

Benoit Coasne

(CNRS Research Director, Section 15)



PART A : CURRICULUM VITAE

Benoit COASNE (Male, 47 ans, 2 children, benoit.coasne@univ-grenoble-alpes.fr)

Laboratoire Interdisciplinaire de Physique,

CNRS/Université Grenoble Alpes, Grenoble, France

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

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

Site Web: benoitcoasne.github.io

Research Theme

« Adsorption, Phase Transitions and Transport in Nanoporous Materials »

Academic Records and Education

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

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

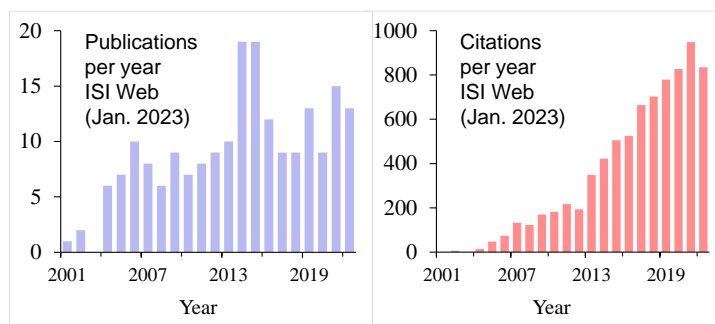
203 Articles (3 Nature Mat, 6 Nat Comm,
2 Chem Soc Rev, 2 PNAS, 2 JACS,
4 PRL., 3 J Phys Chem Lett)

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

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RESPONSIBILITIES, MANAGEMENT AND SCIENTIFIC ANIMATION

Responsibilities, Collective Tasks

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

Commission of Trust

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

Organization of scientific meetings

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

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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. Kelouai, 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. Tabacchini, 12. Z. Zaafour, 13. M. Barbagero, 14. K. Olson, 15. P. Sanchez-Moreno Royer

PhD and Habilitation Jurys (46 including R = Reviewer, P = President)

46. **K. Wang** (P, Montpellier), 45. **HDR R. Semino** (R, Paris), 44. **F. Rizk** (R, Lyon), 44. **K. Ariskina** (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. Hafreager** (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. Louisfremea** (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.

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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

- 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).
- P190.** W. Kellouai, P. Judeinstein, M. Plazanet, J. M. Zanolli, Q. Berrod, M. Drobek, A. Julbe, **B. Coasne**, [Free Volume Theory of Self-diffusion in Zeolite: Molecular simulation and Experiment](#), To be submitted (2022).
- P189.** M. Luciola, 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).

Submitted

- 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.*, To be submitted (2022).
- P187.** C. Zhang, **B. Coasne**, D. Derome, J. Carmeliet, [Adsorption/percolation model for water diffusion in deformable nanoporous polymers](#), To be submitted (2022).

2023

P186. A. J. Souana, 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*, in press (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*, in press (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. Zaafour, 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).

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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 CO₂ 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](#)

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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**, eab8919 (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. Zaafouri, 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 H₂ 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

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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).

P152. Z. Zaafouri, D. Bauer, G. Batot, C. Nieto-Draghi, **B. Coasne**, [Cooperative Effects Dominating the Thermodynamics and Kinetics of Surfactant Adsorption in Porous Media: From Lateral Interactions to Surface Aggregation](#), *J. Phys. Chem. B* **124**, 10841-10849 (2020).

P151. M. Chen, **B. Coasne**, D. Derome, J. Carmeliet, [Coupling of Sorption and Deformation in Soft Nanoporous Polymers: Molecular Simulation and Poromechanics](#), *J. Mech. Phys. Sol.* **137**, 103830 (2020).

P150. C. Hadji, B. Dollet, H. Bodiguel, W. Drenckan, **B. Coasne**, E. Lorenceau, [Impact of fluorocarbon gaseous environments on the permeability of soap films to air](#), *Langmuir* **36**, 13236-13243 (2020).

P149. R. Bey, B. Coasne, C. Picard, [Probing the concept of line tension down to the molecular scale](#), *J. Chem. Phys.* **152**, 094707 (2020).

P148. C. Zhang, A. Shomali, R. Guyer, S. Keten, **B. Coasne**, D. Derome, J. Carmeliet, [Disentangling Heat and Moisture Effects on Biopolymer Mechanics](#), *Macromolecules* **53**, 1527 (2020).

P147. C. Zhang, **B. Coasne**, R. Guyer, D. Derome, J. Carmeliet, [Moisture induced crossover in the thermodynamic and mechanical response of hydrophilic biopolymer](#), *Cellulose* **27**, 89 (2020).

2001 – 2019

P146. A. Monpezat, S. Topin, L. Deliere, D. Farrusseng, **B. Coasne**, [Evaluation methods of adsorbents for air purification and gas separation at low concentration. Case studies on xenon and krypton](#), *Ind. Chem. Eng. Res.* **58**, 4560 (2019).

P145. A. Schlaich, **B. Coasne**, [Dispersion truncation affects the phase behavior of bulk and confined fluids: coexistence, adsorption and criticality](#), *J. Chem. Phys.* **150**, 154104 (2019).

P144. N. Ben Abdelouahab, A. Gossard, S. Rodts, B. Coasne, P. Coussot, [Drying: a simple suction process](#), *Eur. Phys. J. E* **42**, 66 (2019).

Benoit Coasne

(CNRS Research Director, Section 15)

P143. M. Chen, **B. Coasne**, R. Guyer, D. Derome, J. Carmeliet, [Molecular simulation of sorption-induced deformation in atomistic nanoporous materials](#), *Langmuir* **35**, 7751 (2019).

P142. I. C. Medeiros-Costa, C. Laroche, J. Perez-Pellitero, **B. Coasne**, [Characterization of hierarchical zeolites: Combining adsorption/intrusion, electron microscopy, diffraction and spectroscopic techniques \(invited paper; special issue J. Patarin\)](#), *Microsc. Mesop. Mater.* **287**, 167 (2019).

P141. **B. Coasne**, D. Farrusseng, [Gas oversolubility in nanoconfined liquids: Review and perspectives \(invited review paper\)](#), *Microsc. Mesop. Mater.* **288**, 109561 (2019).

