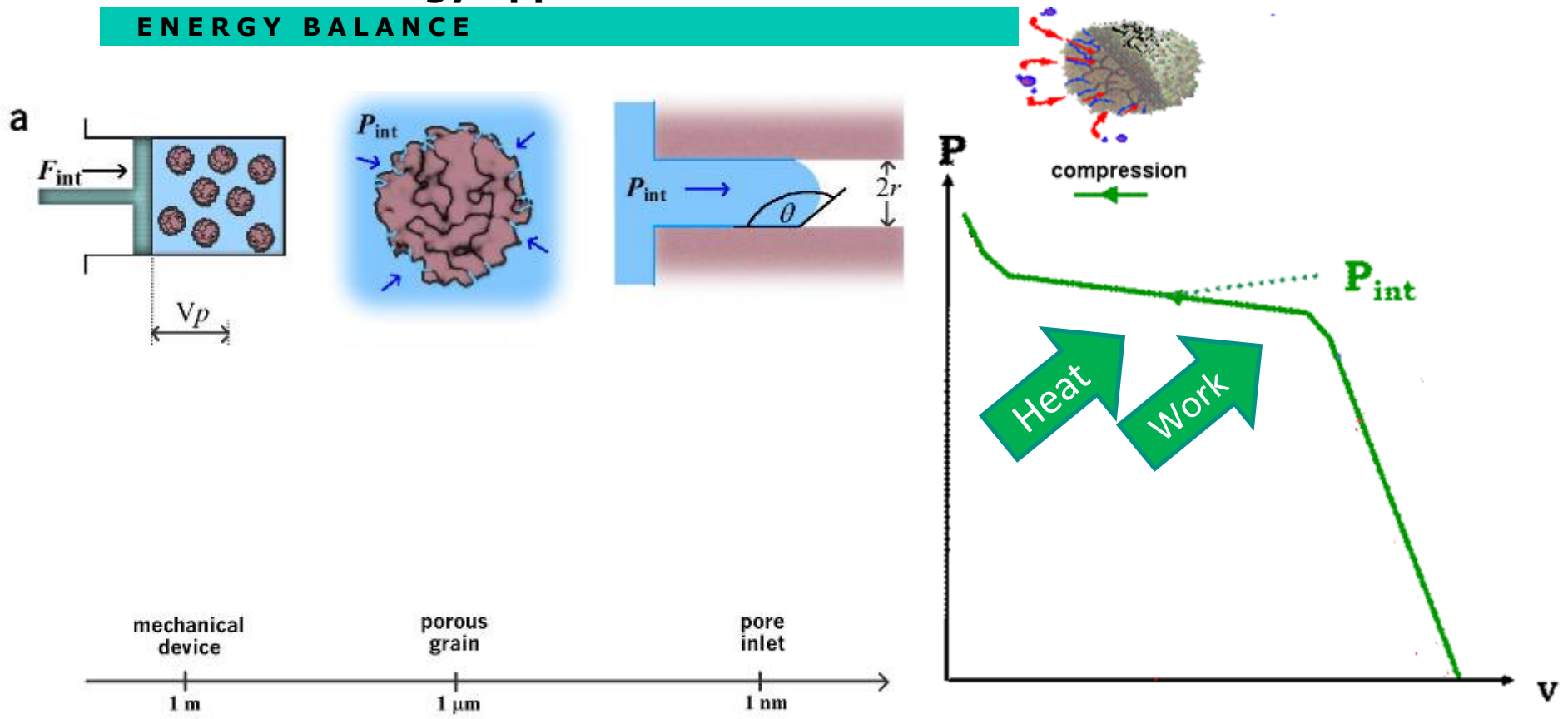
> Intrusion-extrusion for energy applications

ENERGY BALANCE



$$W_{intrusion} = P_{intrusion} \cdot \Delta V = P_{intrusion} \cdot V_{pores}$$

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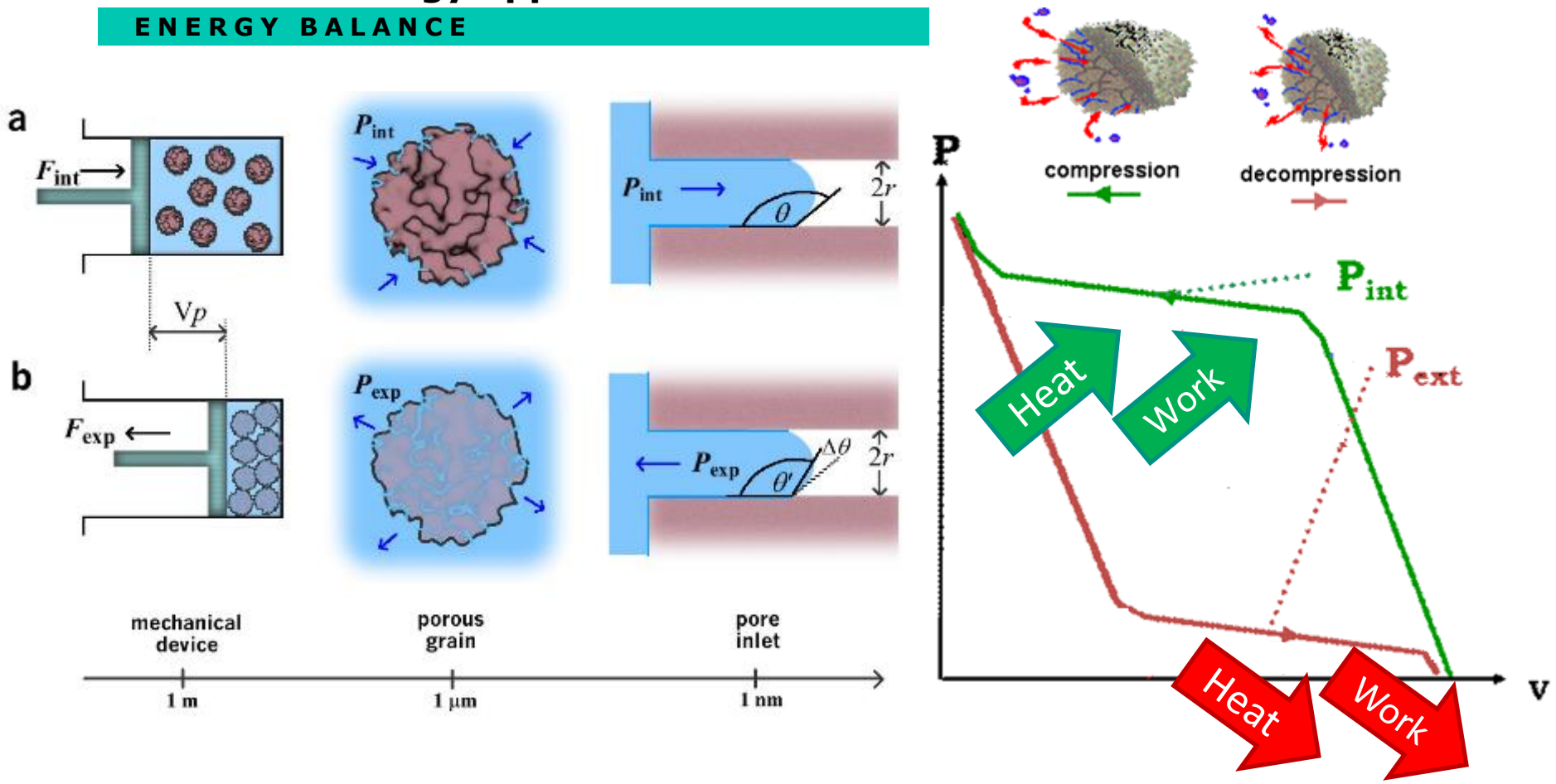
> Intrusion-extrusion for energy applications

