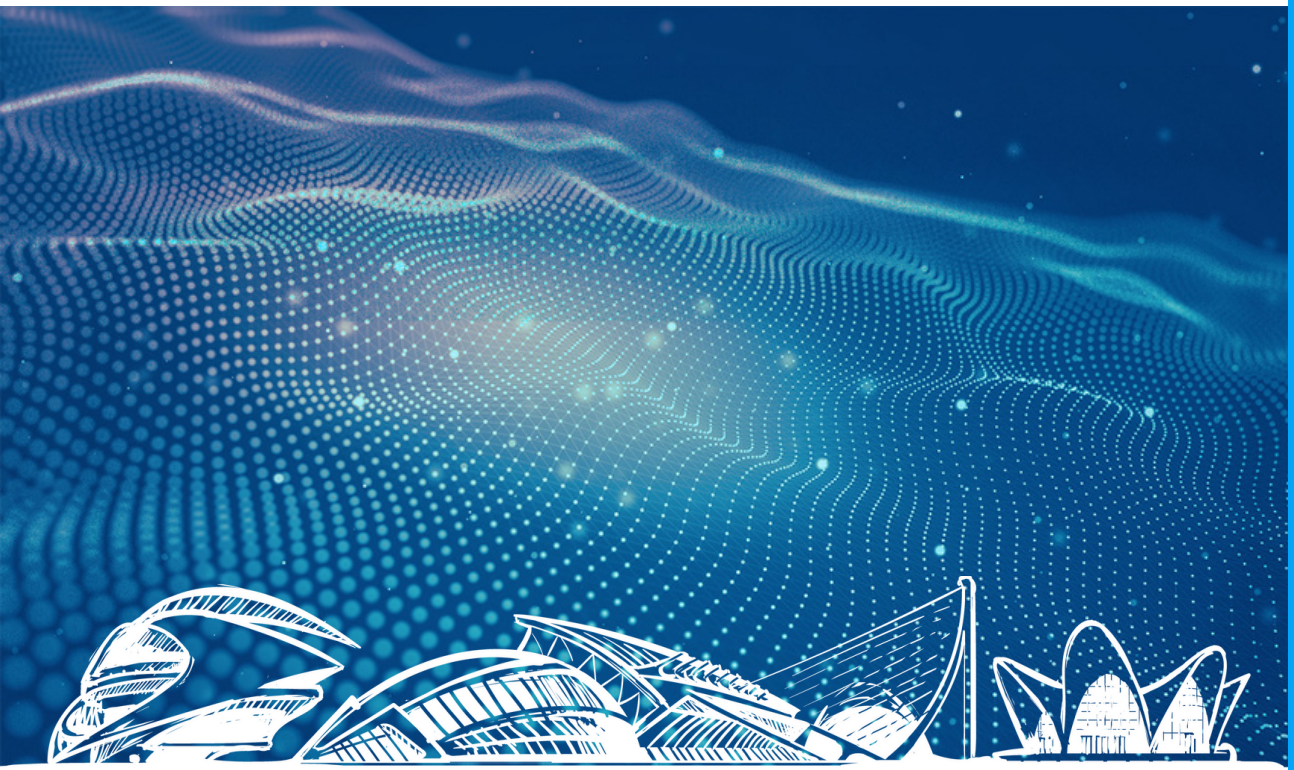
# 42 RIA

## XLII Reunión Ibérica de Adsorción

## VALENCIA, SPAIN

13 - 16 September, 2022



SCIENTIFIC PROGRAM

# 42 RIA

XLII Reunión Ibérica de Adsorción

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13 - 16 September, 2022

INSTITUTO DE TECNOLOGÍA QUÍMICA

CSIC

Consejo Superior de Investigaciones Científicas

UNIVERSITAT POLITÈCNICA DE VALÈNCIA

ADS Adsorción grupo especializado

Real Sociedad Española de Química

Sociedade Portuguesa de Química

Real Sociedad Española de Física

R.S.E.F.

Anton Paar

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# Bienvenida

El Grupo Especializado de Adsorción de la Real Sociedad Española de Química y la Real Sociedad Española de Física le invita cordialmente a participar en la XLII Reunión Ibérica de Adsorción, 42RIA.

Desafortunadamente, la Reunión prevista inicialmente para septiembre de 2020 se canceló debido a la pandemia. Ahora, la situación sanitaria ha mejorado notablemente en España y Portugal y, por ello, hemos retomado la organización de la XLII Reunión Ibérica de Adsorción. Se celebrará del 13 al 16 de septiembre de 2022 en Valencia, que es una de las ciudades más atractivas de la costa mediterránea de España.