P140. M. Santoro, V. Veremeienko, M. Polisi, R. Fantini, F. Alabarse, R. Arletti, S. Quatieri, V. Svitlyk, A. van der Lee, J. Rouquette, B. Alonso, F. Di Renzo, **B. Coasne**, J. Haines, [Insertion and Confinement of H₂O in the hydrophobic siliceous zeolites TON and MFI at high pressure](#), *J. Phys. Chem. C* **123**, 17432 (2019).

P139. M. Chen, C. Zhang, A. Shomali, **B. Coasne**, J. Carmeliet, D. Derome, [Wood-moisture relationships studied with molecular dynamics - methodological guidelines](#), *Forests* **10**, 628 (2019).

P138. G. Gor, **B. Coasne**, [Editorial overview: Separations engineering – Advances in adsorption](#), *Curr. Op. Chem. Eng.* **24**, A4-A6 (2019).

P137. A. Monpezat, G. Couchaux, V. Thomas, A. Artheix, L. Deliere, C. Greau, **B. Coasne**, D. Farrusseng, S. Topin, [Effect of chlorine-containing VOCs on silver migration and sintering in ZSM-5 used in a TSA process](#), *Catalysis* **9**, 686 (2019).

P136. I. Deroche, C. Picard, T. J. Daou, **B. Coasne**, [Reminiscent Capillarity in Subnanopores](#), *Nature Comm.* **10**, 4642 (2019).

+ CNRS communication: <https://inc.cnrs.fr/index.php/fr/cnrsinfo/materiaux-poreux-capillarite-persistante-lechelle-moleculaire>

+ Nature Comm. Editor's highlight: <https://www.nature.com/articles/s41467-019-12418-9>

P135. M. Brun-Cosme-Bruny, E. Bertin, **B. Coasne**, P. Peyla, S. Rafai, [Effective diffusivity of microswimmers in a crowded environment](#), *J. Chem. Phys.* **150**, 104901 (2019).

P134. M. Bah, E. D. Manga, H. Blasco, P. Da Costa, M. Drobek, **B. Coasne**, A. Ayrál, G. Despaux, E. Le Clezio, A. Julbe, [Characterization of porous ceramic membranes by acoustic emission monitoring during gas permeation](#), *J. Membrane Sci.* **555**, 88 (2018).

P133. J. M. Thibaud, J. Rouquette, K. Dziube, F. A. Gorelli, M. Santoro, G. Garbarino, S. Clément, O. Cambon, A. van der Lee, F. Di Renzo, **B. Coasne**, J. Haines, [Saturation of the siliceous zeolite TON with neon at high-pressure](#), *J. Phys. Chem. C* **122**, 8455 (2018).

P132. Z. Chaker, A. Bouzid, **B. Coasne**, C. Massobrio, M. Boero, G. Ori, [The structure and dipolar properties of CO₂ adsorbed in a porous glassy chalcogel: insights from first-principles molecular dynamics](#), *J. Non Cryst. Sol.* **498**, 288 (2018).

Benoit Coasne

(CNRS Research Director, Section 15)

P131. M. Chen, **B. Coasne**, J. Carmeliet, D. Derome, [Role of hydrogen bonding in hysteresis observed in sorption-induced swelling of soft nanoporous polymers](#), *Nature Comm.* **9**, 3507 (2018).

+ Nature Comm. Editor's highlight: <https://www.nature.com/articles/s41467-018-05897-9>

+ CNRS communication: <https://inp.cnrs.fr/fr/cnrsinfo/pourquoi-le-gonflement-de-la-cellulose-lors-de-son-hydratation-est-irreversible>

P130. D. Mehlhorn, J. Rodriguez, T. Cacciaguerra, A. Radu-Dorin, F. Guenneau, A. Gedeon, **B. Coasne**, M. Thommes, D. Minoux, C. Aquino, J.-P. Dath, F. Fajula, A. Galarneau, [Revelation on the complex nature of mesoporous FAU-Y zeolites](#), *Langmuir* **34**, 11414 (2018).

P129. L. Bruschi, G. Mistura, F. Negri, **B. Coasne**, Y. Mayamei, W. Lee, [Adsorption on alumina conical nanopores](#), *Nanoscale* **10**, 18300 (2018).

P128. A. Galarneau, D. Mehlhorn, F. Guenneau, **B. Coasne**, F. Villemot, D. Minoux, C. Aquino, J.-P. Dath, [Specific surface area determination of microporous/mesoporous materials: the case of mesoporous FAU-Y zeolites](#), *Langmuir* **34**, 14134 (2018).

P127. I. Maruyama, J. Rymes, M. Vandamme, **B. Coasne**, [Cavitation in hardened cement paste under short-term desorption measurements](#), *Materials and Structures* **51**, 159 (2018).

P126. V. Kaiser, J. Comtet, A. Nigues, A. Siria, **B. Coasne**, L. Bocquet, [Electrostatic interactions between ions near Thomas-Fermi substrates and the surface energy of ionic crystal at imperfect metals](#), *Faraday Discussions* **199**, 129-158 (2017).

P125. J. Comtet, A. Nigues, V. Kaiser, **B. Coasne**, L. Bocquet, A. Siria, [Nanoscale capillary freezing of ionic liquids confined between metallic interfaces and the role of electronic screening](#), *Nature Materials* **16**, 634 (2017).

P124. A. Vioux, **B. Coasne**, [From Ionogels to Biredox Ionic Liquids: Some Emerging Opportunities for Electrochemical Energy Storage and Conversion Devices](#), *Adv. Energy Mater.*, 1700883 (2017).

P123. G. Hantal, L. Brochard, R. J. M. Pellenq, F. -J. Ulm, **B. Coasne**, [Role of Interfaces in Elasticity and Failure of Clay-Organic Nanocomposites: Toughening upon Interface Weakening?](#), *Langmuir* **33**, 11457 (2017).

P122. D. Jin, **B. Coasne**, [Molecular Simulation of the Phase Diagram of Methane Hydrate: Free Energy Calculations, Direct Coexistence Method, and Hyper Parallel Tempering](#), *Langmuir* **33**, 11217 (2017).

P121. J. S. Bender, J. T. Fourkas, **B. Coasne**, [On the Empirical Analysis of Optical Kerr Effect Spectra: A Case for Constraint](#), *J. Phys. Chem. C* **121**, 11376 (2017).