ENERGY BALANCE



$$W_{intrusion} = P_{intrusion} \cdot \Delta V = P_{intrusion} \cdot V_{pores}$$

$$W_{extrusion} = P_{extrusion} \cdot \Delta V = P_{extrusion} \cdot V_{pores}$$

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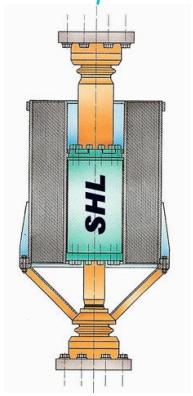
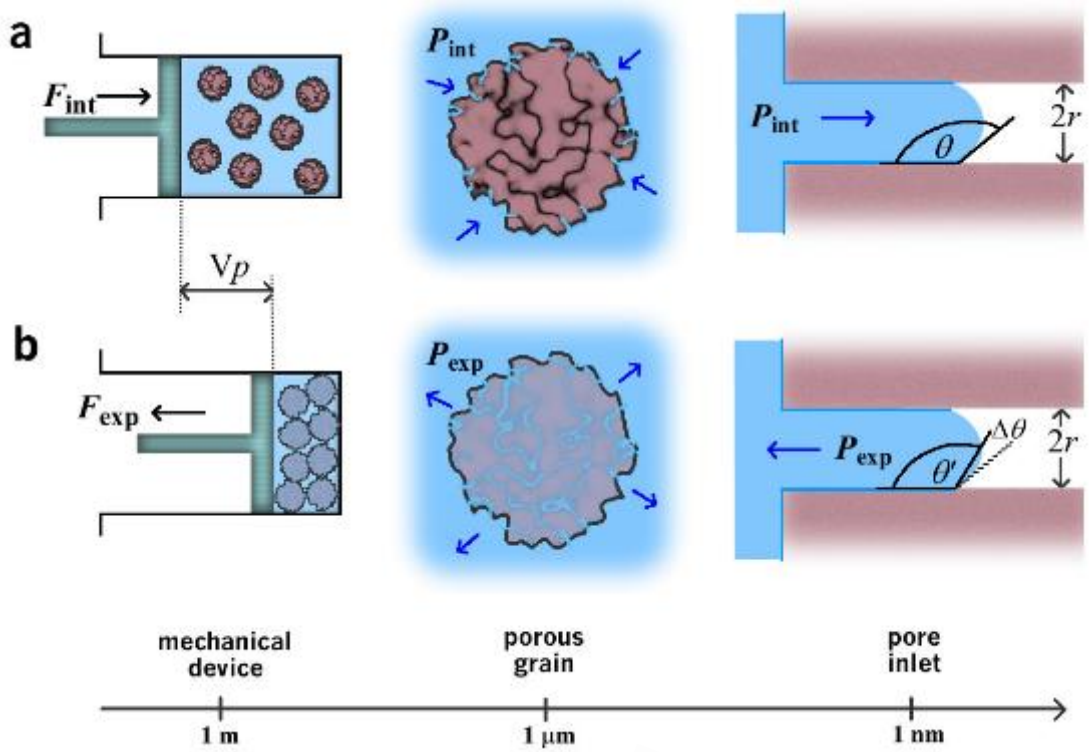
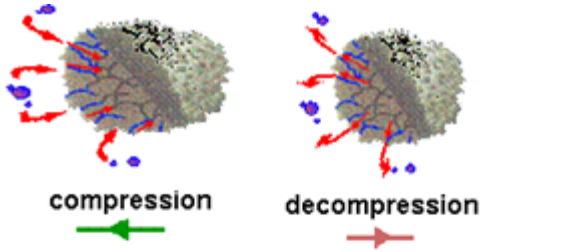
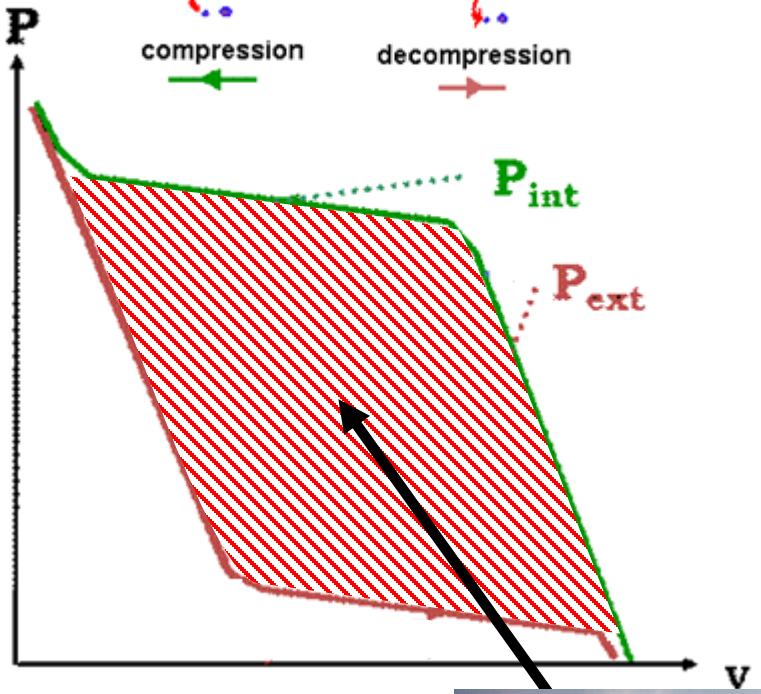
> Intrusion-extrusion for energy applications

ENERGY BALANCE









Eroshenko VA, Piatiletov I, Coiffard L, Stoudenets V. Proc. Inst. Mech. Eng. D. 2007.

