

## PART A : CURRICULUM VITAE

**Benoit COASNE**<sup>1,2</sup> (Male, 47 ans, 2 children, [benoit.coasne@univ-grenoble-alpes.fr](mailto:benoit.coasne@univ-grenoble-alpes.fr))

CNRS Research Director 2nd classe (section 15, CNRS)

<sup>1</sup> Lab. Interdisciplinaire de Physique, CNRS/Univ. Grenoble Alpes, Grenoble, France

<sup>2</sup> ILL Theory Group, Institute Laue Langevin (Neutron Source), Grenoble, France

Researcher id: <http://scholar.google.com/citations?user=-rO1SkUAAAAJ&hl=en&oi=ao>

Site Web: [benoitcoasne.github.io](http://benoitcoasne.github.io)

**Research Theme:** « Adsorption and Transport in Nanoporous Materials »

### Academic Records and Education

2015/... **CNRS Research Director (2nd Class)**

Lab. Interdisciplinaire de Physique, CNRS/Univ. Grenoble Alpes, France.

2023/... **Leader Soft Matter** (ILL Permanent Affiliate)

ILL Theory Group, Institute Laue Langevin, Grenoble, France

2012/15 **CNRS Research 1st class + MIT Visiting Associate Prof.**

CNRS/MIT Lab, USA. **Group leader « Multiscale adsorption/transport »**

2011 **Habilitation** à diriger des recherches, *Thermodynamics/dynamics of fluids, electrolytes and solids in porous materials*. Univ Montpellier

2005/12 **CNRS Researcher** (1st class since 01/2009)

Institut Charles Gerhardt, Montpellier, France

2003/04 **Postdoctoral Researcher**, Department of Chemical Engineering,  
North Carolina State University, Raleigh, NC, USA

2003 **PhD Physics**, *Adsorption and condensation of fluids in porous silicon*  
Groupe de Physique des Solides, Univ Paris 7, France

### Science/International Recognition

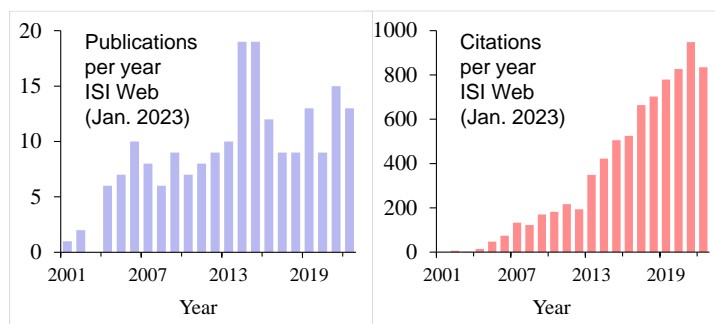
**203** Articles (3 Nature Mat, 6 Nat Comm,  
2 Chem Soc Rev, 2 PNAS, 2 JACS,  
4 PRL, 3 J Phys Chem Lett)

**47** H-index (**54** Google Scholar)

**7396** Citations

**51** Invited Conferences

**77** Seminaires, Schools, etc.



### Awards and Distinctions

2019 **Invited Professor**, Chair Saint-Gobain, Institut Navier, France

2016/22 **Board of Directors**, International Adsorption Society

2015/19 **Prime d'encadrement doctoral et de recherche**, CNRS et MENESR

2012/15 **Visiting Associate Professor**, MIT, Cambridge, USA

2011/17 **Cofounder** of the French Adsorption Society

2010/14 **Prime d'Excellence Scientifique**, CNRS et MENESR

2013 **Scientific Collaborator**, Faculté Polytechnique de Mons, Belgium

2011 **Award "Chercheur d'Avenir 2011"** in Languedoc Roussillon, France

2006 **Visiting Scholar**, Adam Mickiewicz University, Poznan, Poland

## Benoit Coasne

(CNRS Research Director, Section 15)

### RESPONSIBILITIES, MANAGEMENT AND SCIENTIFIC ANIMATION

#### Responsibilities, Collective Tasks

2022/...	<b>Steering Committee</b> , New Joint Laboratory CNRS - PetroChina
2022/...	<b>ILL Review Panel</b> , Institut Laue Langevin (Neutron Center), Grenoble
2022/...	<b>Committee “Young Researcher Award”</b> , Int. Adsorption Society
2022/...	<b>Board Member Division Chimie Physique</b> , Société Chimique de France
2022/24	<b>Scientific Council Expert</b> , IFP Energies Nouvelles
2022/...	<b>French Chair</b> , French/German Adsorption Initiative ( <a href="http://www.adsorption.eu">www.adsorption.eu</a> )
2019/...	<b>Principal Science Advisor</b> , VEOLIA Design Center, St Maurice, France
2019/22	<b>Panel Chair IAS Carbon neutrality</b> , International Adsorption Society
2016/...	Nominated Member <b>LIPhy Council</b> , CNRS/University Grenoble Alpes
2011/17	<b>President</b> of the French Adsorption Society (elected and then reelected)
2012/15	Group Leader « <b>Multiscale Adsorption and Transport</b> » CNRS/MIT Lab., Boston, USA
2015/20	Member <b>Poromechanics Committee</b> , Am. Soc. Civil Engineers
2011/14	Member <b>Institute Charles Gerhardt Council</b> , CNRS/Univ. Montpellier
2009/12	Head of the <b>Communication Commission</b> of Institute Charles Gerhardt
2009/12	Member <b>Scientific Animation</b> of the Institute Charles Gerhardt
2010/16	Board member, <b>French Zeolite Society</b>
2009/12	Board member, <b>Local section LR of the French Chemical Society SCF</b>

#### Commission of Trust

2019/20	<b>M-ERA.NET strategy expert group</b> (21 pers.) Roadmapping 2020 call
2020	<b>Science Council Expert</b> , IFP Energies Nouvelles
2018	<b>Guest Editor</b> , Issue “Adsorption” in Curr. Op. Chem. Eng. (Elsevier)
2017/18	<b>Panel ANR</b> , French National Science Agency « Matériaux inorganiques »
2015/21	<b>Panel FWO</b> , Flanders Res. Foundation « Chem Eng & Material Sci. »
2014	Review Editor in the Editorial Board of <b>Frontiers   Energy Research</b> - Open Access Journal, partner of <b>Nature Publishing Group (NPG)</b>
2014	Co-Guest Editor, « Design/modeling porous materials », <b>Eur Phys J</b>
Since 2009	External expert in Sections 31 et 33 of CNU

#### Organization of scientific meetings

2023	<b>Conference co-chair</b> “FRA/GER Adsorption meeting”, Strasbourg, France
2018	<b>Colloquium Chair</b> “Matériaux poreux, granulaires, à grande surface spécifique”, Conference Matériaux 2018, Strasbourg, France (~ 100 people)
2018	<b>Symp. Chair</b> “Soft Porous Materials”, Interpore2018, N. Orleans, USA
2010/17	Journées Annuelles <b>Association Française de l’Adsorption</b> (~ 70 people)
2011/16	Journées Annuelles <b>Groupe Français des Zéolithes</b> (~ 80 people)
2013	<b>Ionic Liquids for Materials</b> (~ 100 people) ILMAT2013, Montpellier
2010	<b>Journées SCF Grand Sud Ouest</b> (~80 people), Montpellier

# Benoit Coasne

(CNRS Research Director, Section 15)

## Student and postdoc supervision (17 PhD, 18 postdocs, 15 undergrad)

• **17 PhD Students** 1. J. Dweik, 2. C. Abrioux, 3. P. Bonnaud, 4. F. Villemot, 5. M. Lepinay (St Micro), 6. P. Billefont (UMons, Belgique), 7. L. Deliere (CEA), 8. H. Getachew, 9. D. Jin, 10. R. Bey, 11. I. C. M. Costa (IFPEN), 12. M. Chen (ETH medal award, Switzerland), 13. Z. Zaafour (IFPEN), 14. S. Cohen (U. Maryland, Chateaubriand Fellow), 15. W. Kel-louai, 16. N. Ferreira de Souza, 17. L. Didier • **18 Postdocs** 1. P. Cazade, 2. G. Ori, 3. L. Ngoc Ho, 4. R. Hartkamp, 5. A. Botan, 6. G. Hantal, 7. K. Falk, 8. C. Bousige, 9. P. Billefont, 10. T. Lee, 11. A. Obliger, 12. G. Couchaux, 13. D. Mehlhorn, 14. A. Schlaich, 15. R. Manokaran, 16. A. Sam, 17. V. Prasad, 18. S. Gravelle • **15 Undergrad.** 1. L. Naamar, 2. G. Pallares, 3. D. Horlait, 4. P. Epicoco, 5. I. Aydogdu, 6. J. Nigon, 7. F. Freitag, 8. L. Atmani, 9. H. Meyer, 10. J. Mohan, 11. D. Tabacchio-ni, 12. Z. Zaafour, 13. M. Barbagero, 14. K. Olson, 15. P. Sanchez-Moreno Royer