P120. A. Galarneau, F. Guenneau, A. Gedeon, D. Mereib, J. Rodriguez, F. Fajula, **B. Coasne**, [Probing Interconnectivity in Hierarchical Microporous/Mesoporous Materials using Adsorption and Nuclear Magnetic Resonance Diffusion](#), *J. Phys. Chem. C* **120**, 1562 (2016).

Benoit Coasne

(CNRS Research Director, Section 15)

P119. A. Galarneau, A. Sasche, B. Said, C. H. Pelisson, P. Boscaro, N. Brun, L. Courthoux, N. Olivi-Tran, **B. Coasne**, F. Fajula, [Hierarchical Porous Silica Monoliths: a Novel Class of Microreactors for Process intensification in Catalysis and Adsorption](#), *Comptes Rendus Chimie* **19**, 231 (2016).

P118. C. Bousige, C. Ghimbeu, C. Vix, A. E. Pomerantz, A. Suleimenova, G. Vaughan, G. Garbarino, M. Feygenson, C. Wildgruber, F. J. Ulm, R. J. M. Pellenq, **B. Coasne**, [Realistic molecular model of kerogen's nanostructure](#), *Nature Materials* **15**, 576-582 (2016).

+ CNRS Communication Release: <http://www.cnrs.fr/inp/spip.php?article4297>

+ ESRF Highlight www.esrf.fr/home/UsersAndScience/Publications/Highlights/highlights-2016/MEX/MEX09.html

P117. S. Hocine, R. Hartkamp, B. Siboulet, M. Duvail, **B. Coasne**, P. Turq, J. F. Dufrêche, [How ion condensation occurs at a charged surface: a molecular dynamics investigation of the Stern layer for water-silica interfaces](#), *J. Phys. Chem. C* **120**, 963 (2016).

P116. **B. Coasne**, [Multiscale adsorption and transport in hierarchical porous materials \(perspective paper\)](#), *New J. Chem.* **40**, 4078-4094 (2016).

P115. L. Deliere, **B. Coasne**, S. Topin, C. Greau, C. Moulin, D. Farrusseng, [Break-through in Xenon Capture and Purification Using Adsorbent-Supported Silver Nanoparticles](#), *Chem. A Eur. J.* **22**, 9660-9666 (2016).

P114. L. Deliere, F. Villemot, D. Farrusseng, A. Galarneau, S. Topin, **B. Coasne**, [Adsorption in heterogeneous microporous materials](#), *Microsp. Mesosp. Mater.* **229**, 145-154 (2016).

P113. T. Lee, L. Bocquet, **B. Coasne**, [Activated desorption at heterogeneous interfaces and long-time kinetics of hydrocarbon recovery from nanoporous media](#), *Nature Comm* **7**, 11890 (2016).

P112. G. Ori, C. Massobrio, A. Pradel, M. Ribes, **B. Coasne**, [Nanoporous chalcogenides for adsorption and gas separation](#), *Phys. Chem. Chem. Phys.* **18**, 13449-13458 (2016).

P111. J. Bender, S. Cohen, X. He, J. Fourkas, **B. Coasne**, [Toward In Situ Measurement of the Density of Liquid Benzene using Optical Kerr Effect Spectroscopy](#), *J. Phys. Chem. B* **120**, 9103 (2016).

P110. A. Obliger, R. J. M. Pellenq, F. J. Ulm, **B. Coasne**, [Free Volume Theory of Hydrocarbon Mixture Transport in Nanoporous Materials](#), *J. Phys. Chem. Lett.* **7**, 3712 (2016).

P109. J. S. Bender, **B. Coasne**, J. T. Fourkas, [Assessing Polarizability Models for the Simulation of Low-Frequency Raman Spectra of Benzene](#), *J. Phys. Chem. B* **119**, 9345 (2015).

P108. F. G. Alabarse, J. Rouquette, **B. Coasne**, A. Haidoux, C. Paulmann, O. Cambron, J. Haines, [Mechanism of H₂O Insertion and Chemical Bond Formation in AlPO₄-54.xH₂O at high pressure](#), *J. Am. Chem. Soc.* **137**, 584 (2015).

Benoit Coasne

(CNRS Research Director, Section 15)

- P107.** B. Coasne, [Effect of surface texture on freezing of argon in nanopores: Surface-induced versus homogeneous crystallization](#), *Langmuir* **37**, 2706 (2015).
- P106.** M. Lepinay, L. Broussous, K. Courouble, C. Licitra, F. Bertin, V. Rouessac, A. Ayral, B. Coasne, [Predicting Adsorption on Bare and Modified Silica Surfaces](#), *J. Phys. Chem. C* **119**, 6009 (2015).
- P105.** A. Botan, B. Coasne, R. Pellenq, F. J. Ulm, [A bottom-up approach of multiscale transport in porous media](#), *Phys. Rev. E* **91**, 032133 (2015).
- P104.** C. Bousige, A. Botan, F. -J. Ulm, R. J.-M. Pellenq, B. Coasne, [Optimized atomic reconstruction procedure combining Hybrid Reverse Monte Carlo and Molecular Dynamics](#), *J. Chem. Phys.* **142**, 114112 (2015).
- P103.** K. Falk, B. Coasne, R. Pellenq, F. -J. Ulm, L. Bocquet, [Subcontinuum mass transport of condensed hydrocarbons in nanoporous media](#), *Nature Comm.* **6**, 6949 (2015).
- P102.** M. L. Bocquet, B. Coasne, R. Pellenq, F. J. Ulm, [Organic-clay interfacial chemical bonds probed by ab initio calculations](#), *J. Phys. Chem. C* **119**, 6511 (2015).
- P101.** M. Lepinay, L. Broussous, C. Licitra, F. Bertin, V. Rouessac, A. Ayral, B. Coasne, [Probing the microporosity of low-k organosilica films: MP and t-plot methods applied to ellipsometric porosimetry data](#), *Microp. Mesop. Mater.* **217**, 119 (2015).
- P100.** G. Ori, C. Massobrio, A. Pradel, M. Ribes, [Structure and Dynamics of Ionic Liquids Confined in Amorphous Porous Chalcogenides](#), *Langmuir* **31**, 6742 (2015).
- P99.** M. Barboiu, P. A. Cazade, Y. Le Duc, Y. M. Legrand, A. van der Lee, B. Coasne, [Polarized water-wires under confinement inside chiral nanochannels](#), *J. Phys. Chem. B* **119**, 8707 (2015).
- P98.** E. Secret, C. C. Wu, A. Chaix, A. Galarneau, P. Gonzalez, D. Cot, M. J. Sailor, J. Jestin, J. M. Zanolli, F. Cunin, B. Coasne, [Control of the Pore Texture in Nanoporous Silicon via Chemical Dissolution](#), *Langmuir* **31**, 8121 (2015).
- P97.** A. Ayral, S. Calas-Etienne, B. Coasne, A. Deratani, A. Evstratov, A. Galarneau, D. Grande, M. Hureau, H. Jobic, C. Morlay, J. Parmentier, B. Prelot, S. Rossignol, A. Simon-Masseron, F. Thibault-Starzyk, [Advances in Design and Modeling of Porous Materials](#), *Eur. Phys. J. Special Topics* **224**, 1653 (2015).
- P96.** L. Ho, Y. Schuurman, D. Farrusseng, B. Coasne, [Solubility of Gases in Water Confined in Nanoporous Materials: ZSM-5, MCM-41, MIL-100](#), *J. Phys. Chem. C* **119**, 21547 (2015).
- P95.** R. Hartkamp, B. Siboulet, J. F. Dufreche, B. Coasne, [Ion-Specific Adsorption and Electroosmosis in Charged Amorphous Porous Silica](#), *Phys. Chem. Chem. Phys.* **17**, 24683 (2015).
- P94.** A. Ayral, S. Calas-Etienne, B. Coasne, A. Deratani, D. Grande, D. Quemener, S. Rossignol, [Les matériaux poreux : un domaine scientifique et technologique pluridisciplinaire au futur radieux](#), *Matériaux et Techniques* **103**, 701 (2015).