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Smart pressure transmitting fluids

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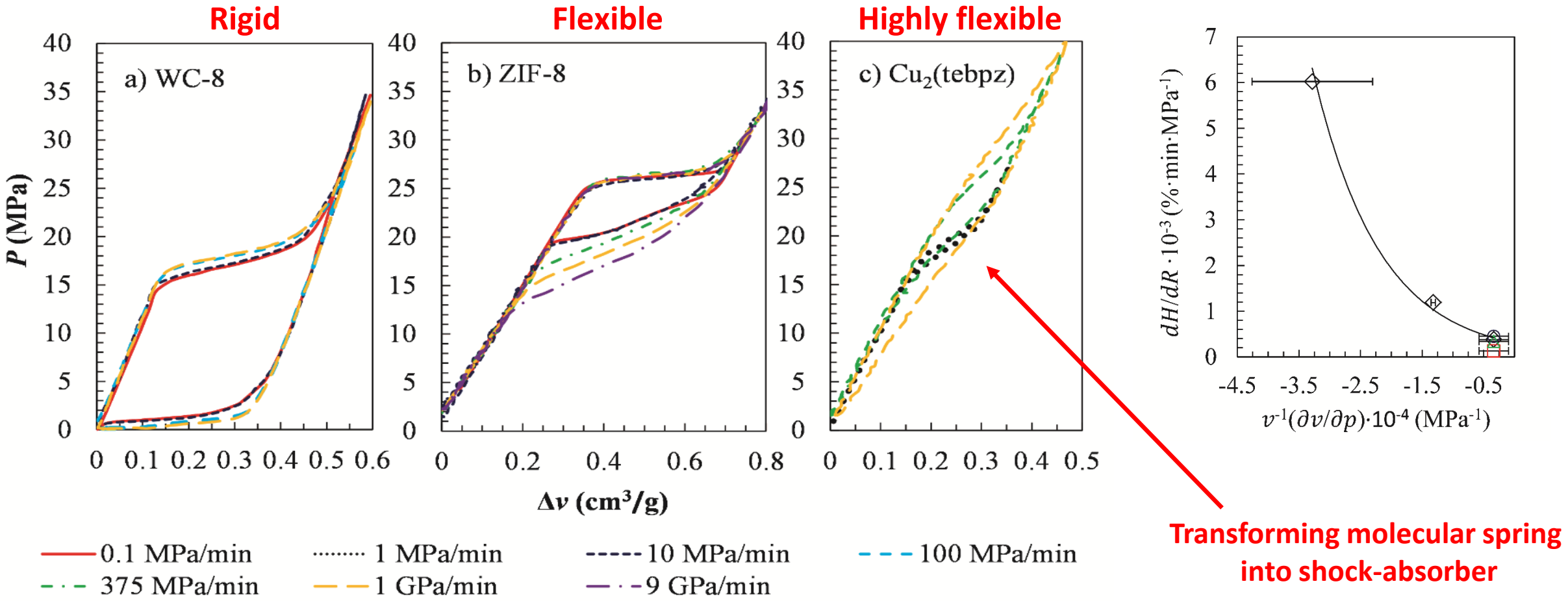
> Flexibility of porous material on the hysteresis of int-ext process

SMART PRESSURE TRANSMITTING FLUIDS



ACS Appl. Mater. & Interf. 2019

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Negative compressibility

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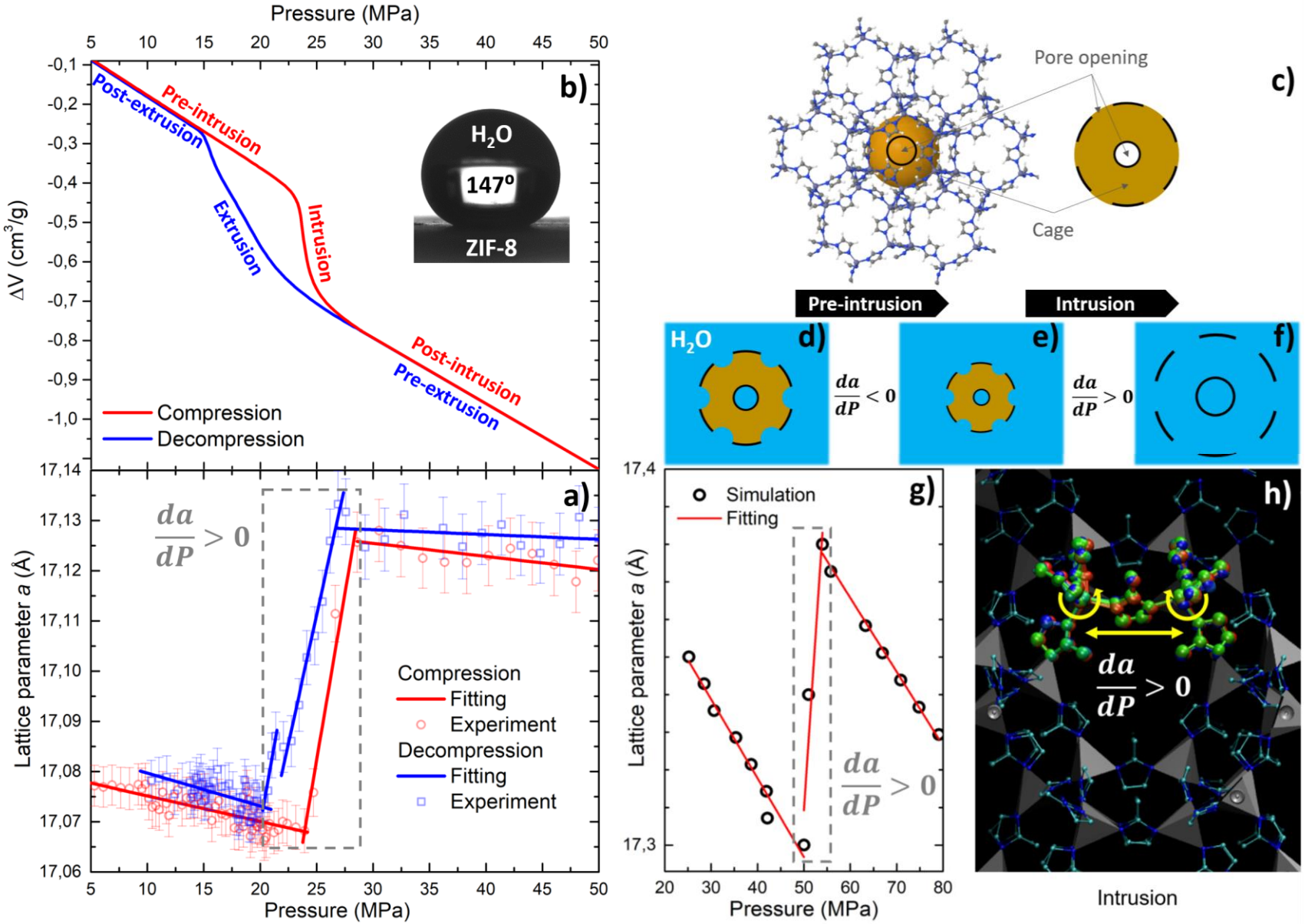
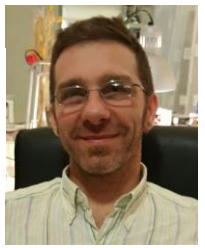
Negative compressibility