## PhD and Habilitation Jurys (47 including R = Reviewer, P = President)

47. Y. Khaldouni (R, Pau), 46. K. Wang (P, Montpellier), 45. HDR R. Semino (R, Paris), 44. F. Rizk (R, Lyon), 44. K. Ariski-na (R, Pau), 42. A. Hammoumi (R, Cavaillon), 41. M. Ducamp (R, Cavaillon), 40. M. Benchaabane (R, Paris), 40. A. Robert (Paris), 39. M. Ducamp (R, Paris), 38. A. Marcotte (P, ENS Paris), 37. A. Mishra (R, Univ. Metz), 36. F. Guy (P, Chambéry), 35. C. Methais (R, Besançon), 34. M. Sperra (R, SP, Brazil), 34. G. El Tabbal (R, Paris), 32. T. Virdis (R, VUB Brussels), 31. J. B. Pigot (R, Paris), 30. A. Patt (R, Dijon), 29. A. Håreager (R, Oslo), 28. R. Bingre (P, Strasbourg), 27. K. L. Nguyen (R, Marseille), 26. A. Coste (Montpellier), 25. N. Ganfoud (R, Paris), 24. C. Cabaud (P, Paris), 23. M. Chen (R, ETH Zurich), 22. HDR M. Vandamme (R, Paris), 21. B. K. Xiong (Tours), 20. E. Perrin (R + P, Berlin + Paris), 19. J. Wolanin (R, Paris), 18. HDR J. Jacquemin (R, Tours), 17. P. Bacle (R, Paris), 16. W. Louisfreme (R, Paris), 15. W. Goncalves (R, Lyon), 14. S. Dutta (R, Rennes), 13. J. M. Vanson (R, Paris), 12. M. Ciantar (R, Paris), 11. C. Péan (R, Paris), 10. C. Sempere (R, Lyon), 9. M. Michelin-Jamais (R, Lyon), 8. B. Farbos (R, Bordeaux), 7. G. Aubry (R, Grenoble), 6. A. Bouzid (Strasbourg), 5. M. De Toni (R, Paris), 4. L. Brochard (R, Paris), 3. M. Amrouche (R, Manchester), 2. A. Botan (R, Paris), 1. M. Jeffroy (Orsay)

## VALORISATION, TECHNOLOGICAL TRANSFER, INDUSTRIAL RELATIONS

### Contracts and Research Grants (\* = total funding unknown)

Contrat	Période	Organisme	Partners	Montant	Responsabilité
SESAME	2022/26	ANR	4	~50 k€	Partner
ACOUFEN	2021/25	ANR	3	~500 k€	Coordinator
MENIHR	2021/25	ANR	3	106 k€	Partner
IRGA21	2021/23	Univ. Grenoble Alpes	3	43 k€	Co-Coordinator
MODYTICS	2019/23	ANR Astrid	4	130 k€	Partner
CATCALL	2019/23	ANR	2	130 k€	Partner
2FDN	2019/23	PhD grant	2	103 k€	Coordin.
IFPEN	2017/20	Research contract	1	30 k€	Coordin.
TWIST	2017/20	ANR	5	80 k€	Partner
CEA	2017/20	Research contract	3	40 k€	Partner
EUROKIN4	2017/18	Research contract	1	12.5 k€	Coordin.
IFPEN	2016/19	Research contract	1	18 k€	Coordin.
TOTAL	2017/18	Research contract	3	7 k€	Partner
TAMTAM	2011/15	ANR	4	~500 k€	Coordin.
X-Shale	2012/15	Industry	3	~1 M€/year	Co-coordin.
OCTAPPOM	2014	NEEDS	2	~100 k€	Coordin.
GENESIS	2013/16	ANR	3	~400 k€	Partner
TARG-E-D	2013/16	ANR	3	~376 k€	Partner
Transport_ion	2012/15	Cherch. Avenir	2	~70 k€	Coordin.
NanoChalco	2011/15	ANR	3	~500 k€	Coordin.
Structuring_IL	2012/15	CINES	1	CPU Time	Coordin.
IDDILIQ	2009/12	ANR	1	200 k€	Partner
ATILH	2008/10	Industry	5	100 k€*	Partner
SiMoNanoMem	2008/10	ANR	4	400 k€	Partner
Eau, Electro	2009/10	CINES	1	CPU Time	Coordin.

## Benoit Coasne

(CNRS Research Director, Section 15)

### Partnership with industry/Consulting

- 2009/20 Saint Gobain, Consulting « Adsorption/transport in porous materials »  
2019/20 EUROKIN consortium, 200 page report on transport in porous media  
2012/15 Shell and Schlumberger, « Adsorption, Transport, Mechanics properties of Gas Shale ». Collab. Industry/Academia  
2015/17 Gaztransport & Technigaz (GTT) Report on Adsorption (2015) + Report on Knudsen diffusion (2017) + Technical calculations (2017)  
2008/2010 Association Technique de l'Industrie des Liants Hydrauliques (ATILH), « Porosity, transport and resistance of concrete ». (2008-2010)

### FORMATION, TEACHING, DISSEMINATION

#### Teaching, Training

- 2022/... International Master Week, Qingdao University/China, Adsorption and transport in porous materials (6 h/year)  
2016/... Research Training Master Nanosciences, University Grenoble Alpes, Molecular modeling (40 h/year)  
2018/... Res. Seminar for Master 2 Nanophysics, U. Grenoble Alpes (1 h/year)  
2018 Collège École Polytechnique X, Multiscale porous materials (4h)  
2014 Formation Arkema, Characterization techniques of porous solids (8h)  
2013 Formation ST Microelectronics, Molecular simulation (16h)  
2012 Collège École Polytechnique X, Multiscale porous materials (4h)  
2012 Formation IRCELYON, Molecular simulation (16h)  
2011 Course, Institute of Separative Chemistry, Molecular modeling (2h)  
2009 Tutorat Bénévole auprès d'élèves en primaire/collège/lycée, Association de quartier Boutonnet, Montpellier (2 h/week)  
2005/11 Master Phys/Chem, U. Montpellier, Molecular modeling (8 h/year)  
2000/02 IUT, Univ. Paris 7, Classical Mechanics (115h)  
2000/01 DEUG, Univ. Marne la Vallée, Electromagnetism (45h)  
1999/00 DEUG, Univ. Paris 7, Electronics (70h)

#### Communication/Dissemination

- 2020 Les matériaux nanoporeux: de l'utilité des trous en chimie des matériaux, Chimie Étonnante CNRS (Farrusseng, Coasne)  
2020 Des matériaux fonctionnels à l'échelle du nanomètre, Usine Nouvelle 1035, Oct. 2020 (Farrusseng, Coasne)  
2016 Article P. Passebon in Industrie & Technologies, <https://www.industrie-techno.com/comprendre-les-gaz-de-schiste-pour-mieux-les-exploiter.42366>  
2012 L'eau dans les mésopores du ciment, Ciments, Bétons, Plâtres et Chaux 907, 64, 2012. (Bonnaud, Pellenq, Coasne)  
2010 Internship L'Express.fr. 2 articles « Nous comprenons les consommateurs d'eau en bouteilles » et « Le triplement du nucléaire doit être débattu »  
2010 Seminar for University Students on Research in France  
2008 Seminar for High School Students on Research in France

**PART B : SCIENTIFIC PRODUCTION**

**1. Publications in peer-reviewed journals (183)**

**including 6 invited review articles (titles in red)**

**Communication releases are indicated in green**

## **In Preparation**

**P194.** W. Kellouai, P. Judeinstein, M. Plazanet, J. M. Zanotti, Q. Berrod, M. Drobek, A. Julbe, **B. Coasne**, [Free Volume Theory of Self-diffusion in Zeolite: Molecular simulation and Experiment](#), To be submitted (2022).

**P193.** A. Schlaich, M. Vandamme, M. Plazanet, **B. Coasne**, [Bridging Microscopic Dynamics and Hydraulic Permeability in Mechanically-Deformed Nanoporous Materials](#), To be submitted (2022).