Benoit Coasne

(CNRS Research Director, Section 15)

- P93.** K. Falk, R. Pellenq, F. J. Ulm, **B. Coasne**, [Effect of Chain Length and Pore Accessibility on Alkane Adsorption in Kerogen](#), *Energy Fuels* **29**, 7889 (2015).
- P92.** **B. Coasne**, K. E. Gubbins, Y. Long, [Pressure effects in confined nanophases \(Invited review paper\)](#), *Mol. Simul.* **40**, 721 (2014).
- P91.** K. I. Falk, **B. Coasne**, R. J. M. Pellenq, [Effect of temperature on adsorption of mixtures in porous materials](#), *Mol. Simul.* **40**, 45 (2014).
- P90.** C. Tourne-Peteilh, **B. Coasne**, M. In, D. Brevet, J. –M. Devoisselle, A. Vioux, L. Viau, [Surfactant Behavior of Ionic Liquids Involving a Drug: From Molecular Interactions to Self-Assembly](#), *Langmuir* **30**, 1229 (2014).
- P89.** P. Billemont, **B. Coasne**, G. De Weireld, [Adsorption of carbon dioxide-methane mixture in porous carbons: effect of surface chemistry](#), *Adsorption* **20**, 453 (2014).
- P88.** P. A. Cazade, R. Hartkamp, **B. Coasne**, [Structure and dynamics of an electrolyte solution confined in charged nanopores](#), *J. Phys. Chem. C* **118**, 5061 (2014).
- P87.** G. Ori, F. Villemot, L. Viau, A. Vioux, **B. Coasne**, [Ionic liquid confined in silica nanopores: Molecular Dynamics in the isobaric-isothermal ensemble](#), *Mol. Phys.* **112**, 1350 (2014).
- P86.** F. Villemot, A. Galarneau, **B. Coasne**, [Adsorption-based characterization of hierarchical metal-organic frameworks](#), *Adsorption* **20**, 349 (2014).
- P85.** G. Hantal, L. Brochard, H. Laubie, D. Ebrahimi, R. J.-M. Pellenq, F. J. Ulm, **B. Coasne**, [Atomic-scale modeling of elastic and failure properties of clays](#), *Mol. Phys.* **112**, 1294 (2014).
- P84.** F. Villemot, A. Galarneau, **B. Coasne**, [Adsorption and dynamics in hierarchical Metal Organic Frameworks](#), *J. Phys. Chem. C* **118**, 7423 (2014).
- P83.** J. Canivet, J. Bonnefoy, C. Daniel, **B. Coasne**, D. Farrusseng, [Structure-property relationships of water adsorption in Metal-Organic Frameworks](#), *New J. Chem.* **38**, 3102 (2014).
- P82.** S. Clauzier, L. Ngoc Ho, M. Pera-Titus, D. Farrusseng, **B. Coasne**, [Enhanced H₂ solubility in n-alkane confined in mesoporous materials](#), *J. Phys. Chem. C* **118**, 10720 (2014).
- P81.** M. Barboiu, A. Gilles, Y. Le Duc, P. A. Cazade, M. Michau, Y. M. Legrand, A. Van der Lee, **B. Coasne**, J. Post, T. Fyles, [An artificial primitive mimic of the Gramicidin-A channel](#), *Nature Comm.* **5**, 4142 (2014).
- P80.** J. Canivet, A. Fateeva, Y. Guo, **B. Coasne**, D. Farrusseng, [Water adsorption in MOFs: fundamentals and applications \(Invited review paper\)](#), *Chem. Soc. Rev.* **43**, 5594 (2014).
- P79.** G. Ori, C. Massobrio, A. Bouzid, M. Boero, **B. Coasne**, [Surface of glassy GeS₂: a model based on a first-principles approach](#), *Phys. Rev. B* **90**, 045423 (2014).
- P78.** E. D. Manga, H. Blasco, P. Da Costa, M. Drobek, A. Ayral, E. Le Clezio, G. Despaux, **B. Coasne**, A. Julbe, [Effect of Gas Adsorption on Acoustic Propagation in Zeolites: Experiment and Molecular Simulation](#), *Langmuir* **30**, 10336 (2014).