La 42RIA tiene como objetivo fomentar la ciencia fundamental y aplicada sobre adsorción y separación de gases o líquidos, simulación molecular de fenómenos de adsorción, materiales adsorbentes que incluyen zeolitas, carbones, sílices y compuestos metal-orgánicos, aplicaciones energéticas de adsorción, etc.

El propósito de la 42RIA es reunir a investigadores con el objetivo de explorar, reflexionar y compartir ideas sobre el impacto de la investigación y la tecnología en los procesos de adsorción y separación. El desarrollo de estas tecnologías requerirá de investigación integradora para un mejor entendimiento de los procesos que permita contribuir a la solución de los desafíos científicos y tecnológicos presentes y futuros.

**Comité Organizador 42RIA**



# Apresentação

O Grupo Especializado de Adsorção da Real Sociedade Espanhola de Química e da Real Sociedade Espanhola de Física convida-o cordialmente a participar da XLII Reunião Ibérica de Adsorção, 42RIA.

Infelizmente, a reunião originalmente agendada para setembro de 2020 foi cancelada devido à pandemia. Agora, a situação da saúde melhorou notavelmente na Espanha e em Portugal e, por isso, retomamos a organização da XLII Reunião Ibérica de Adsorção. Será realizada de 13 a 16 de setembro de 2022 em Valência, que é uma das cidades mais atraentes da costa mediterrânea da Espanha.

O 42RIA visa promover a ciência fundamental e aplicada sobre adsorção e separação de gases ou líquidos, simulação molecular de fenômenos de adsorção, materiais adsorventes incluindo zeólitos, carbonos, sílicas e MOFs, aplicações energéticas de processos adsortivos, etc.

Além das conferências e pôsteres apresentados, o objetivo da 42RIA é reunir pesquisadores com o objetivo de explorar, refletir e compartilhar ideias sobre o impacto da pesquisa e da tecnologia nos processos de adsorção e separação. O desenvolvimento dessas tecnologias exigirá pesquisas integrativas para um melhor entendimento dos processos que contribuirão para a solução dos desafios científicos e tecnológicos presentes e futuros.

**Comissão Organizadora 42RIA**

# Welcome

The Specialized Group of Adsorption of the Royal Spanish Society of Chemistry and the Royal Spanish Society of Physics cordially invites you to participate in the XLII Iberian Adsorption Meeting, 42RIA.

The meeting initially scheduled for September 2020 was unfortunately cancelled due to the pandemic. Now, the health situation has notably improved in Spain and Portugal and, thus, we have retaken the organization of the XLII Iberian Adsorption Meeting. It will be held from 13th to 16th September 2022 in Valencia, which is one of the most attractive cities on the Mediterranean coast of Spain.

The 42RIA aims to encourage fundamental and applied science on adsorption and separation of gases or liquids, molecular simulation of adsorption phenomena, adsorbent materials including zeolites, carbons, silicas, and metal organic frameworks, energy applications of adsorption, etc.

The purpose of the 42RIA is to bring together researchers with the objective of exploring, reflecting and sharing ideas about the impact of the research and technology on adsorption and separation processes. The development of these technologies will require integrative research for a better understanding of the processes that will contribute to the solution of present and future scientific and technological challenges.

**42RIA Organizing Committee**



# Local Committee

- Susana Valencia
- Fernando Rey
- Miguel Palomino
- Eduardo Andrés
- Teresa Blasco
- Alberto Barros
- Inmaculada García (Technical Secretary)

# Scientific Committee

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- Conchi Ania (CNRS Orleans, Francia)
- Ana Arenillas (INCAR CSIC, Oviedo)
- Diana Azevedo (UFC, Brasil)
- Carmen Blanco (Univ. Cantabria)
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- Jorge Gascón (KAUST, Arabia Saudi)
- Carlos Grande (KAUST, Arabia Saudi)
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# Scientific Committee

- José Bernardo Parra (retirado, antes INCAR CSIC, Oviedo)
- Eduardo Pérez Botella (Vrije Univ. Brussels)
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- Carmen Pesquera (Univ. Cantabria)
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- Teresa Valdés-Solís (INCAR CSIC, Oviedo)

# Scientific Program

## Wednesday, 14 September

**9:00** Plenary Lecture **PL2 / Ana Arenillas** (Institute of Carbon Science and Tecnology, INCAR-CSIC, Oviedo, Spain)
"Designing nanostructured materials by sol-gel synthesis"