**P192.** M. Rajasekaran, A. Schlaich, M. Vandamme, S. Brisard, J. M. Pereira, **B. Coasne**, [Enhanced Self-Diffusion and Collective Transport of Water in Thermalized Nanoporous Materials: From hydrogen-Bond Softening to Correlated Solid-Fluid Dynamics](#), To be submitted (2023).

**P191.** S. Dutta, A. Nossov, A. Galarneau, Y. Didi, B. Said, R. Denoyel, V. Wernert, **B. Coasne**, F. Guenneau, [Apparent Anomalous Temperature Behavior of Self-Diffusion in Hierarchical Monolithic Zeolites: A Pulsed-Field Gradient Nuclear Magnetic Resonance and Thermodynamic Study](#), To be submitted (2022).

## **Submitted**

**P190.** A. Streb, R. Lively, P. Llewellyn, A. Matsumoto, M. Mazzotti, R. Pini, **B. Coasne**, [Towards carbon neutral scientific societies: A case study with the International Adsorption Society](#), Submitted (2023).

**P189.** M. Lucioli, M. Rescigno, F. G. Alabarse, U. Ranieri, B. Frick, **B. Coasne**, L. E. Bove, [Low Temperature Dynamics of Water Confined in Hydrophilic Zeolite Nanopores](#), To be submitted (2023).

**P188.** A. Sam, M. Barbagero, R. Venegas, **B. Coasne**, [Multiscale Acoustic Properties of Nanoporous Materials: From Microscopic Dynamics to Mechanics and Wave Propagation](#), *J. Mech. Phys. Sol.*, Submitted (2023).

**P187.** C. Zhang, **B. Coasne**, D. Derome, J. Carmeliet, [Adsorption/percolation model for water diffusion in deformable nanoporous polymers](#), Submitted (2023).



## 2023

**P186.** A. J. Souna, S. R. Cohen,, C. A. Rivera, K. Manfred, **B. Coasne**, J. T. Fourkas, [The Role of Resonant Coupling in Vibrational Sum-Frequency-Generation Spectroscopy: Liquid Acetonitrile at the Silica Interface](#), *J. Mol. Liq.*, in press (2023)

**P185.** S. Dutta, A. Galarneau, D. Minoux, C. Aquino, J. P. Dath, F. Guenneau, **B. Coasne**, [Molecular Diffusion in Hierarchical Zeolites with Ordered Mesoporosity: Pulsed Field Gradient Nuclear Magnetic Resonance combined with Thermodynamic Modeling](#), *J. Phys. Chem. C* **127**, 1548 (2023).

**P184.** A. Obliger, C. Bousige, J. M. Leyssale, **B. Coasne**, [Mini-review on the development of atomistic kerogen models and their applications in gas adsorption and diffusion \(Invited Review Paper\)](#), *Energy Fuels* **37**, 1678 (2023).

+ ACS Editor's Choice, <https://pubs.acs.org/page/policy/editorchoice/index.html>

## 2022

**P183.** V. Wernert, **B. Coasne**, P. Levitz, K. Nguyen, E. J. Garcia, R. Denoyel, [Tortuosity of hierarchical porous materials: diffusion experiments and random walk simulations](#), *Chem. Eng. Sci.* **264**, 118136 (2022).

**P182.** D. Bauer, Z. Zaafouri, G. Batot, **B. Coasne**, [From Transient to Stationary Transport in Porous Networks under Various Adsorption Conditions and Kinetics](#), *J. Phys. Chem. B* **126**, 6125 (2022).

**P181.** C. O'Sullivan, C. Arson, **B. Coasne**, [A Perspective on Darcy's Law across the Scales: From Physical Foundations to Particulate Mechanics](#), *J. Eng. Mech.* **148**, 11 (2022).

+ Editor's Choice section of the *Journal of Engineering Mechanics* page in the ASCE Library <https://ascelibrary.org/journal/jenmdt>

**P180.** I. C. Medeiros-Costa, C. Laroche, **B. Coasne**, J. Pérez-Pellitero, [Xylene Selectivity at the External Surface of Hierarchical Zeolites: Experiment and Molecular Modeling](#), *Ind. Eng. Chem. Res.* **61**, 10184 (2022).

**P179.** C. Pagis, D. Laprune, Lucian Roiban, T. Epicier, C. Daniel, D. Farrusseng, **B. Coasne**, [Morphology and topology assessment in hierarchical zeolite materials: adsorption hysteresis, scanning behavior, and domain theory](#), *Inorg. Chem. Frontiers* **9**, 2903 (2022).

**P178.** W. Kellouai, P. Judenstein, M. Plazanet, S. Baudoin, M. Drobek, A. Julbe, **B. Coasne**, [Gas Adsorption in Zeolite and Thin Zeolite Layers: Molecular Simulation, Experiment and Adsorption Potential Theory](#), *Langmuir* **38**, 5428 (2022).

## Benoit Coasne

(CNRS Research Director, Section 15)

**P177.** S. Ghojavand, **Benoit Coasne**, R. Guillet-Nicolas, P. Bazin, M. Desmurs, L. J. Aguilera, V. Ruaux, S. Mintova, [The role of alkali metal cations on the CO<sub>2</sub> adsorption behavior of nanosized chabazite](#), *ACS Appl. Nano. Mater.* **5**, 5578 (2022).

**P176.** J. W. M. Osterrieth et al., [How reproducible are surface areas calculated from the BET equation?](#), *Adv. Materials*, 2201502 (2022).

**P175.** D. T. Bowron, D. A. Keen, M. Kint, C. Weigel, L. Konczewicz, S. Contreras, **B. Coasne**, G. Garbarino, M. Beaudhuin, J. Haines, J. Rouquette, [Atomic-Spring Effect in Amorphous Silica-Helium Composite](#), *J. Phys. Chem. C* **126**, 5722 (2022).

**P174.** Z. Zaafour, G. Batot, C. Nieto-Draghi, B. Rotenberg, **B. Coasne**, D. Bauer, [Impact of adsorption kinetics on pollutant dispersion in water flowing in nanopores](#), *Adv. Water Res.* **162**, 104143 (2022).

**P173.** V. Wernert, K. L. Nguyen, P. Levitz, **B. Coasne**, R. Denoyel, [Impact of surface diffusion on transport through porous materials](#), *J. Chrom. A* **1665**, 462823 (2022).

**P172.** M. Dopke, F. Westerbaan van der Meij, **B. Coasne**, R. Hartkamp, [Surface Protolysis and its Kinetics Impact the Electrical Double Layer](#), *Phys. Rev. Lett.* **128**, 056001 (2022).

**P171.** S. R. Cohen, M. Plazanet, S. Rols, D. J. Voneshen, J. T. Fourkas, **B. Coasne**, [Structure and Dynamics of Acetonitrile: Molecular Simulation and Neutron Scattering](#), *J. Mol. Liq.* **348**, 118423 (2022).

**P170.** C. Zhang, M. Chen, **B. Coasne**, S. Keten, D. Derome, J. Carmeliet, [Hygromechanics of Composite with Intramolecular Interactions at Fiber-Matrix Interface Investigated with Molecular Dynamics](#), *Composites Part B* **228**, 109449 (2022).

**P169.** A. Schlaich, D. Jin, L. Bocquet, **B. Coasne**, [Electronic screening using a virtual Thomas–Fermi fluid for predicting wetting and phase transitions of ionic liquids at metal surfaces](#), *Nature Materials* **21**, 237 (2022).

+ CNRS communication: <https://www.inp.cnrs.fr/index.php/fr/cnrsinfo/un-fluide-virtuel-pour-simuler-des-liquides-charges-confines>

## 2021

**P168.** M. Lions, C. Daniel, B. Coasne, F. Meunier, A. Tuel, D. Farrusseng, [The Pivotal Role of Critical Hydroxyl Concentration in Si-rich zeolites for Switching Vapor Adsorption](#), *J. Phys. Chem. C* **125**, 22890 (2021).

**P167.** J. Wolanin, L. Michel, D. Tabacchioni, J. M. Zanotti, J. Peters, I. Imaz, **B. Coasne**, M. Plazanet, C. Picard, [Heterogeneous Microscopic Dynamics of Water Nanoconfined in a Ultra-hydrophobic Environment: Neutron Scattering and Molecular Modeling](#), *J. Phys. Chem. B* **125**, 136 (2021).