ZIF-8 + WATER



Simone Meloni
University
of Ferrara



Marco Tortora
Sapienza
University
of Rome

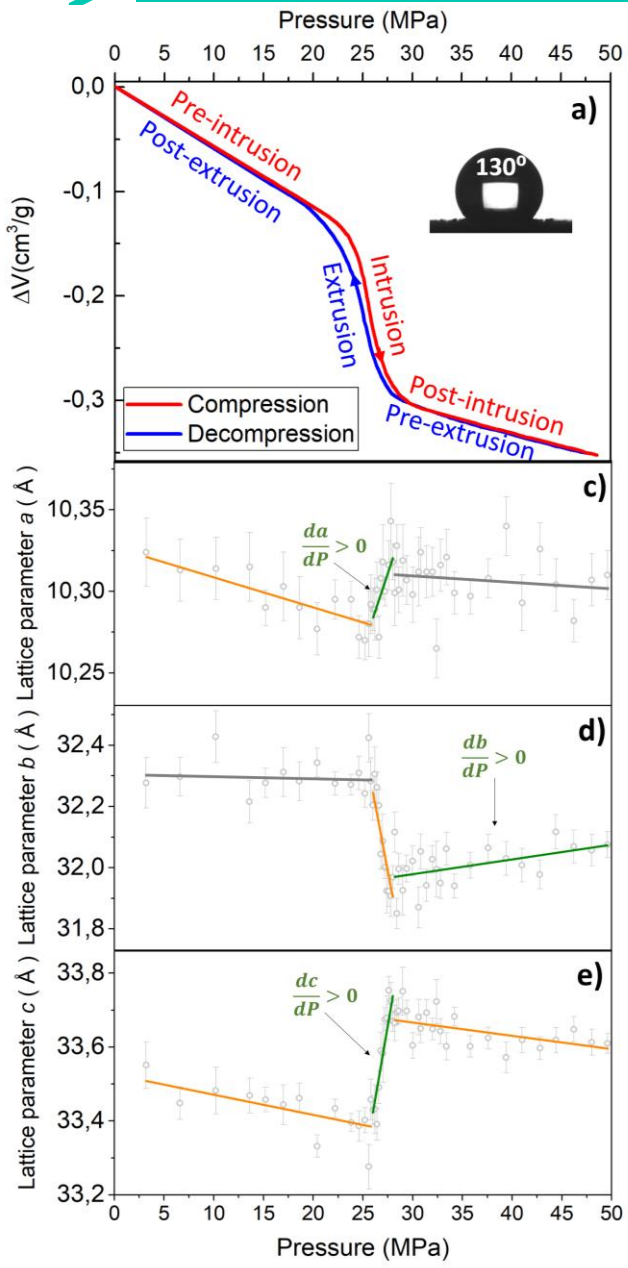
Alberto Giacomello
Sapienza
University
of Rome

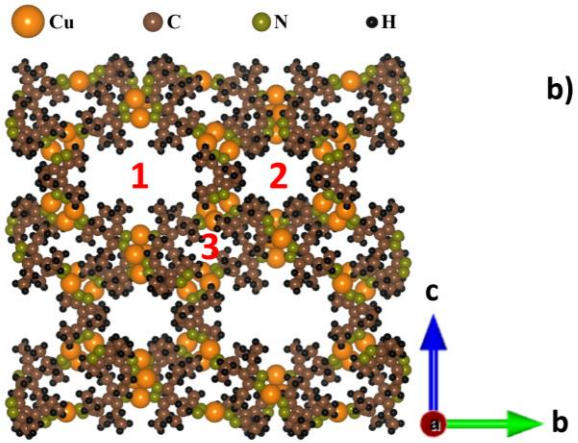
Carlo Massimo Casciola
Sapienza University
of Rome