Benoit Coasne

(CNRS Research Director, Section 15)

- P77.** R. Hartkamp, **B. Coasne**, [Structure and transport of aqueous electrolytes: from simple halides to radionuclide ions](#), *J. Chem. Phys.* **141**, 124508 (2014).
- P76.** L. Deliere, S. Topin, **B. Coasne**, D. Farrusseng, J. P. Fontaine, S. De Vito, C. Den Auwer, P. L. Solari, C. Daniel, Y. Schuurman, [Role of Silver Nanoparticles in Enhanced Xenon Adsorption using Silver loaded Zeolites](#), *J. Phys. Chem. C* **118**, 25032 (2014).
- P75.** A. Galarneau, F. Villemot, J. Rodriguez, F. Fajula, **B. Coasne**, [Validity of the t-plot Method to Assess Microporosity in Hierarchical Micro/Mesoporous Materials](#), *Langmuir* **30**, 13266 (2014).
- P74.** **B. Coasne**, C. Weigel, A. Polian, M. Kint, J. Rouquette, J. Haines, M. Foret, R. Vacher, B. Ruffle, [Poroelastic Theory Applied to the Adsorption-induced Deformation of Vitreous Silica](#), *J. Phys. Chem. B* **118**, 14519 (2014).
- P73.** **B. Coasne**, A. Galarneau, R. J. M. Pellenq, F. Di Renzo, [Adsorption, intrusion and freezing in porous silica: the view from the nanoscale \(Invited review paper\)](#), *Chem. Soc. Rev.* **42**, 4141 (2013).
- P72.** P. Billemont, **B. Coasne**, G. De Weireld, [Adsorption of carbon dioxide, methane, and their mixture in porous carbons: effect of surface chemistry, water content and pore disorder](#), *Langmuir* **29**, 3328 (2013).
- P71.** A. F. Cosseron, T. J. Daou, L. Tzanis, H. Nouali, I. Deroche, **B. Coasne**, V. Tchaber, J. Patarin, [Adsorption of Volatile Organic Compounds in pure silica CHA, *BEA, MFI and STT-type zeolites](#), *Microsp. Mesop. Mater.* **173**, 144, (2013).
- P70.** P. Epicoco, **B. Coasne**, A. Gioia, P. Papet, I. Cabodi, M. Gaubil, [Mesoscopic Monte Carlo simulations of microstructure and conductivity of ZrO₂-glass composites](#), *Acta Materialia* **61**, 5018 (2013).
- P69.** **B. Coasne**, A. Galarneau, C. Gerardin, F. Fajula, F. Villemot, [Molecular simulation of adsorption and transport in hierarchical porous materials](#), *Langmuir* **29**, 7864 (2013).
- P68.** L. N. Ho, S. Clauzier, Y. Schuurman, D. Farrusseng, **B. Coasne**, [Gas uptake in solvents confined in mesopores: Adsorption versus enhanced solubility](#), *J. Phys. Chem. Lett.* **4**, 2274 (2013).
- P67.** P. Levitz, P. A. Bonnaud, P. A. Cazade, R. J. M. Pellenq, **B. Coasne**, [Molecular intermittent dynamics of interfacial water: probing adsorption and bulk confinement](#), *Soft Matter* **9**, 8654 (2013).
- P66.** Y. Long, J. C. Palmer, **B. Coasne**, M. Sliwinska-Bartkowiak, G. Jackson, E. A. Muller, K. E. Gubbins, J. C. Palmer, M. Sliwinska-Bartkowiak, [On the Molecular Origin of High Pressure Effects in Nanoconfinement: Effects of Surface Chemistry and Roughness](#), *J. Chem. Phys.* **139**, 144701 (2013).
- P65.** M. Celino, S. Le Roux, A. Bouzid, G. Ori, **B. Coasne**, M. Boero, C. Massobrio, [First-principles molecular dynamics study of glassy GeS₂: Atomic structure and bonding properties](#), *Phys. Rev. B* **88**, 174201 (2013).

Benoit Coasne

(CNRS Research Director, Section 15)

- P64.** B. Siboulet, **B. Coasne**, J. F. Dufreche, J. Molina, P. Turq, [Influence of hydrophilicity on water self-diffusion at irradiated glass interfaces](#) (invited paper), *Mol. Phys.* **111**, 3410 (2013).
- P63.** J. Dweik, **B. Coasne**, J. Palmeri, P. Jouanna, P. Gouze, [Inner and subsurface distribution of water and ions in weakly and highly hydrophilic uncharged nanoporous materials: a molecular dynamics study of a confined NaI electrolyte solution](#), *J. Phys. Chem. C* **116**, 726 (2012).
- P62.** Y. Long, J. C. Palmer, **B. Coasne**, M. Sliwinska-Bartkowiak, K. E. Gubbins, [Under pressure : Quasi-high pressure effects in nanopores](#), *Microsp. Mesop. Mater.* **154**, 19 (2012).
- P61.** A. Sachse, R. Ameloot, B. Coq, F. Fajula, **B. Coasne**, D. De Vos, A. Galarneau, [In situ synthesis of Cu-BTC \(HKUST-1\) in macro/mesoporous silica monoliths for continuous flow catalysis](#), *Chem. Comm.* **48**, 4749 (2012).
- P60.** A. Boutin, **B. Coasne**, A. H. Fuchs, A. Galarneau, F. Di Renzo, [Experiment and Theory of Low Pressure Nitrogen Adsorption in Organic Layers Supported or Grafted on Inorganic Adsorbents: Towards a Tool to Characterize Surfaces of Hybrid Organic/Inorganic Systems](#), *Langmuir* **28**, 9526 (2012).
- P59.** F. Alabarse, J. Haines, O. Cambon, C. Levelut, D. Bourgoigne, A. Haidoux, D. Granier, **B. Coasne**, [Freezing of water confined at the nanoscale](#), *Phys. Rev. Lett.* **109**, 035701 (2012).
- P58.** P. A. Bonnaud, Q. Li, **B. Coasne**, R. J. M. Pellenq, K. J. Van Vliet, [Thermodynamics of water confined in porous calcium-silicate-hydrates](#), *Langmuir* **28**, 11422 (2012).
- P57.** **B. Coasne**, P. Ugliengo, [Atomistic model of micelle-templated mesoporous silicas: structural, morphological and adsorption properties](#), *Langmuir*, **28**, 11131 (2012).
- P56.** P. A. Bonnaud, **B. Coasne**, R. J. M. Pellenq, [Solvated Calcium Ions in Charged Silica Nanopores](#), *J. Chem. Phys.* **137**, 064706 (2012).
- P55.** S. Clauzier, L. Ngoc Ho, M. Pera-Titus, **B. Coasne**, D. Farrusseng, [Enhanced H₂ uptake in solvents confined in mesoporous metal-organic framework](#), *J. Am. Chem. Soc.* **134**, 17369 (2012).
- P54.** **B. Coasne**, R. Metz, [Mesoscopic Monte Carlo simulations of interfacial films in ZnO-Bi₂O₃ ceramics](#), *J. Eur. Ceram. Soc.* **311**, 597 (2011).
- P53.** P. Billefont, **B. Coasne**, G. De Weireld, [An experimental and molecular simulation study of the adsorption of carbon dioxide and methane in nanoporous carbons in presence of water](#), *Langmuir* **27**, 1015 (2011).
- P52.** **B. Coasne**, C. Alba-Simionesco, F. Audonnet, G. Dosseh, K. E. Gubbins, [Adsorption, structure, and dynamics of benzene in ordered and disordered porous carbons](#), *Phys. Chem. Chem. Phys.* **13**, 3748 (2011).
- P51.** **B. Coasne**, L. Viau, A. Vioux, [Loading-controlled stiffening in nanoconfined ionic liquids](#), *J. Phys. Chem. Lett.* **2**, 1150 (2011).