**P166.** M. Santoro, M. Morana, D. Scelta, J. Rouquette, K. Dziubek, F. A. Gorelli, R. Bini, G. Garbarino, A. van der Lee, F. Di Renzo, B. Coasne, J. Haines, [Insertion of](#)

## Benoit Coasne

(CNRS Research Director, Section 15)

Oxygen and Nitrogen in the Siliceous Zeolite TON at High-Pressure, *J. Phys. Chem. C* **125**, 19517 (2021).

**P165.** C. Zhang, M. Chen, S. Keten, **B. Coasne**, D. Derome, J. Carmeliet, Hygromechanical mechanisms of wood cell wall revealed by molecular modeling and mixture rule analysis: Role of components, interphases and hydrogen bonding, *Sci. Adv.* **7**, ea-bi8919 (2021).

**P164.** T. Rego, S. Spagnoli, M. C. Fauré, C. Allain, **B. Coasne**, J. Malinge, C. Shen, P. Fontaine, M. Goldmann, Unexpected order-disorder transition in Diacetylene alcohol Langmuir film, *Langmuir* **37**, 30 (2021).

**P163.** Z. Zaafour, G. Batot, C. Nieto-Draghi, B. Rotenberg, D. Bauer, **B. Coasne**, Lattice Boltzmann method for adsorption under stationary and transient conditions: Interplay between transport and adsorption kinetics in porous media, *Phys. Rev. E* **104**, 015314 (2021).

**P162.** R. Bey, **B. Coasne**, C. Picard, Carbon dioxide as a line active agent: its impact on line tension and nucleation rate, *Proc. Nat. Acad. Sci.* **118**, e2102449118 (2021).

+ CNRS communication: <https://inp.cnrs.fr/fr/cnrsinfo/le-co2-comme-tensioactif-de-ligne-dans-un-nanopore>

**P161.** F. G. Alabarse, B. Baptiste, M. Jimenez-Ruiz, **B. Coasne**, J. Haines, J. B. Brubach, P. Roy, H. E. Fischer, S. Klotz, L. E. Bove, Different Water Networks Confined in Unidirectional Hydrophilic Nanopores and Transitions with Temperature, *J. Phys. Chem. C* **125**, 14378 (2021).

**P160.** D. Jin, **B. Coasne**, Reduced phase stability and faster formation/dissociation kinetics in confined methane hydrate, *Proc. Nat. Acad. Sci.* **118**, e2024025118 (2021).

**P159.** W. Xu, X. Liu, M. Pena-Alvarez, H. C. Jiang, P. Dalladay-Simpson, **B. Coasne**, J. Haines, E. Gregoryanz, M. Santoro, High Pressure Insertion of Dense H<sub>2</sub> into a Model Zeolite, *J. Phys. Chem. C* **125**, 7511 (2021).

**P158.** L. Scalfi, **B. Coasne**, B. Rotenberg, On the Gibbs-Thomson equation for the crystallization of confined fluids, *J. Chem. Phys.* **154**, 114711 (2021).

**P157.** P. Judeinstein, M. Zeghal, D. Constantin, C. Iojoiu, **B. Coasne**, Interplay of Structure and Dynamics in Lithium/Ionic Liquid Electrolytes: Experiment and Molecular Simulation, *J. Phys. Chem. B* **125**, 1618 (2021).

**P156.** C. Bousige, P. E. Levitz, **B. Coasne**, Bridging scales in disordered porous media by mapping molecular dynamics onto intermittent Brownian motion, *Nature Comm.* **12**, 1043 (2021).

## 2020



## Benoit Coasne

(CNRS Research Director, Section 15)

**P155.** M. Chen, **B. Coasne**, R. Guyer, D. Derome, J. Carmeliet, [A Poromechanical Model for Sorption Hysteresis in Nanoporous Polymers](#), *J. Phys. Chem. B* **124**, 8690-8703 (2020).

**P154.** Y. Long, J.C. Palmer, B. Coasne, K. Shi, M. Sliwinska-Bartkowiak and K. E. Gubbins, [Reply to Comment on “Pressure enhancement in carbon nanopores: a major confinement effect”](#), *Phys. Chem. Chem. Phys.* **22**, 9826 (2020).

**P153.** M. Chen, **B. Coasne**, D. Derome, J. Carmeliet, [Role of cellulose nanocrystals on hysteretic sorption and deformation of nanocomposites](#), *Cellulose* **27**, 6945 (2020).

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## 2. Conference Proceedings with peer-review (20)

- A20.** A. Sam, **B. Coasne**, R. Venegas, [Towards bridging nanoscale and macroscale acoustics of porous solids](#), Proceedings of the Internoise Conference (2022).
- A19.** D. Derome, M. Chen, C. Zhang, A. Shomali, **B. Coasne**, J. Carmeliet, [Modeling wood long term performance? The challenge of using natural materials](#), Poromechanics VI: Proceedings of the Sixth Biot Conference on Poromechanics, *ASCE Proc.* (Am. Soc. Civil Engineers), 427-434 (2017).
- A18.** M. Chen, **B. Coasne**, R. Guyer, D. Derome, J. Carmeliet, [Analysis of Sorption and Mechanical Hysteresis of Nano-Porous Materials: Upscaling Molecular Simulations with the Dependent Domain Theory](#), Poromechanics VI: Proceedings of the Sixth Biot Conference on Poromechanics, *ASCE Proc.* (Am. Soc. Civil Engineers), 427-434 (2017).
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**A8.** R. J. –M. Pellenq, **B. Coasne**, “Testing the validity of small – angle and adsorption – based characterization techniques by atomic – scale simulation”, Technical proceedings of the 2006 NSTI Nanotechnology Conference **1**, 819 – 822 (2006).

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### 3. Book or Book Chapters (3)

**B3.** D. Farrusseng, **B. Coasne**, [Solides nanoporeux: de l'utilité des trous en science des matériaux](#), Etonante Chimie !, Ouvrage de Vulgarisation, *CNRS Editions* (2020).

**B2.** G. Ori, C. Massobrio, **B. Coasne**, [Molecular modeling of glassy surfaces](#), Molecular dynamics of disordered systems, *Springer* (2015).

**B1.** R. J. M. Pellenq, **B. Coasne**, P. E. Levitz “[Adsorption and Condensation of Xenon in Mesopores having a Microporous Texture or a Surface Roughness](#)”, *Molecular Simulation of Adsorption Phenomena* Eds. N. Quirke and D. Nicholson, Taylor and Francis, London (2005).

### 4. Invited conferences (51)

**I51. B. Coasne**, [Bridging Molecular Dynamics and Macroscopic Transport in Nanoporous Materials](#) (invited talk), *CECAM Workshop “Fluids in porous materials: from fundamental physics to engineering applications”*, EPFL Lausanne, Switzerland (2023).

**I50. B. Coasne**, [Dynamics in compliant nanoporous materials: Coupling multiscale dynamics and mechanics](#) (invited talk), *Modelling Complexity in Mechanics*, Alghero, Sardinia, Italy (2023).

**I49. B. Coasne**, [Oversolubility in nanoconfinement: from adsorption in porous media to wetting of interfaces](#) (invited talk, symposium ‘Reactivity in nanoconfined interfaces’), *ACS Meeting 2023*, Indianapolis, IN, USA (2023).

**I48. B. Coasne**, [Reduced phase stability and faster formation/dissociation kinetics in confined methane hydrate](#) (invited talk), *GDR Hydrates*, Rueil Malmaison (Paris), France (2022).

**I47. B. Coasne**, [Adsorption and Transport in Nanoporous Materials](#) (keynote, colloque 10), *Matériaux 2022*, Lille, France (2022).