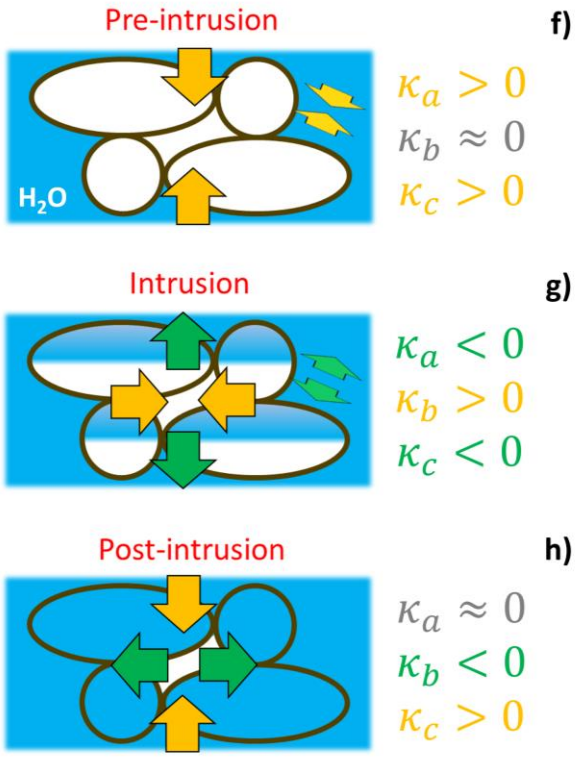
Nano letters 2021

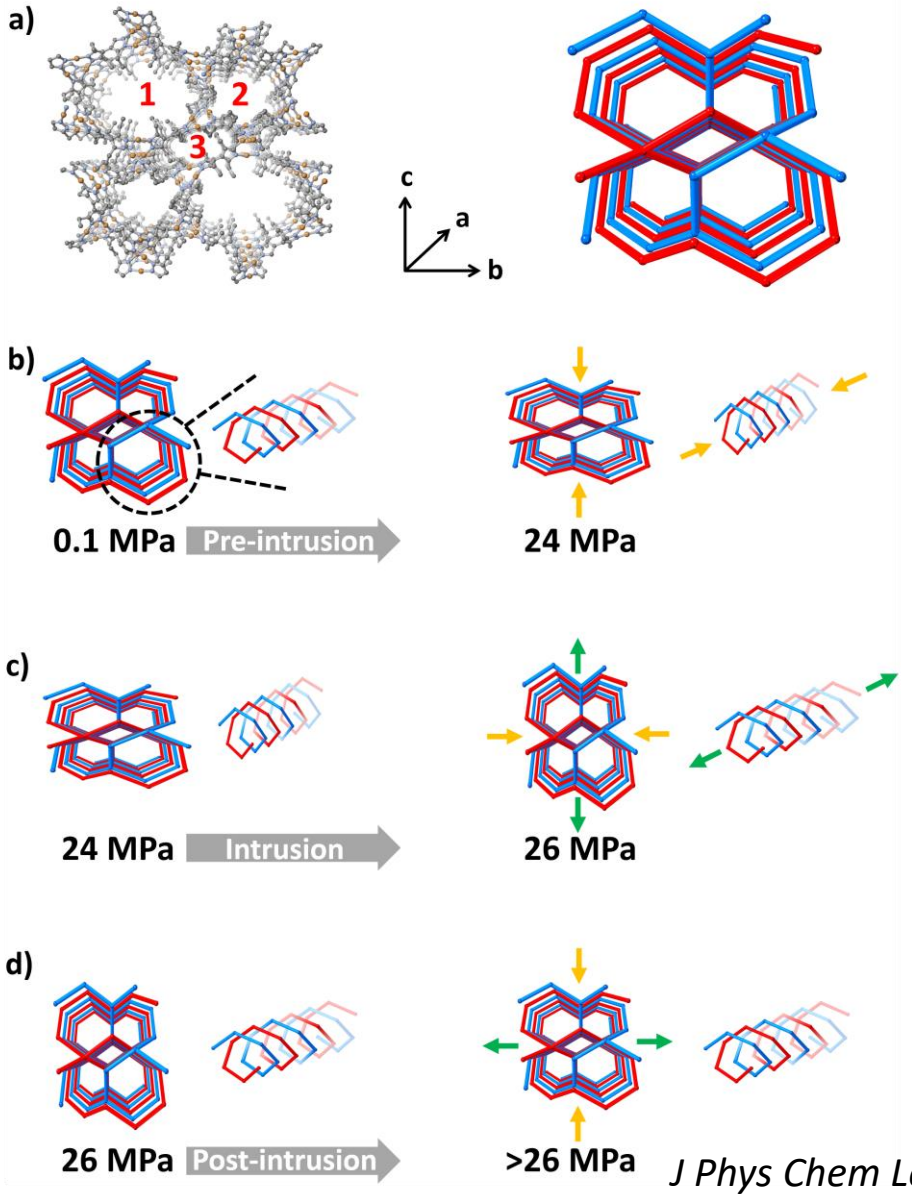
Negative compressibility

CU2(TEBPZ) + WATER









J Phys Chem Lett 2021

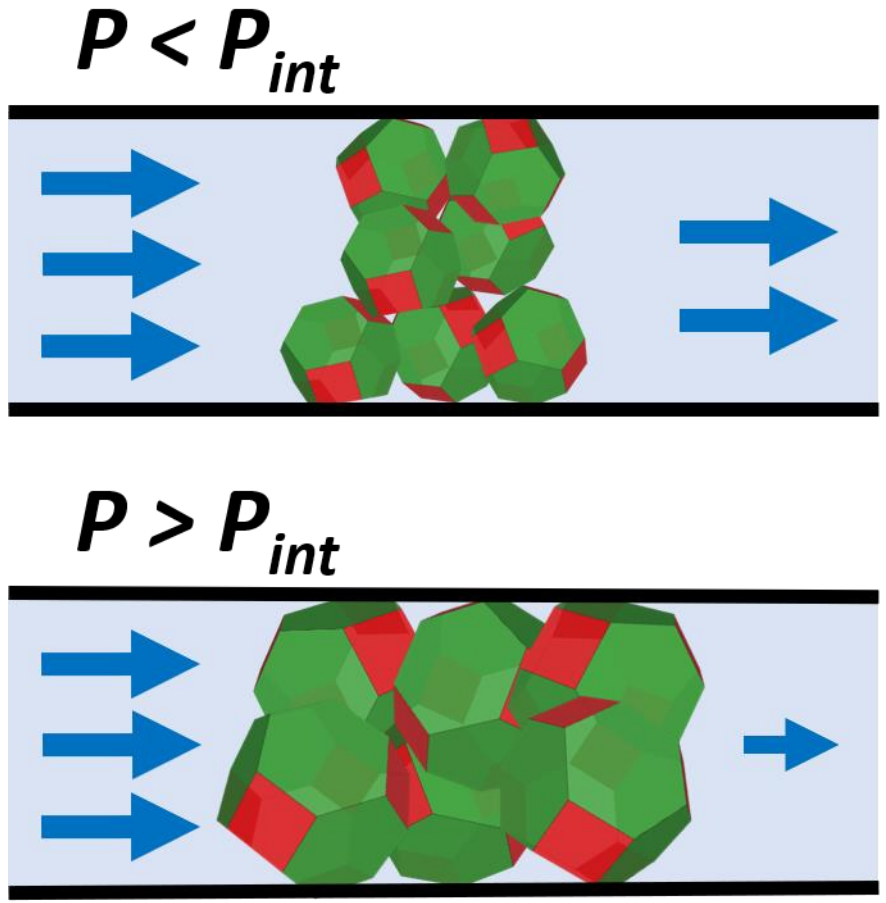
> Negative compressibility

ZIF-8 + WATER

Table 1. Experimental Linear Compressibility Coefficients for Materials with a Pronounced NLC Effect

Material	κ_l, TPa^{-1}	ref
BiB_3O_6 (0–5 GPa)	−6.7(3)	1
BiB_3O_6 ($P \rightarrow 0$)	−12.5	1
MIL-53 MOF	−28	20
$[Ag(en)]NO_3$	−28.4(18)	25
$Zn[Au(CN)_2]_2$	−42(5)	26
MCF-34 MOF	−47.3	22
$InH(BDC)_2$	−62.4	27
$[Zn(L)_2(OH)_2]_n$	−72[a]	23
$Ag_3[Co(CN)_6]$	−76.9	28
ZIF-8 MOF	−37.2[b]	19
ZIF-8 MOF (intrusion)	−1020(130)[b]	this work
ZIF-8 MOF (extrusion 1)	−770(120)[b]	this work
ZIF-8 MOF (extrusion 2)	−610(40)[b]	this work

[a]Negative area compressibility was reported. [b]Negative volumetric compressibility was reported



Negative compressibiloty of more than 1 order of magnitude higher compared to the state – of – the – art

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Thermal actuation

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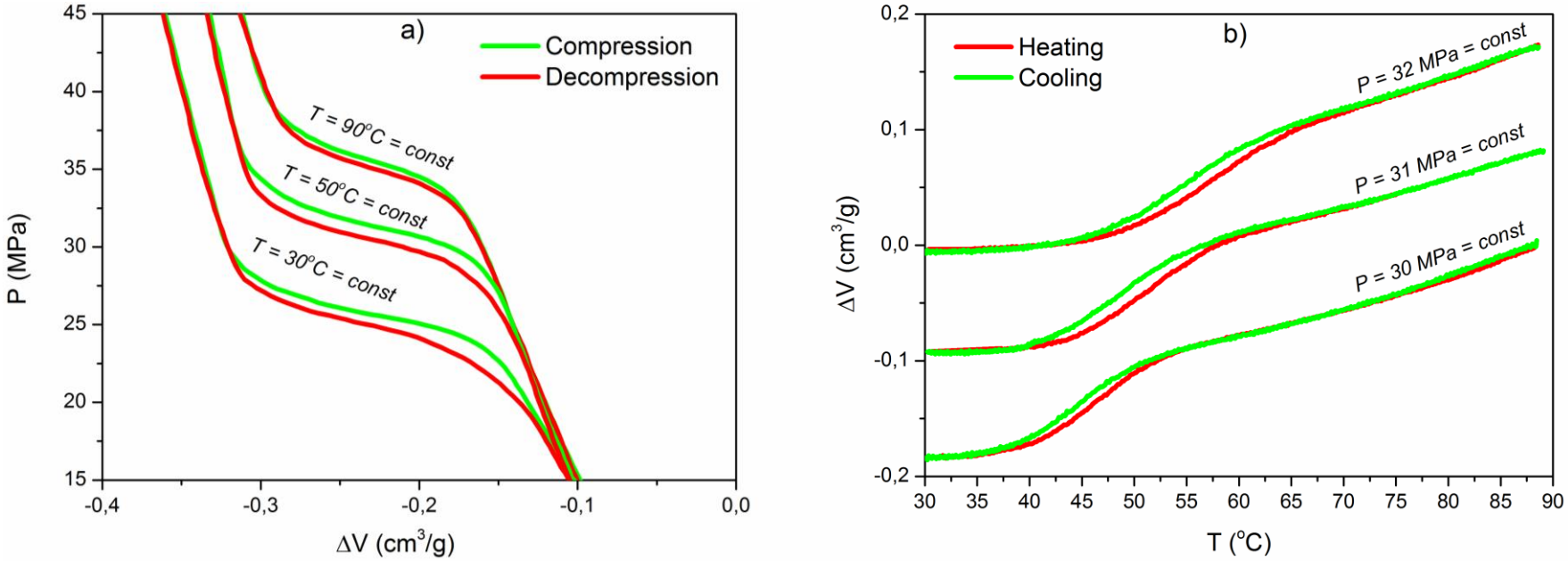
Thermal actuation