Benoit Coasne

(CNRS Research Director, Section 15)

- P50.** B. Siboulet, **B. Coasne**, J. F. Dufrêche, P. Turq, [Hydrophobic Transition in Porous Amorphous Silica](#), *J. Phys. Chem. B* **115**, 7881 (2011).
- P49.** **B. Coasne**, J. T. Fourkas, [Structure and dynamics of benzene confined in silica nanopores](#), *J. Phys. Chem. C* **115**, 15471 (2011).
- P48.** Y. Long, J. C. Palmer, **B. Coasne**, M. Sliwinska-Bartkowiak, K. E. Gubbins, [Pressure enhancement in nanopores: a major confinement effect](#), *Phys. Chem. Chem. Phys.* **13**, 17163 (2011).
- P47.** **B. Coasne**, J. Haines, C. Levelut, O. Cambon, M. Santoro, F. Gorelli, G. Garbarino, [Enhanced mechanical strength of zeolites by adsorption of guest molecules](#), *Phys. Chem. Chem. Phys.* (communication) **13**, 20096 (2011).
- P46.** C. Abrioux, S. Balme, **B. Coasne**, S. Devautour-vinot, M. Kharroubi, G. Maurin, F. Henn, [Effect of water adsorption on ion dynamics in confined geometry: Na⁺ faujasites and homoionic alkali exchanged montmorillonite](#), *J. Phys. Soc. Jpn* **79**, 19 (2010).
- P45.** P. Bonnaud, **B. Coasne**, R. J. M. Pellenq, [Molecular simulation of water confined in nanoporous silica](#), *J. Phys. Condens. Matter* **22**, 284110 (2010).
- P44.** **B. Coasne**, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, [Molecular simulation of nitrogen adsorption in nanoporous silica](#), *Langmuir* **26**, 10872 (2010).
- P43.** L. Bruschi, G. Mistura, L. Liu, W. Lee, U. Gosele, **B. Coasne**, [Capillary condensation and evaporation in ordered nanopores with controlled modulations](#), *Langmuir* **26**, 11894 (2010).
- P42.** P. -A. Cazade, J. Dweik, **B. Coasne**, F. Henn, J. Palmeri, [Molecular simulation of ion-specific effects in confined electrolyte solutions using polarizable forcefields](#), *J. Phys. Chem. C* **114**, 12245 (2010).
- P41.** D. Horlait, **B. Coasne**, A. Mezy, D. Ravot, J. C. Tedenac, [Zinc oxide nanostructures confined in carbon nanotubes](#), *Mol. Sim.* **36**, 1045 (2010).
- P40.** **B. Coasne**, J. Czwartos, M. Sliwinska-Bartkowiak, K. E. Gubbins, [Freezing of mixtures confined in silica nanopores: Experiment and molecular simulation](#), *J. Chem. Phys.* **133**, 08470 (2010).
- P39.** B. Ratajczak, M. Sliwinska-Bartkowiak, T. Koziol, **B. Coasne**, K. E. Gubbins, [An apparent critical point in binary mixtures of nitrotoluene with alkanes: experimental and simulation study](#), *J. Comp. Meth. Sc. Eng.* **10**, 561 (2010).
- P38.** R. J. M. Pellenq, **B. Coasne**, R. Denoyel, O. Coussy, [Simple Phenomenological Model for Phase Transitions in Confined Geometry. 2: Capillary Condensation/Evaporation in Cylindrical Nanopores](#), *Langmuir* **25**, 1393 (2009).
- P37.** S. Bhattacharya, **B. Coasne**, F. R. Hung, K. E. Gubbins, [Modeling Micelle-Templated Mesoporous Material SBA-15: Atomistic Model and Gas Adsorption Studies](#), *Langmuir*, **25**, 5802 (2009).

Benoit Coasne

(CNRS Research Director, Section 15)