## Benoit Coasne

(CNRS Research Director, Section 15)

- I46. B. Coasne, [Wetting and phase transitions of ionic liquids at metal surfaces: Electronic screening using a virtual Thomas–Fermi](#), *CECAM Workshop on Ion adsorption and electrokinetic transport at interfaces*, Marcoule (Avignon), France (2022).
- I45. B. Coasne, [Gas Adsorption in Zeolite and Thin Zeolite Layers: Molecular Simulation, Experiment and Adsorption Potential Theory](#), *8th Workshop “Prospects & Challenges in Zeolites and Related Porous Materials”*, Cabourg/Caen, France (2022).
- I44. B. Coasne, [Multiscale diffusion in carbonaceous materials](#), *CECAM Workshop on adsorption in microporous carbons for a range of societal and emerging applications*, Bordeaux, France (2022).
- I43. B. Coasne, [Adsorption and diffusion in zeolitic materials](#), *Groupe Français des Zeolithes (GFZ)*, Vogue (Ardeche), France (2022). [Keynote Invitation](#).
- I42. B. Coasne, [Fluid adsorption and diffusion in zeolitic materials](#), *First International Edition of the 21st Chinese Zeolite Conference (21CZC)*, Qingdao, Shandong Province, China (2021). [Visioconference](#).
- I41. B. Coasne, [Adsorption and transport in nanoconfinement](#), *Summer Workshop nanoCAFÉ group* (Sapienza Università di Roma), Siena (Tuscany), Italy (2021). [3 seminars on “Adsorption and criticality in nanoconfined fluids”, “Wetting and phase transitions at metallic surface”, “Bottom up model of dynamics/transport in porous media”](#)
- I40. B. Coasne, [Fluid adsorption and transport in nanoporous materials](#), *Annual meeting of the German Adsorption Society*, Frankfurt, Germany (2021)..
- I39. B. Coasne, [Adsorption et transport de fluides dans des angstropores](#), *Rencontres Francophones de l’Association Française de l’Adsorption*, France (2021). [Visioconference](#).
- I38. B. Coasne, [Fluid adsorption and diffusion in nanoporous materials](#), *US DOE Res. Center for Enhanced Nanofluidics Transport*, MIT, Boston, USA (2021). [Visioconference](#).
- I37. B. Coasne, [Fluid adsorption and diffusion in nanoporous materials](#), *2021 Biot-Bazant Conferenc eon Engineering Mechanics and Physics of Porous Materials*, Northwestern University, Chicago, USA (2021). [Visioconference](#).
- I36. B. Coasne, [Fluid adsorption and diffusion in nanoporous materials](#), *APS March Meeting*, USA (2021). [Visioconference](#).
- I35. B. Coasne, [Adsorption and diffusion in porous materials](#), *10<sup>th</sup> International Symposium on Heat Transfer*, Beijing, China (2020). [Postponed 2022 due to COVID-19](#).
- I34. B. Coasne, [Adsorption and diffusion in porous materials](#), *8<sup>th</sup> Workshop NIMS-UR1-CNRS-SG*, Tsukuba, Japan (2019).
- I33. B. Coasne, [Multiscale adsorption and transport in porous materials](#), *Workshop Modèles cinétiques pour les milieux poreux*, Bordeaux, France (2019).
- I32. B. Coasne, [Atom-scale simulation of adsorption and transport in nanoporous media \(keynote\)](#), *Symposium on Acoustics of Nanoporous Materials*, Salford University, Manchester, UK (2019).
- I31. B. Coasne, [Multiscale adsorption and transport in porous materials](#), *Colloque Matériaux poreux: Synthèse, Propriétés, Applications*, College de France, Paris, France (2019).



## Benoît Coasne

(CNRS Research Director, Section 15)

- I30. B. Coasne**, [Hydrocarbon adsorption and transport in realistic molecular model of kerogen's structure](#), *2018 MRS International Materials Research Congress*, Cancun, Mexico (2018).
- I29. B. Coasne**, [Adsorption et transport dans les milieux nanoporeux](#), *Journées de la Matière Condensée 2018*, Molecular liquids under micro/mesoporous confinement, Grenoble, France (2018).
- I28. B. Coasne**, [Realistic molecular model of kerogen in gas shales: hydrocarbon adsorption and transport \(keynote 30'\)](#), *Matériaux 2018 – Symposium Matériaux Carbonés*, Strasbourg, France (2018).
- I27. B. Coasne**, [Desorption: drying at the nanoscale?](#), *The Physics of Drying*, Marne-La-Vallée, France (2018).
- I26. B. Coasne**, [Molecular Approach to Adsorption in Multiscale Porous Materials](#), *1st International GFZ edition*, Cabourg, France (2018).
- I25. B. Coasne**, [Oversolubility effects in nanoconfined solvents](#), *2018 MRS International Materials Research Congress*, Cancun, Mexico (2018).
- I24. B. Coasne**, [Modeling Adsorption and Transport in Multiscale Porous Materials](#), *Materials, Characterization, Catalysis*, Zurich, Switzerland (2018).
- I23. B. Coasne**, [Adsorption and Transport in Multiscale Porous Materials](#), *American Institute of Chemical Engineers*, Minneapolis, MN, USA (2017).
- I22. B. Coasne**, [Poroelastic Theory Applied to the Adsorption-Induced Deformation of Vitreous Silica](#) (plenary talk), *6th Biot Conference on Poromechanics*, Paris, France (2017).
- I21. B. Coasne**, [Molecular Modeling of Porous Materials: Structure, Texture and Adsorption Properties](#), *Energy Materials Nanotechnology Mesoporous Materials*, Prague, Czech Republic (2016).
- I20. B. Coasne**, [Adsorption and Transport in Multiscale Porous Media](#), *Multiscale high-performance computational modelling*, EMPA Topical Day, Zurich, Switzerland (2015).
- I19. B. Coasne**, [Atom-scale modelling of elastic and failure properties of clays and clay/organic hybrid materials](#), *Reactive Force Fields: From Development and Implementation to Applications*, RSC Faraday Division and CCP5, Manchester, UK (2015).
- I18. B. Coasne**, [Adsorption and transport in hierarchical porous materials](#), *Fourth Workshop on Zeolites: Prospects & Challenges*, Caen, France (2015).
- I17. B. Coasne**, [Multiscale adsorption and transport in porous materials](#), *6th International Symposium "Advanced microporous and mesoporous materials"*, Black Sea Coast, Bulgaria (2015).
- I16. B. Coasne**, [Adsorption and transport in multiscale porous materials](#), *CECAM Workshop "Simulation of systems under thermodynamic-like gradients"*, Zaragoza, Spain (2015).
- I15. B. Coasne**, [Adsorption and transport in multiscale porous materials](#), *Workshop MultiScale Porous Materials*, San Sebastian, Spain (2014).

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- I13. B. Coasne, [Adsorption and Transport in Hierarchical Zeolites: The view from the NanoScale](#), *1st International Symposium on Energy Challenges and Mechanics*, Aberdeen, Scotland (2014).
- I12. B. Coasne, [A bottom-up model of adsorption and transport in multiscale porous media](#), *American Society of Mechanical Engineering Annual Meeting*, Montreal, Canada (2014).
- I11. B. Coasne, [Crystallization in porous materials: the view from the nanoscale](#), *4<sup>th</sup> International Workshop on Crystallization in Porous Media*, Amsterdam, Netherlands (2014).
- I10. B. Coasne, [Chemistry of interfaces between inorganic minerals and porous carbons: implications for the mechanical properties of gas shale](#), *Society of Engineering Science and American Society of Mechanical Engineering Annual Meetings*, Providence, RI, USA (2013).
- I9. B. Coasne, [“Adsorption, intrusion, and freezing in porous silica: the view from the nanoscale”](#). *3<sup>rd</sup> International Conference on Nanotek (Nanotek 2013)*, Las Vegas, NV, USA.
- I8. B. Coasne, [“Pressure effects in nanoconfined phases”](#). *5<sup>th</sup> Biot Conference on Poromechanics*, Vienna, Austria (2013).
- I7. B. Coasne, [“Adsorption and transport in hierarchical zeolites: the view from the nanoscale”](#). *2<sup>nd</sup> Workshop on Zeolites*, Caen, France (2013).
- I6. B. Coasne, [Adsorption and dynamics of ions confined in nanopores: from simple ions to ionic liquids](#), *CECAM Workshop on Aging of Materials*, Zurich, Switzerland (2012).
- I5. B. Coasne, [“Surface chemistry and performance of carbon materials”](#). *Surface Chemistry and Performance of Carbon materials*, Budapest, Hungary (2012).
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- I3. B. Coasne, [“Simulation moléculaire de l’adsorption et confinement de fluides dans des adsorbants microporeux et mesoporeux”](#). *26<sup>e</sup> Réunion du Groupe Français des Zéolithes*, Presqu’île de Giens, France (2010).
- I2. B. Coasne, [“Development of realistic models of MCM-41 materials for gas adsorption studies”](#). *CECAM Workshop on Surfactant Templated Porous Materials: Synthesis and Characterisation*, Zurich, Switzerland (2008).
- I1. B. Coasne, [“Transition de phase dans des matériaux nanoporeux”](#). *Matériaux Hybrides Organisés Multifonctionnels (HMOM)*, La Grande Motte, France (2006).