CU2(TEBPZ) + WATER



ACS Nano 2021

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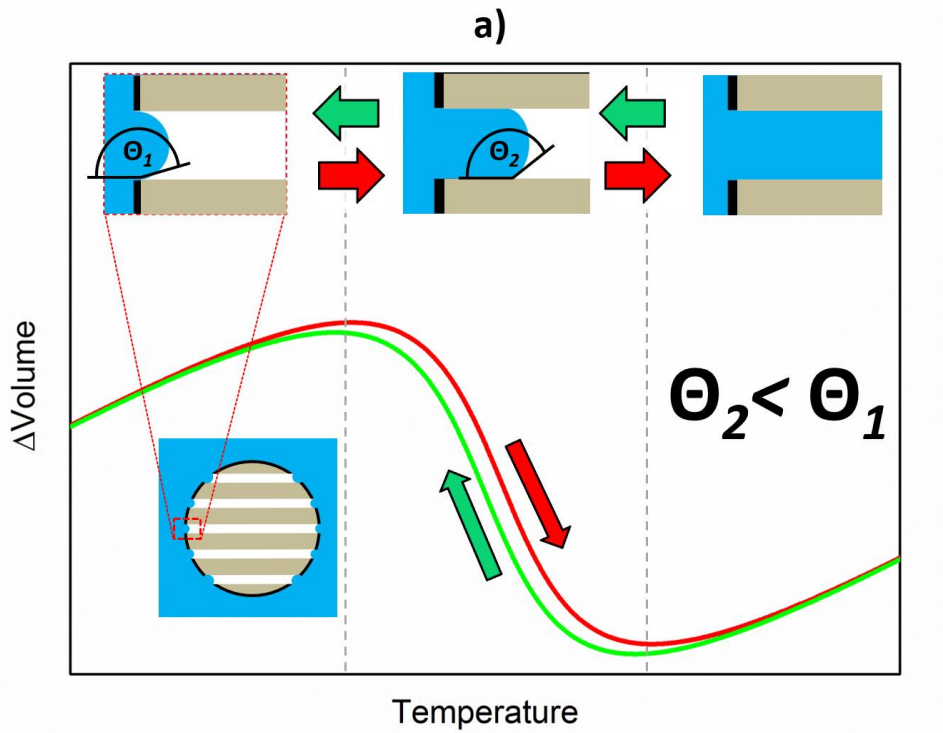
> Thermal actuation

CU2(TEBPZ) + WATER



$$E_{heating} = \frac{W_{ext} - W_{exp}}{C_P \cdot \Delta T + Q_{ext}} \cdot 100\%$$

$$E_{cooling} = \frac{W_{int} - W_{con}}{C_P \cdot \Delta T + Q_{int}} \cdot 100\%$$

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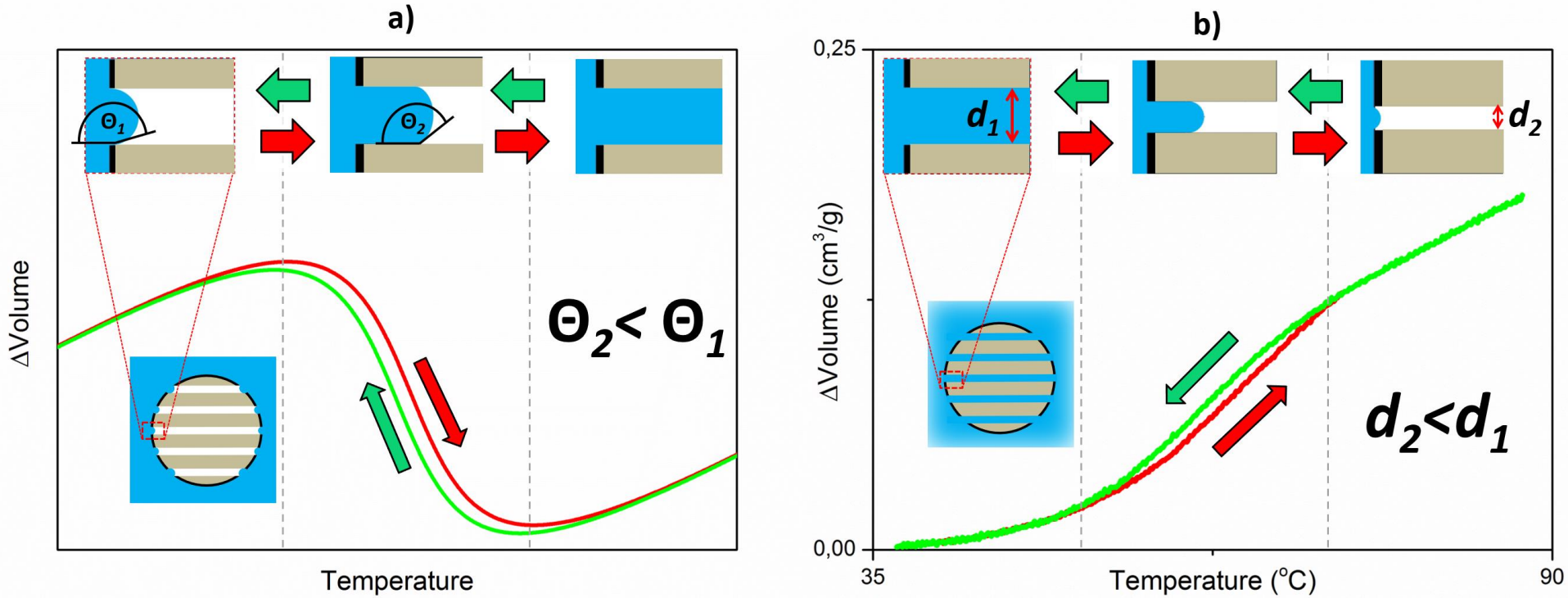
> Thermal actuation