- P36. B. Coasne**, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, [Intrusion and retraction of fluids in nanopores: Effect of morphological heterogeneity](#), *J. Phys. Chem. C* **113**, 1953 (2009).
- P35. B. Coasne**, A. Mezy, R. J. M. Pellenq, D. Ravot, J. C. Tedenac, [Zinc oxide nanostructures confined in porous silicas](#), *J. Am. Chem. Soc.* **131**, 2185 (2009).
- P34. A. Galarneau**, N. Calin, J. Iapichella, M. Barrande, R. Denoyel, **B. Coasne**, F. Fajula, [Optimization of the properties of macroporous chromatography silica supports through surface roughness control](#), *Chem. Mater.* **21**, 1884 (2009).
- P33. C. Abrioux**, **B. Coasne**, G. Maurin, F. Henn, M. Jeffroy, A. Boutin, [Cation behavior in Faujasite zeolites upon water adsorption: A combination of Monte Carlo and Molecular Dynamics simulations](#), *J. Phys. Chem. C* **113**, 10696 (2009).
- P32. B. Coasne**, C. Alba-Simionesco, F. Audonnet, G. Dosseh, K. E. Gubbins, [Adsorption and structure of benzene on silica surfaces and nanopores](#), *Langmuir* **25**, 10648 (2009).
- P31. B. Coasne**, J. Czwartos, M. Sliwinska-Bartkowiak, K. E. Gubbins, [Effect of pressure on freezing of pure fluids and mixtures confined in nanopores](#), *J. Phys. Chem. B* **113**, 13874 (2009).
- P30. J. Czwartos**, M. Sliwinska-Bartkowiak, **B. Coasne**, K. E. Gubbins, [Melting of mixtures confined in nanoporous silicas](#), *Pure Appl. Chem.* **81**, 1953 (2009).
- P29. B. Coasne**, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, [Molecular simulation of adsorption and intrusion in nanopores](#), *Adsorption* **14**, 215 – 221 (2008).
- P28. B. Kuchta**, L. Firlej, R. Denoyel, S. Rols, M. R. Johnson, **B. Coasne**, [Melting mechanism of monolayers adsorbed in cylindrical pores: The influence of the pore wall roughness](#), *J. Chem. Phys.* **128**, 184703 (2008).
- P27. C. Abrioux**, **B. Coasne**, G. Maurin, F. Henn, A. Boutin, A. Di Lella, C. Nieto-Draghi, Ph. Ungerer, A. H. Fuchs, [A molecular simulation study of the cation distribution in zeolites](#), *Adsorption* **14**, 743 (2008).
- P26. B. Coasne**, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, [Adsorption of simple fluid on silica surface and nanopore: Effect of surface chemistry and pore shape](#), *Langmuir* **24**, 7285 (2008).
- P25. A. Galarneau**, B. Lefevre, H. Cambon, **B. Coasne**, S. Valange, Z. Gabelica, J. P. Bellat, F. Di Renzo, [Pore-shape effects in the determination of the pore size of ordered mesoporous silicas by nitrogen adsorption and mercury intrusion](#), *J. Phys. Chem. C* **112**, 12921 (2008).
- P24. B. Coasne**, S. K. Jain, L. Naamar, K. E. Gubbins, [Freezing of argon in ordered and disordered porous carbons](#), *Phys. Rev. B* **76**, 085416 (2007).
- P23. B. Ratajczak**, M. Sliwinska-Bartkowiak, **B. Coasne**, K. E. Gubbins, [Apparent critical point in binary mixtures of m-nitrotoluene and n-alkanes: Experimental and simulation study](#), *J. Non Crystal. Sol.* **353**, 4565 – 4569 (2007).

Benoit Coasne

(CNRS Research Director, Section 15)

P22. B. Coasne, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, [Effect of morphological defects on gas adsorption in nanoporous silicas](#), *J. Phys. Chem. C*, **111**, 15759 – 15770 (2007).

P21. B. Coasne, C. Alba-Simionesco, F. Audonnet, G. Dosseh, K. E. Gubbins, [Molecular simulation of the adsorption and structure of benzene confined in mesoporous silicas](#), *Adsorption* **13**, 485 - 490 (2007).

P20. F. R. Hung, **B. Coasne**, S. Bhattacharya, M. Thommes, K. E. Gubbins, [Argon and Krypton adsorption on templated mesoporous silicas: Molecular simulation and experiment](#), *Adsorption* **13**, 425 – 437 (2007).

P19. B. Coasne, F. R. Hung, R. J. –M Pellenq, F. R. Siperstein, K. E. Gubbins, [Adsorption of simple gases in MCM-41 materials: the role of surface roughness](#), *Langmuir* **22**, 194 (2006).

P18. C. Alba-Simionesco, **B. Coasne**, G. Dosseh, G. Dudziak, K. E. Gubbins, R. Radhakrishnan, M. Sliwinska-Bartkowiak, [Effects of Confinement on Freezing and Melting \(Invited review paper\)](#), *J. Phys.: Condens. Matter* **18**, R15 – R68 (2006).

P17. B. Coasne, K. E. Gubbins, F. R. Hung, S. K. Jain, [Adsorption and structure of argon in activated porous carbons](#), *Mol. Sim.* **32**, 557 – 566 (2006).

P16. B. Coasne, S. K. Jain, K. E. Gubbins, [Freezing of fluids confined in a disordered nanoporous structure](#), *Phys. Rev. Lett.* **97**, 105702 (2006).

P15. B. Coasne, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, [Gas adsorption in mesoporous templated silicas: MCM-41, MCM-48 and SBA-15](#), *Langmuir* **22**, 11097 (2006).

P14. B. Coasne, S. K. Jain, K. E. Gubbins, [Adsorption, structure and dynamics of fluids in ordered and disordered models of porous carbons](#), *Mol. Phys.* **104**, 3491 (2006).

P13. B. Coasne, K. E. Gubbins, R. J. M. Pellenq, [Temperature effect on adsorption/desorption isotherms for a simple fluid confined within various nanopores](#), *Adsorption* **11**, 289 – 294 (2005).

P12. M. Sliwinska-Bartkowiak, F. R. Hung, E. E. Santiso, **B. Coasne**, K. E. Gubbins, F. R. Siperstein, [Effect of confinement on freezing in cylindrical pores](#), *Adsorption* **11**, 391 – 396 (2005).

P11. B. Coasne, J. Czwartos, K. E. Gubbins, F. R. Hung, M. Sliwinska-Bartkowiak, [Freezing of mixtures confined in a slit nanopore](#), *Adsorption* **11**, 301 – 306 (2005).

P10. F. R. Hung, **B. Coasne**, E. E. Santiso, K. E. Gubbins, F. R. Siperstein, M. Sliwinska-Bartkowiak, [Molecular modeling of freezing of simple fluids confined within carbon nanotubes](#), *J. Chem. Phys.* **122**, 144706 (2005).

P9. B. Coasne, F. R. Hung, F. R. Siperstein, K. E. Gubbins, [Molecular simulation of gas adsorption in realistic models of silica nanopores](#), *Ann. Chim. Sci. Mat.* **30**, 375 – 383 (2005).