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- O170.** B. Coasne, [Confinement de fluides dans des matériaux nanoporeux](#), *Journée des utilisateurs GRICAD*, Grenoble, France (2021).
- O169.** M. Chen, B. Coasne, R. Guyer, D. Derome, J. Carmeliet, [Where lies hysteresis in materials undergoing sorption-induced swelling?](#), *POROTEC*, Germany (2019).
- O168.** A. Gossard, B. Coasne, M. Nidal Ben Abdelouahab, P. Coussot, [Drying thanks to nano-films?](#), *INTERPORE 2019*, Valencia, Spain (2019).
- O167.** A. Schlaich, B. Coasne, [Coupling of Adsorption and Transport in Hierarchical Porous Materials](#), *INTERPORE 2019*, Valencia, Spain (2019).
- O166.** M. Bah, E. D. Manga, P. da Costa, M. Drobek, A. Ayril, G. Despau, E. Le Clezio, A. Julbe, B. Coasne, [Acoustic Footprint of Gas Permeation through Porous Materials](#), *Groupe Français des Zéolithes 2019*, Ile de Porquerolles, France (2019).
- O165.** D. Jin, B. Coasne, [Phase Stability and Formation Kinetics of Methane Hydrate in Nanoporous Media](#), *Fundamentals of Adsorption 2019*, Cairns, Australia (2019).
- O164.** Z. Zaafouri, B. Coasne, G. Batot, C. Nieto-Draghi and D. Bauer, [TRT-Lattice Boltzmann simulation of transport and adsorption in porous media](#), *14th World Congress in Computational Mechanics (WCCM)*, Paris, France (2019).
- O163.** I. C. Medeiros-Costa, C. Laroche, J. Perez-Pellitero, B. Coasne, [Advanced characterization of hierarchical zeolites for optimal xylene separation](#), *Materials, Characterization, and Catalysis Workshop*, Zurich, Switzerland (2018).
- O162.** B. Coasne, [Transport as a tool to characterize multiscale porous media](#), *8th International Workshop on Characterization of Porous Materials: From Ångströms to Millimeters*, Delray Beach, FL (2018).
- O161.** M. Bah, E.D. Manga, M. Drobek, E. Le Clezio, G. Despau, P. Da Costa, A. Ayril, B. Coasne, A. Julbe, [Acoustic emission monitoring: A novel diagnostic tool for characterization of porous ceramic membranes during gas permeation](#), Keynote Oral presentation, *15th International Conference on Inorganic Membranes*, Dresden, Germany (2018).
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- O159.** C. Zhang, B. Coasne, D. Derome, J. Carmeliet, [Hygro-thermo-mechanical behavior of softwood lignin studied by molecular dynamics](#), EMI 2018, Boston, MA, USA (2018).
- O158.** A. C. Bueno, L. Roiban, B. Coasne, Y. Schuurman, M. Klotz, D. Farrusseng, [Materials with oriented hierarchical porosity as catalyst support](#), *12th International Symposium on the Scientific Bases for the Preparation of Heterogeneous Catalysts*, Louvain-la-neuve, Belgium (2018).

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- O156.** D. Jin, B. Coasne, [Effects of Confinement and Surface Force on Methane Hydrate in Porous Media](#), *Interpore 10th Annual Meeting*, New Orleans, LA, USA (2018).
- O155.** B. Coasne, [Adsorption and Transport in Multiscale Porous Media](#), *Interpore 10th Annual Meeting*, New Orleans, LA, USA (2018).
- O154.** M. Bah, E. D. Manga, M. Drobek, E. Le Clezio, G. Despaux, P. Da-Costa, B. Coasne, A. Ayral, A. Julbe, [L'émission acoustique comme outil de diagnostic en temps réel lors de la perméation gazeuse au travers de membranes céramiques poreuses](#), *Journées du Groupe Français de la Céramique 2018*, Bordeaux, France (2018).
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- O151.** M. Chen, B. Coasne, R. Guyer, D. Derome, J. Carmeliet, [A multi-scale study of sorption-induced swelling of wood and related hysteresis](#), Eighteenth European Conference on Composite Materials (ECCM 18), Athens, Greece (2018).
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- O144.** M. Chen, B. Coasne, R. Guyer, D. Derome, J. Carmeliet, [Coupling behavior between adsorption and deformation of nano-porous materials: a multiscale study](#), *9th International Conference on Porous Media*, Rotterdam, Netherlands (2017).

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- O136.** B. Coasne, [Adsorption and Transport in Hierarchical Porous Materials](#), *Workshop Rational Design for Improved Functionalities of Porous Inorganic Materials*, Cavaillon, France (2016).
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- C84.** R. Hartkamp, R. J. M. Pellenq, **B. Coasne**, [Adsorption and transport of ions confined in realistic porous materials: from simple to radioactive ions](#), *9<sup>th</sup> Liquid Matter Conference*, Lisboa, Portugal (2014).
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**C75.** D. Brevet, **B. Coasne**, J. M. Devoisselle, M. In, P. Judeinstein, C. Tourné-Péteilh, A. Vioux, L. Viau, [Aggregation in Water of Unusual Imidazolium-Based Ionic Liquids Containing Ibuprofenate Anion: a Combined Experimental and Molecular Dynamic Study](#), *6<sup>th</sup> Congress on Ionic Liquids*, Algarve, Portugal (2013).

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**C50.** P. Bonnaud, B. Coasne, P. Levitz, R. J. M. Pellenq, [Dynamics of water in hydroxylated and calcium silica nanopores](#). *4<sup>th</sup> International Workshop on Dynamics in Confinement*, Grenoble, France (2010).

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**C39.** P. A. Cazade, J. Dweik, B. Coasne, F. Henn, J. Palmeri, [Dynamics of electrolyte solutions confined in nanopores](#). *Diffusion Fundamentals III: Basic principles of theory, experiment and application*, Athens, Greece (2009).

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- C22.** N. Bibent, N. Fekkar-Nemliche, S. Devautour-Vinot, G. Silly, P. Gaveau, **B. Coasne**, F. Henn, R. Mouawia, A. Mehdi, C. Reye, R. J. P. Corriu, "[Mobilité des charges ioniques dans des silices mésoporeuses fonctionnalisées sous l'influence d'adsorption d'eau](#)". *23<sup>e</sup> Réunion du Groupe Français des Zéolithes*, La Grande Motte, France (2007).
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- C10.** N. Fekkar-Nemmiche, S. Devautour-Vinot, **B. Coasne**, F. Henn, A. Mehdi, C. Reye, R. Corriu, "Water dynamics in silica nanopores from conductivity measurements: Effect of the surface chemistry". *9<sup>th</sup> International Conference on Dielectric and Related Phenomena*, Poznan, Poland (2006).
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- C7.** M. Sliwinska-Bartkowiak, M. Jazdzewska, F. R. Hung, **B. Coasne**, K. E. Gubbins, "Freezing of CCl<sub>4</sub> within carbon nanotubes: a combined experimental and simulation approach". *Thermodynamics 2005*, Sesimbra, Portugal (2005).
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- C5.** S. Bhattacharya, **B. Coasne**, F. R. Hung, K. E. Gubbins, "Modeling and Characterization of Triblock Surfactant Templated Mesoporous Silicas". *7<sup>th</sup> international symposium on the characterization of porous solids*, Aix-en-Provence, France (2005).
- C4.** G. Maurin, **B. Coasne**, A. Nicolas, S. Devautour-Vinot, J. C. Giuntini, F. Henn, "Effect of water adsorption on thermodynamics and dynamics of the extra-framework cations in zeolite systems". *Diffusion Fundamentals: Experiment and Application*, Leipzig, Germany (2005).
- C3.** F. R. Hung, **B. Coasne**, K. E. Gubbins, F. R. Siperstein, M. Sliwinska-Bartkowiak, "Effect of confinement on freezing in cylindrical pores". *8<sup>th</sup> International Conference on Fundamentals of Adsorption*, Sedona, USA (2004).

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**C2. B. Coasne**, A. Grosman, C. Ortega, "[Study of capillary condensation hysteresis in mesoscopic pores: Comparison between adsorption in P + type porous silicon and adsorption in SBA](#)". *6<sup>th</sup> international symposium on the characterization of porous solids*, Alicante, Spain (2002).