CU2(TEBPZ) + WATER



$$E_{heating} = \frac{W_{ext} - W_{exp}}{C_P \cdot \Delta T + Q_{ext}} \cdot 100\%$$

$$E_{heating} = \frac{W_{ext} + W_{exp}}{C_P \cdot \Delta T - Q_{ext}} \cdot 100\%$$

$$E_{cooling} = \frac{W_{int} - W_{con}}{C_P \cdot \Delta T + Q_{int}} \cdot 100\%$$

$$E_{cooling} = \frac{W_{int} + W_{con}}{C_P \cdot \Delta T - Q_{int}} \cdot 100\%$$

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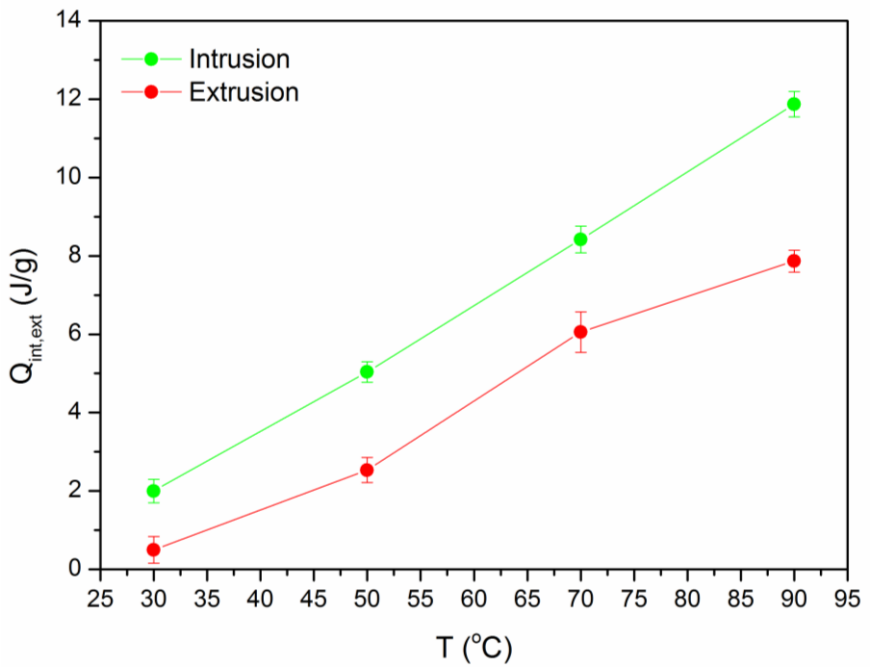
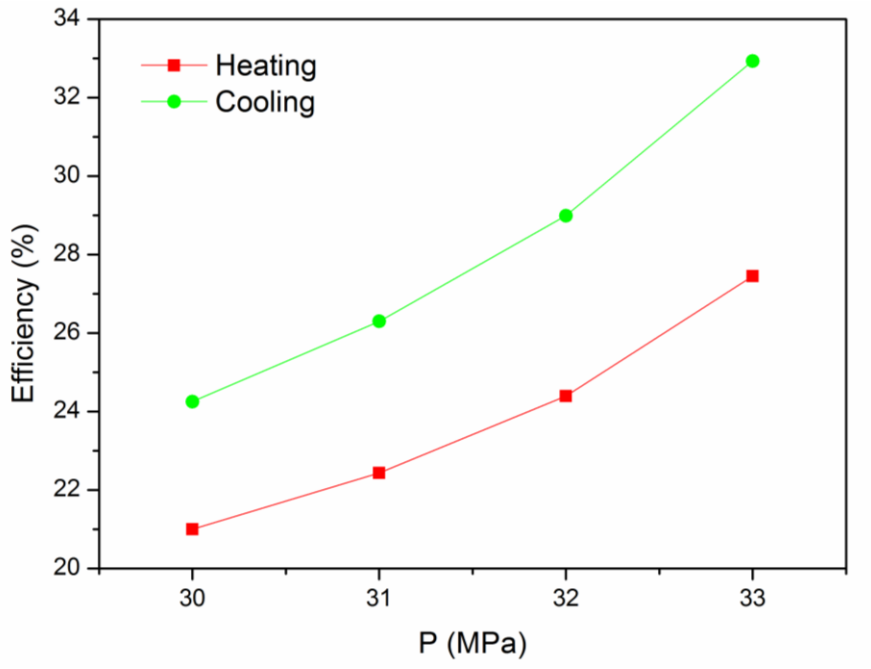
Thermal actuation