**10:00** Oral Communications **(S1)**

10:00-10:15 **O-01**
Optimizing the insulation performance of hybrid materials through their chemical and structural properties.
Samantha L. Flores-López, Natalia Rey-Raap, Ana Arenillas.
*INCAR-CSIC, Oviedo, Spain*

10:15-10:30 **O-02**
Assessing $CO_2$ capture of amino-modified silica sorbents via solid-state NMR-assisted adsorption techniques.
Marina Ilkaeva, Ricardo Vieira, João Pereira, Mariana Sardo, Ildefonso Marin-Montesinos, Luís Mafra.
*University of Aveiro, Portugal*

# Scientific Program

## Wednesday, 14 September

10:30-10:45 **O-03**

Separation Performance of Shaped MOF MIL-160(Al) for Double Applications of Pre and Post Combustion Carbon Capture.

Mohsen Karimi, Alexandre Ferreira, Alírio E. Rodrigues, Farid Nouar, Kyung-Ho Cho, U-Hwang Lee, Christian Serre, José A. C. Silva.

*Universidade do Porto, Portugal*

10:45-11:00 **O-04**

Novel flexible MOFs to revolutionize gas separation industry.

Eduardo Andrés-García, Isabel Abánades Lázaro, Eleni Mazarakioti, Guillermo Mínguez Espallargas.

*ICMol, Valencia, Spain*

11:00-11:15 **O-05**

Investigation of Industrial Adsorbents for Direct Air Capture by Gas Flow Methods.

Francesco Walenszus, Robert Eschrich, Carsten Blum, Sebastian Ehrling.

*3P Instruments, Leipzig, Germany*

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# Separation Performance of Shaped MOF MIL-160(Al) for Double Applications of Pre and Post Combustion Carbon Capture

**Mohsen Karimi [1,2,3,*] , Alexandre Ferreira [1,2], Alírio E. Rodrigues [1,2], Farid Nouar[4] d, Kyung-Ho Cho[5], U-Hwang Lee[5], Christian Serre[4], , José A. C. Silva[3]**

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*[2] ALiCE - Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.*
*[3] Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal.*
*[4] Institut des Matériaux Poreux de Paris, ESPCI Paris, Ecole Normale Supérieure, CNRS, PSL University, Paris, France.*
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The world currently faces the dual challenges: climate changes caused by global warming and a high energy demand regarding the exponential population expansion and industrial development [1, 2]. Carbon dioxide, methane, nitrogen oxide and halogenated components are the main anthropogenic greenhouse gases (GHGs) [1]. The challenge of reducing GHGs emission can be overcome by successful developing post-combustion CO2 capture also advancing the green and renewable sources of energy including biogas [3]. Nevertheless, the main drawback concerning the biogas is its high content on carbon dioxide (it might be as high as 40% or more), which significantly reduces its heating capacity. Therefore, for biogas applications, a previous separation step is required to reduce the $CO_2$ content [2,3]. Among the different methodologies for biogas upgrading and post-combustion $CO_2$ capture, adsorption is among the most attractive ones [1].

**Theory:**

Accordingly, In this study, a hydrothermally stable Al-based MOF MIL-160(Al), made under scalable green conditions in shaped form, is being studied experimentally for gas adsorption and separation for biogas upgrading strategies [4,5]. This MOF is constructed from aluminum hydroxide chains linked via a five-membered ring 2,5-furan dicarboxylate ligand delimiting 1D microporous channels of 5-6Å. Its technico-economic cost production analysis has recently been assessed [6]. In the current study, the breakthrough experiments regarding the separation of CO2/CH4 and CO2/N2 have firstly been accomplished. Afterwards, the pressure swing adsorption (PSA) processes have been designed, which the developed PSA revealed that obtaining CH4 with the purity of 99% and recovery of 68% are possible. Figure 1 illustrates the loading capacity of CO2 and CH4 in various cycles. Further, the outcomes specified the promising potential of Al-based MOF MIL-160(Al) for separation of CO2 and N2, which N2 with 98% purity and 80% recovery are accessible. The flowrate changes of N2 and CO2 at product and waste flows, respectively, are depicted in Figure 2. Currently, performing the PSAs experiments regarding designed PSAs are ongoing for engineering perspective processes.