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(CNRS Research Director, Section 15)

### 7. Seminars, practical schools (77)

- S77. B. Coasne**, [Adsorption et transport de fluides dans des matériaux nanoporeux](#), *Séminaire donné dans le cadre de la Chaire Innovation du Collège de France (Pr. Lydéric Bocquet)*, Collège de France, Paris, France (2023).
- S76. B. Coasne**, [Adsorption and transport in nanoporous materials](#), *TOTAL Energies*, Pau, France (2022).
- S75. B. Coasne**, [Transport dans les matériaux poreux: de l'échelle nanométrique au milieu continu](#), *TEC21*, Grenoble, France (2022).
- S74.** ["Fluid Adsorption and Transport in Nanoporous Materials"](#), *Manchester University*, Manchester, UK (March 01, 2021). On-line seminar due to COVID-19.
- S73.** ["Fluid Adsorption and Transport in Nanoporous Materials"](#), *Univ. Caen/ENSICAEN*, Caen, France (Feb. 02, 2021).
- S72.** ["Adsorption and Transport in Subnanoporous Media: Theory and Molecular Modeling"](#), *ETH Zurich*, Zurich, Switzerland (February 18, 2020).
- S71.** ["Adsorption and Transport in Multiscale Porous Media"](#), *Oslo University*, Oslo, Norway (August 29, 2019).
- S70.** ["Physique des Gaz de Schiste: Une Vision Moléculaire"](#), *Université François Rabelais de Tours*, Tours, France (March 22, 2018).
- S69.** ["Adsorption and Transport in Multiscale Porous Media"](#), *Université Franche Comté*, Besançon, France (February 12, 2018).
- S68.** ["Adsorption dans les matériaux poreux multiéchelles"](#), *Institut de Chimie et des Matériaux de Paris Est*, Thiais, France (January 13, 2017).
- S67.** ["Adsorption and Transport in Multiscale Porous Media"](#), *Freie Universität*, Berlin, Germany (February 15, 2017).
- S66.** ["Adsorption and Transport in Multiscale Porous Media"](#), *Laboratoire Charles Coulomb*, Montpellier, France (April 18, 2017).
- S65.** ["Adsorption and Transport in Multiscale Porous Media"](#), *New Jersey Institute of Technology*, Newark, NJ, USA (November 06, 2017).
- S64.** ["Adsorption et transport multiéchelles dans les matériaux poreux"](#), *Science et Ingénierie des Matériaux et Procédés*, Grenoble, France (March 24, 2016).
- S63.** ["Adsorption et transport multiéchelles dans les matériaux poreux"](#), *Institut de Physique de Rennes*, Rennes, France (June 06, 2016).
- S62.** ["Adsorption and transport in multiscale porous materials"](#), *IFPEN Rueil Malmaison*, Rueil Malmaison, France (September 22, 2016).
- S61.** ["Adsorption and condensation in porous materials: The view from the nanoscale"](#), *ST Microelectronics*, Crolles-Grenoble, France (October 05, 2016).
- S60.** ["Adsorption and Transport in Multiscale Porous Media"](#), *Montanuniversitaet Leoben*, Leoben, Austria (December 12, 2016).

## Benoît Coasne

(CNRS Research Director, Section 15)

- S59. "[Adsorption et transport multiéchelles dans les solides poreux](#)", *Saint Gobain CREE*, Cavaillon, France (February 12, 2015).
- S58. "[Multiscale Adsorption and Transport in Porous Media](#)", *IBM Almaden Research Center*, San Jose, CA, USA (June 16, 2015).
- S57. "[Caractérisation des milieux poreux](#)", *Saint Gobain CREE*, Cavaillon, France (October 02, 2015).
- S56. "[Freezing in porous materials: the view from the nanoscale](#)", Heriot-Watt University, School of Engineering and Physical Sciences, Edinburgh, Scotland, UK (Janvier 15, 2014).
- S55. "[Adsorption and transport in porous materials: the view from the nanoscale](#)", Gaztransport & Technigaz, Paris, France (May 12, 2014).
- S54. "[Adsorption and freezing in porous media: the view from the nanoscale](#)", *3rd Practical Summer School of Labex Chemisyst – Fondation Balard*, Montpellier, France (Sep. 17-19, 2014).
- S53. "[Adsorption et transport dans les solides poreux hierarchises](#)", *IFP – Energies Nouvelles*, Solaize, France (Sep. 26, 2014).
- S52. "[Adsorption et transport dans les solides poreux hierarchises](#)", *Laboratoire de Physique Interdisciplinaire de Physique (LIPHY)*, Université Joseph Fourier, Grenoble, France (Oct. 02, 2014).
- S51. "[Multiscale Modeling of Amorphous Porous Materials](#)", *Workshop « Materials Modeling »*, Institut Physique Chimie des Matériaux de Strasbourg, Université Strasbourg, France (Oct. 03, 2014).
- S50. "[Adsorption and transport of simple fluids and ionic liquids in porous media](#)", *Laboratoire Leon Brillouin*, CNRS et CEA Saclay, France (Dec. 10, 2014).
- S49. "[Adsorption and transport in porous materials](#)", *ETH - EMPA*, Zurich, Switzerland (May 08, 2013).
- S48. "[Adsorption and transport in porous materials](#)", *CEA Bruyeres le Chatel*, Arpajon, France (June 03, 2013).
- S47. "[Molecular simulation of adsorption and dynamics in nanopores](#)", *2nd Practical Summer School of Labex Chemisyst – Fondation Balard*, Montpellier, France (Jul 04, 2013).
- S46. "[Approche moléculaire de l'adsorption et du transport dans des matériaux poreux](#)", *Saint Gobain CREE*, Cavaillon, France (September 25, 2013).
- S45. "[Adsorption et transport dans les matériaux poreux hiérarchisés](#)", *LASIR*, Lille, France (September 26, 2013).
- S44. "[Freezing in porous materials: the view from the nanoscale](#)", Princeton University, Civil and Environmental Engineering, Princeton, NJ, USA (October 07, 2013).
- S43. "[Molecular simulation of adsorption and dynamics in nanoporous solids](#)", *ETH - EMPA*, Zurich, Switzerland (January 20, 2012).

## Benoît Coasne

(CNRS Research Director, Section 15)

S42. "High pressure effects in nanoconfined phases", Laboratoire Charles Coulomb (L2C), Montpellier, France (February 20, 2012).

S41. "High pressure effects in nanoconfined phases", Laboratoire Physicochimie des Electrolytes, Colloïdes et Sciences Analytiques (PECSA), Université Pierre et Marie Curie, France (April 24, 2012).

S40. "Simulation et modélisation de la dynamique et du transport dans des nanomembranes", Journées Avenir de la filière membranaire en Languedoc-Roussillon, Pole de Compétitivité TRIMATEC Languedoc-Roussillon, France (April 26, 2012).

S39. "High pressure effects in nanoconfined phases", Département de Chimie, Ecole Normale Supérieure de Lyon, France (June 01, 2012).

S38. "High pressure effects in nanoconfined phases", Institut Physique Chimie des Matériaux de Strasbourg, Université Strasbourg, France (June 28, 2012).

S37. "Molecular simulation of adsorption and dynamics of solvents and ions in nanopores", *1st Practical Summer School of Labex Chemisyst – Fondation Balard*, Montpellier/Cevennes, France (2012).

S36. "Simulation de l'adsorption et de la diffusion de molécules dans des solides poreux", Institut de Science des Matériaux de Mulhouse, Mulhouse, France (April 28, 2011).

S35. "Apport de la modélisation moléculaire à l'étude des matériaux", Journée Scientifique Pole Chimie Balard / Saint Gobain, Montpellier, France (Juin 24, 2011).

S34. "Adsorption and dynamics of water and ions confined in nanopores", *6th European Practical School of Separation and Analytical Chemistry of Marcoule*, Marcoule, France (July 2011).

S33. "Modélisation moléculaire multi-échelle des matériaux: propriétés physiques, chimiques et structurales", Saint Gobain CREE, Cavaillon, France (September 09, 2011).

S32. "Le gel de l'eau dans les mésopores du ciment", *Ecole thématique Physique, Chimie et Mécanique des matériaux cimentaires*, La Grande Motte, France (2011).

S31. "Apport de la simulation moléculaire à l'étude des solides poreux", Institut de Recherches sur la Catalyse et l'Environnement (IRCELYon), Lyon, France (April 26, 2010)

S30. "Apport de la simulation moléculaire à l'étude des solides poreux", Laboratoire de Chimie de la Matière Condensée de Paris, Paris, France (May 19, 2010)

S29. "Théorie et modélisation moléculaire: de la molécule au matériau en passant par les architectures moléculaires", *Journée d'échange scientifique entre l'ICGM et l'ICSM*, Marcoule, France (2010).