CU2(TEBPZ) + WATER





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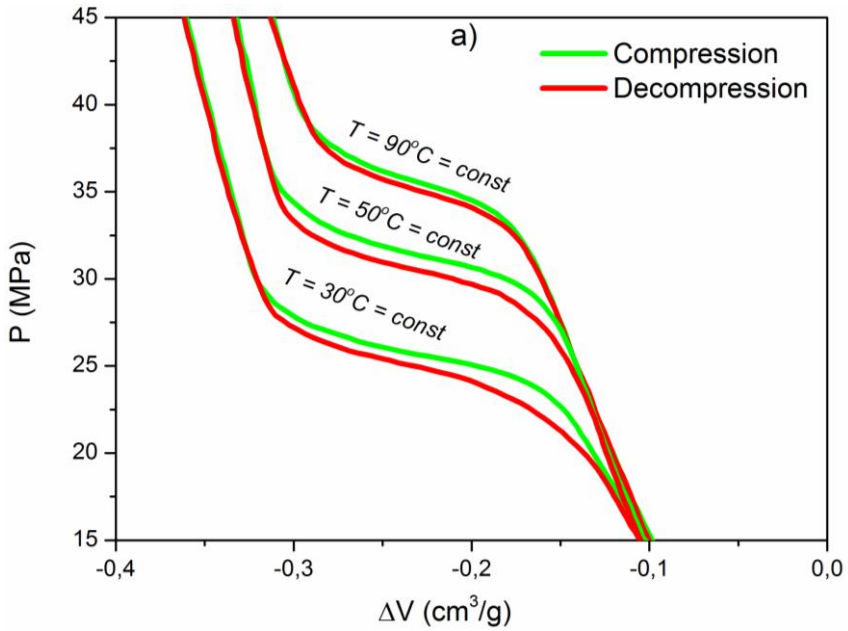
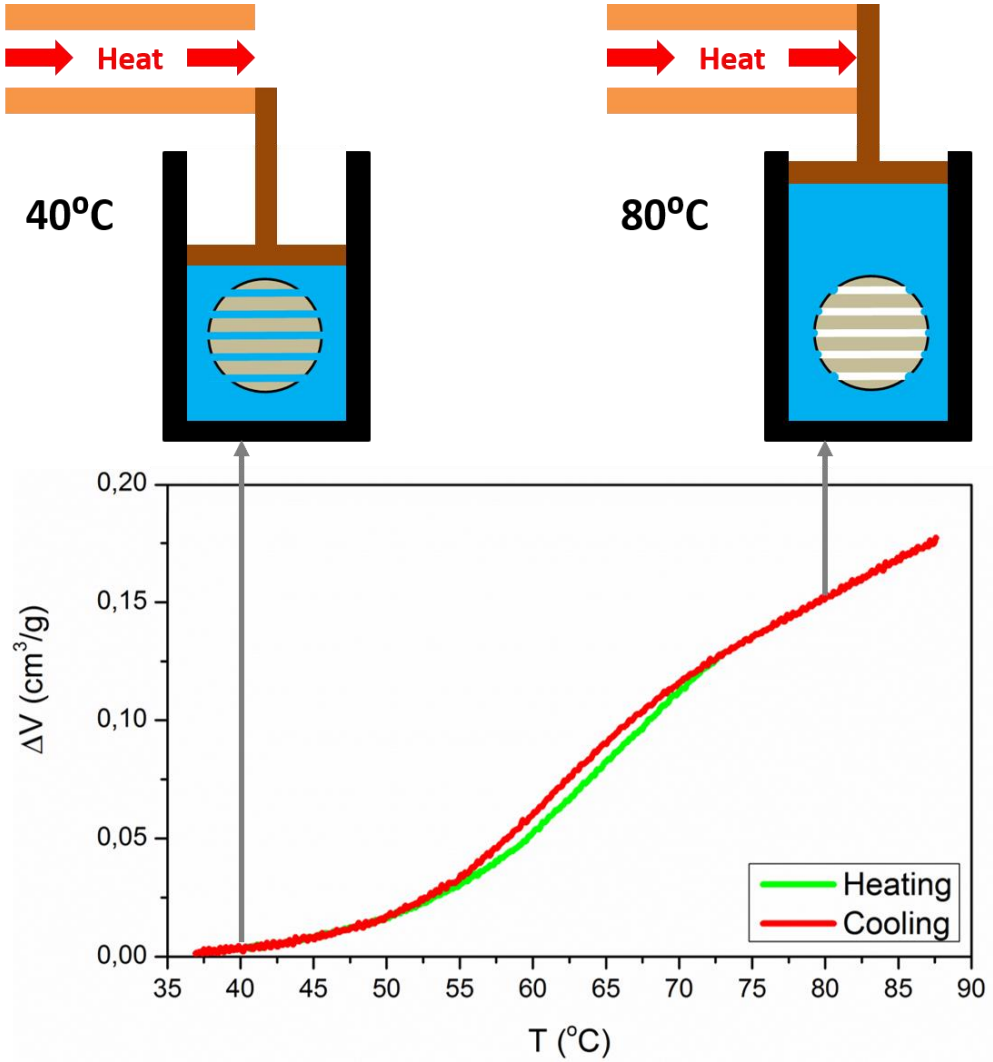
> Thermal actuation

CU2(TEBPZ) + WATER

Temperature regulating valve-actuator





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More information

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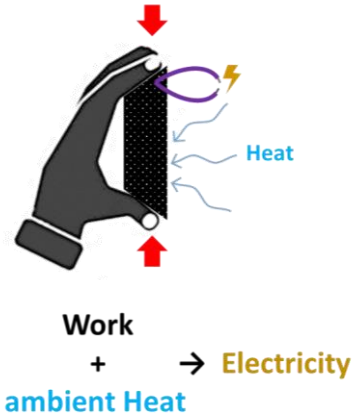
> Additional information

1st July 2021 at 10:30 Seminar at Sapienza:

Converting vibrations and environmental heat into electricity via reversible water intrusion into hydrophobic nanopores

Electro-intrusion FET-proactive project

https://www.electro-intrusion.eu/en



Recent papers

- M. Chorążewski, P. Zajdel, T. Feng, D. Luo, A. R. Lowe, C. M. Brown, J. B. Leão, M. Li, M. Bleuel, G. Jensen, D. Li, A. Faik, Y. Grosu. Compact Thermal Actuation by Water and Flexible Hydrophobic Nanopore. *ACS Nano*. **2021**. Just accepted. DOI: 10.1021/acsnano.1c02175.
- Tortora M., Zajdel P., Lowe A.R., Chorążewski M., Leão J.B., Jensen G.V., Bleuel M., Giacomello A., Casciola C.M., Meloni S., Grosu, Y. Giant Negative Compressibility by Liquid Intrusion into Superhydrophobic Flexible Nanoporous Frameworks. *Nano Letters*, **2021**, 21(7), pp.2848-2853.
- P Zajdel, M Chorążewski, J B Leão, G V Jensen, M Bleuel, H-F Zhang, T Feng, D Luo, M Li, A R Lowe, M Geppert-Rybczynska, D Li, Y Grosu. Inflation Negative Compressibility during Intrusion-Extrusion of a Non-Wetting Liquid into a Flexible Nanoporous Framework. *J. Phys. Chem. Lett.* **2021**. Just accepted.
- Lowe A., Tsyrin N., Chorążewski M., Zajdel P., Mierzwa M., Leão J.B., Bleuel M., Feng T., Luo D., Li M., Li D., Stoudenets V., Pawlus S., Faik A., Grosu Y. Effect of flexibility and nanotriboelectrification on the dynamic reversibility of water intrusion into nanopores: Pressure-transmitting fluid with frequency-dependent dissipation capability. *ACS Appl. Mater. & Interf.* **2019**. 11(43), pp.40842-40849.

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Collaboration opportunities

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Cutting edge Laboratories and Infrastructures

Complete infrastructure and material characterization facilities

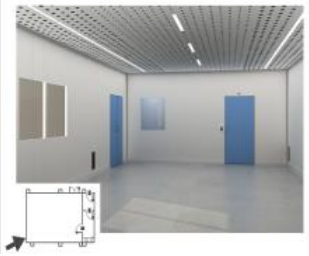
Materials Development

STA

DSC

Rheometer

LFA

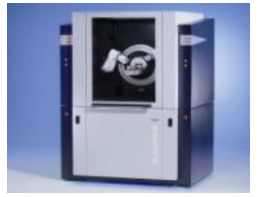


Dry room

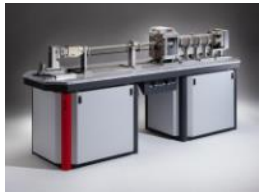
XPS

TEM

SEM



XRD



SAXS

BET

RAMAN

FT IR

PPMS

NMR

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Available testing infrastructure

- ***AIR-Loop Testing Platform**: closed hydraulic loop using air as heat transfer fluid, able to deliver **hot air up to 800ºC** and variable mass flow up to 360 kg/h.*

- ***OIL-Loop Testing Platform**: closed hydraulic loop using thermal oil as heat transfer fluid, able to deliver **hot oil up to 400ºC** and variable mass flow up to 25 m^3/h.*

- ***Steam-Loop Testing Platform**: closed hydraulic loop using water as heat transfer fluid, able to deliver **hot steam up to 300ºC** and variable mass flow up to 50 kg/h.*

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101017858

GRACIAS · THANK YOU · ESKERRIK ASKO

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