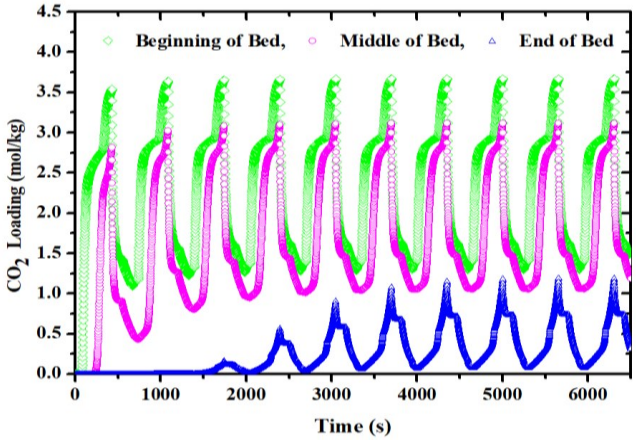


Figure 1a

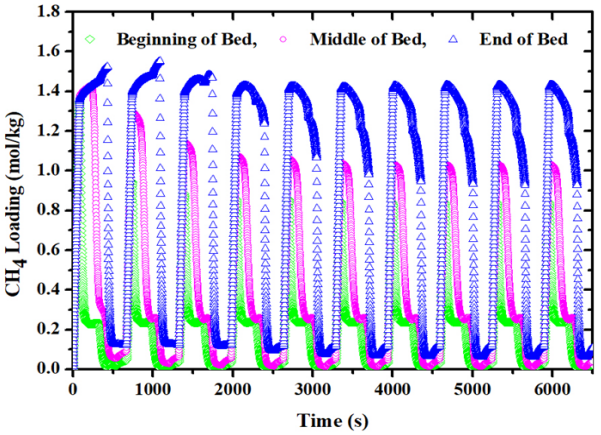


Figure 1b

**Figure 1: (a)** loading capacity of CO2 and **(b)** CH4 in various cycles of designed PSA

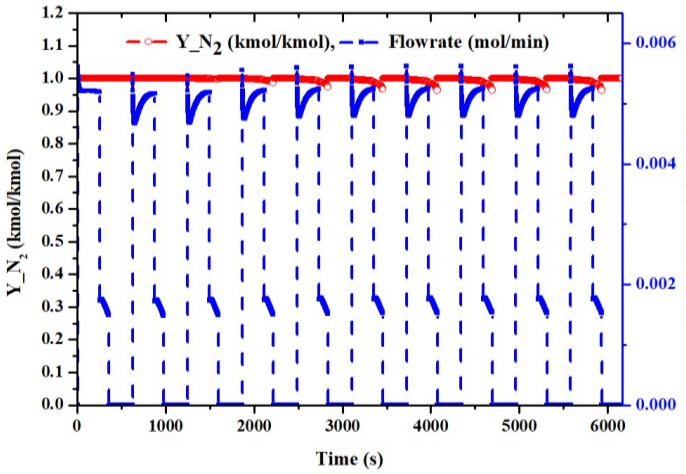


Figure 2a

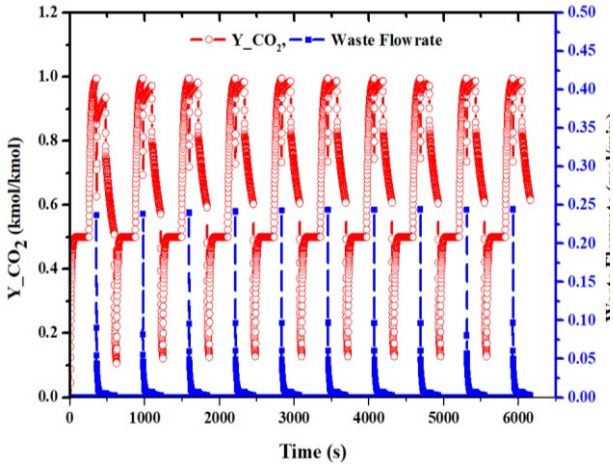


Figure 2b

**Figure 2:** flowrate changes of **(a)** N2 and **(b)** CO2 at product and waste flows, in various cycles of designed PSA.

**Acknowledgments:**

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**References:**

[1] Karimi et al., Journal of CO2 Utilization, 57 (2022) 101890.
[2 Karimi et al., Industrial & Engineering Chemistry Research, 57 (2018) 11154-11166.
[3] Ferreira et al., Chemical Engineering Science 124 (2015) 79–95.
[4] Cadiau et al, Advanced Materials, 2015, 27 (32), 4775−4780.
[5] Permyakova et al, ChemSusChem 2017, 10 (7), 1419−1426.

[6] Severino et al., Faraday Discuss. 2017, 231, 326-341.