S28. "Adsorption, freezing and dynamics of fluids confined in nanoporous materials", Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, USA (October 12, 2010)

S27. "Apport de la modélisation moléculaire aux sciences des matériaux", Saint Gobain CREE, Cavaillon, France (July 02, 2009).

## Benoit Coasne

(CNRS Research Director, Section 15)

**S26.** [Theory and molecular modeling of transport in nanoporous membranes](#), *4th European Practical School of Separation Chemistry*, Marcoule, France (2009).

**S25.** [Théorie et modélisation moléculaire: de la molécule au matériau en passant par les architectures moléculaires](#), *Conseil Scientifique de l'Institut Charles Gerbart Montpellier*, Montpellier, France (2009).

**S24.** ["Modélisation moléculaire de l'adsorption, intrusion, structure et dynamique de fluides dans des nanopores"](#), Faculté Polytechnique de Mons, Mons, Belgique (November 17, 2009).

**S23.** ["Adsorption et dynamique de liquides complexes confinés dans des nanopores"](#), Centre Interdisciplinaire des Nanosciences de Marseille, Marseille, France (November 24, 2009)

**S22.** ["Freezing in nanoporous materials"](#), Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC, USA (December 05, 2008).

**S21.** ["Solidification et structure de fluides confinés dans des nanopores"](#), Laboratoire de Physique Théorique, CNRS - Université Paul Sabatier/Toulouse (February 20, 2007).

**S20.** ["Modélisation moléculaire de l'adsorption et intrusion de fluides dans un milieu nanoporeux"](#), Matériaux Divisés, Revêtements, ELectrocéramiques MADIREL, CNRS - Université de Provence (October 11, 2007).

**S19.** ["Modélisation moléculaire de l'adsorption et intrusion de fluides dans un milieu nanoporeux"](#), Laboratoire de Physique de la Matière Condensée et Nanostructures, CNRS – Université Claude Bernard Lyon I (October 12, 2007).

**S18.** ["Molecular modeling of adsorption and intrusion in nanoporous materials"](#), Institute of Physics, Adam Mickiewicz University, Poznan, Poland (October 17, 2007).

**S17.** ["Molecular modeling of adsorption and intrusion in nanoporous materials"](#), Institute of Chemistry, Stranski Laboratory of Physical and Theoretical Chemistry, Technische Universität Berlin, Berlin, Germany (December 11, 2007).

**S16.** ["Transitions de phase de fluides confinés dans des matériaux nanoporeux"](#), Laboratoire de Chimie Physique, CNRS - Université de Paris-Sud Orsay (January 13, 2006).

**S15.** ["Transitions de phase de fluides confinés dans des matériaux nanoporeux"](#), Séminaire Ecole doctorale, CNRS - Université Montpellier 2 (January 19, 2006).

**S14.** ["Cristallisation dans un milieu poreux"](#), Workshop sur la cristallisation en milieu confiné, Centre de Recherche en Matière Condensée et Nanosciences, CNRS – Marseille (September 08, 2006).

**S13.** ["Transitions de phase de fluides confinés dans des matériaux nanoporeux"](#), Laboratoire des Colloïdes, Verres et Nanomatériaux, CNRS - Université Montpellier 2 (November 09, 2006).

**S12.** ["Molecular simulation of phase transitions in nanoporous materials"](#), Institute of Organic Chemistry and Biochemistry, Center for Complex Molecular Systems and Biomolecules, Prague, Czech Republic (September 17, 2005).

## Benoît Coasne

(CNRS Research Director, Section 15)

- S11.** "[Molecular simulation of phase transitions in nanoporous materials](#)", Institute of Physics, Adam Mickiewicz University, Poznan, Poland (September 23, 2005).
- S10.** "[Etude expérimentale et par simulation moléculaire des transitions de phase dans un milieu nanoporeux](#)", Laboratoire de Chimie de l'école normale supérieure de Lyon (December 09, 2003).
- S9.** "[Etude expérimentale et par simulation moléculaire des transitions de phase dans un milieu nanoporeux](#)", Laboratoire Environnement et Minéralurgie, CNRS/INPL (December 11, 2003).
- S8.** "[Etude expérimentale et par simulation moléculaire des transitions de phase dans un milieu nanoporeux](#)", Laboratoire de Physique Moléculaire, CNRS - Université de Franche Comté (December 12, 2003).
- S7.** "[Etude expérimentale et par simulation moléculaire des transitions de phase dans un milieu nanoporeux](#)", Laboratoire de Physico-chimie de la Matière Condensée, CNRS - Université de Montpellier II (December 15, 2003).
- S6.** "[Etude expérimentale et par simulation moléculaire des transitions de phase dans un milieu nanoporeux](#)", Matériaux Divisés, Revêtements, ELectrocéramiques MADIREL, CNRS - Université de Provence (December 17, 2003).
- S5.** "[Etude expérimentale et par simulation moléculaire des transitions de phase dans un milieu nanoporeux](#)", Laboratoire de Chimie Physique, CNRS - Université de Paris-Sud Orsay (December 18, 2003).
- S4.** "[Etude expérimentale et par simulation moléculaire des transitions de phase dans un milieu nanoporeux](#)", Laboratoire de Physique de la Matière Condensée et Nanostructures, CNRS – Université Claude Bernard Lyon I (December 19, 2003).
- S3.** "[Etude de la physisorption/ condensation de gaz dans un matériau mésoporeux](#)", Centre de Recherche sur la Matière Divisée CRMD, CNRS - Université d'Orléans (June 28, 2002).
- S2.** "[Apport des simulations Monte Carlo dans l'ensemble Grand Canonique à l'étude de la physisorption/condensation de gaz dans un matériau mésoporeux](#)", Laboratoire de Physique Moléculaire, CNRS - Université de Franche Comté (December 10, 2002).
- S1.** "[Adsorption dans des pores non interconnectés ouverts à une ou deux extrémités: origine de l'irréversibilité du phénomène de condensation capillaire](#)", Matériaux Divisés, Revêtements, ELectrocéramiques MADIREL, CNRS - Université de Provence (March 04, 2001).



## 8. Participations à des ouvrages ou revues spécialisés (8)

### Science@ifpen est la lettre d'information scientifique d'IFPEN

**D8.** D. Bauer, **B. Coasne**, [Simulation du couplage adsorption/transport via une approche Lattice-Boltzmann](#), Science@IFPEN, Lettre actualité IFP Energies Nouvelles (2023).

**D7.** D. Farrusseng, **B. Coasne**, [Les matériaux nanoporeux: de l'utilité des trous en chimie des matériaux](#), « Etonante Chimie », Editions CNRS (2020).

**D6.** D. Farrusseng, **B. Coasne**, [Les matériaux poreux « Metal Organic Frameworks »](#), Revue Usine Nouvelle (2020).

**D5.** C. Bousige, C. Matei Ghimbeu, C. Vix-Guterl, A. E. Pomerantz, A. Suleimenova, G. Vaughan, G. Garbarino, M. Feygenson, C. Wildgruber, F. -J. Ulm, R.J.-M. Pellenq, **B. Coasne**, [Revealing the molecular structure of kerogen in gas shale](#), *2016 ESRF Highlights*, Matter at Extremes, 124-125 (2017).

**D4.** J. M. Sobstyl, M. J. Abdolhosseini, **B. Coasne**, R. J. M. Pellenq, F. J. Ulm, [Energy management : city texture matters](#), *Concrete Sustainability Hub MIT*, Research Profile Letter October (2012).

**D3.** P. A. Bonnaud, **B. Coasne**, R. J. M. Pellenq, [Le gel de l'eau dans les mésopores du ciment](#), *Ciments, Bétons, Plâtres et Chaux* 907, 64 (2012).

**D2.** **B. Coasne**, [Le triplement du nucléaire doit être débattu](#), *L'Express* (Edition Web), Mar. 12 (2010),  
[http://www.lexpress.fr/actualite/environnement/le-triplement-du-nucleaire-doit-etre-debattu\\_854755.html](http://www.lexpress.fr/actualite/environnement/le-triplement-du-nucleaire-doit-etre-debattu_854755.html)

**D1.** E. Bousquet, **B. Coasne**, [Nous comprenons les consommateurs d'eau en bouteilles](#), *L'Express* (Edition Web), Mar. 12 (2010),  
[http://www.lexpress.fr/actualite/environnement/nous-comprenons-les-consommateurs-d-eau-en-bouteilles\\_854256.html](http://www.lexpress.fr/actualite/environnement/nous-comprenons-les-consommateurs-d-eau-en-bouteilles_854256.html)