P8. J. Czwartos, **B. Coasne**, F. R. Hung, K. E. Gubbins, M. Sliwinska-Bartkowiak, [Freezing and melting of azeotropic mixtures confined in nanopores: experiment and molecular simulation](#), *Mol. Phys.* **103**, 3103 – 3113 (2005).

Benoit Coasne

(CNRS Research Director, Section 15)

- P7. B. Coasne**, K. E. Gubbins, R. J. –M. Pellenq, [Domain theory for capillary condensation hysteresis](#), *Phys. Rev. B* **72**, 024304 (2005).
- P6. B. Coasne**, R. J. M. Pellenq, [Grand canonical Monte Carlo simulation of argon adsorption at the surface of silica nanopores: Effect of pore size, pore morphology and surface roughness](#), *J. Chem. Phys.* **120**, 2913 – 2922 (2004).
- P5. B. Coasne**, K. E. Gubbins, R. J. M. Pellenq, [A Grand Canonical Monte Carlo Study of Adsorption and Capillary Phenomena in Nanopores of Various Morphologies and Topologies: Testing the BET and BJH Characterization Methods](#) (Invited paper), *Part. Part. Syst. Char.* **21**, 149 – 160 (2004).
- P4. B. Coasne**, R. J. M. Pellenq, [A grand canonical Monte Carlo study of capillary condensation in mesoporous media: Effect of the pore morphology and topology](#), *J. Chem. Phys.* **121**, 3767 – 3774 (2004).
- P3. B. Coasne**, J. Czwartos, K. E. Gubbins, F. R. Hung, M. Sliwinska-Bartkowiak, [Freezing and Melting of Binary Mixtures Confined in a Nanopore](#), *Mol. Phys.* **102**, 2149 – 2163 (2004).
- P2. B. Coasne**, A. Grosman, C. Ortega, M. Simon, [Adsorption in non-interconnected pores open at one or at both ends: a reconsideration of the hysteresis phenomenon](#), *Phys. Rev. Lett.* **88**, 25602 (2002).
- P1. B. Coasne**, A. Grosman, N. Dupont-Pavlovsky, C. Ortega, M. Simon, [Adsorption in an ordered and non-interconnected mesoporous material: Single crystal porous silicon](#), *Phys. Chem. Chem. Phys.* **3**, 1196 – 1200 (2001).

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).
- A17.** C. Weigel, A. Polian, M. Kint, J. Rouquette, J. Haines, M. Foret, R. Vacher, B. Ruffle, **B. Coasne**, [Poroelastic Theory Applied to the Adsorption-induced Deformation of Vitreous Silica](#), Poromechanics VI: Proceedings of the Sixth Biot Conference on Poromechanics, *ASCE Proc.* (Am. Soc. Civil Engineers), 14-19 (2017).

Benoit Coasne

(CNRS Research Director, Section 15)

A16. L. Broussous, M. Lepinay, **B. Coasne**, C. Licitra, F. Bertin, V. Rouessac; A Ayral, “Molecular Simulation Contribution to Porous Low-K Pore Size Determination after Damage by Etch and Wet Clean Processes”, *Solid State Phenomena* **255**, 215 (2016).

A15. P. Billemont, **B. Coasne**, G. De Weireld, Adsorption of carbon dioxide, methane, and their mixture in porous carbons: effect of surface chemistry, water content and pore disorder, *Proceedings of the International Conference on Coal Science & Technology 2013* (2013).

A14. **B. Coasne**, “Pressure effects in phases confined in pores: application to in-pore freezing and mechanical enhancement of porous materials”, *ASCE Proc.* (Am. Soc. Civil Engineers) (2013).

A13. P. Bonnaud, **B. Coasne**, R. J. M. Pellenq, “Molecular simulation of water confined in nanoporous Ca-silica”, *Mat. Res. Soc. Symp. Proc.*, 1227-JJ08-05 (2010).

A12. A. Galarneau, B. Lefevre, H. Cambon, **B. Coasne**, S. Valange, Z. Gabelica, J. P. Bellat, F. Di Renzo, Pore shape affects the determination of the pore size of ordered mesoporous silicas by mercury intrusion, *Studies in Surface Science and Catalysis*, Elsevier Science **174**, 957 – 960 (2008).

A11. **B. Coasne**, S. K. Jain, K. E. Gubbins, “Adsorption and dynamics of argon in porous carbons,” *Eur. Phys J. Special Topics* **141**, 121 – 125 (2007).

A10. N. Fekkar-Nemliche, S. Devautour-Vinot, **B. Coasne**, F. Henn, A. Mehdi, C. Reye, R. Corriu, “Effect of surface chemistry on the thermodynamics and conductivity of water in silica nanopores,” *Eur. Phys J. Special Topics* **141**, 45 – 48 (2007).

A9. S. Bhattacharya, K. E. Gubbins, **B. Coasne**, F. R. Hung, “Molecular simulation of gas adsorption in mesoporous silicas SBA-15,” in *Proceedings of the 4th Pacific Basin Conference on Adsorption Science and Technology* (2006).

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).

A7. F. R. Hung, **B. Coasne**, K. E. Gubbins, F. R. Siperstein, M. Sliwinska-Bartkowiak, A Monte Carlo study of capillary condensation of krypton within realistic models of templated mesoporous silica materials, *Studies in Surface Science and Catalysis* **160**, Elsevier Science, 153 – 160 (2006).

A6. R. J. M. Pellenq, **B. Coasne**, R. O. Denoyel, J. Puibasset, “Effect of pore morphology and topology on capillary condensation in nanopores: a theoretical and molecular simulation study”, *Studies in Surface Science and Catalysis* **160**, Elsevier Science, 1 – 8 (2006).

A5. **B. Coasne**, J. Czwartos, K. E. Gubbins, F. R. Hung, M. Sliwinska-Bartkowiak, “Confinement effect on freezing of binary mixtures”, *Studies in Surface Science and Catalysis* **160**, Elsevier Science, 667 – 674 (2006).

A4. S. Bhattacharya, **B. Coasne**, F. R. Hung, K. E. Gubbins, Modeling and characterization of triblock surfactant templated mesoporous silicas, *Studies in Surface Science and Catalysis*, Elsevier Science **160**, Elsevier Science, 527 – 534 (2006).

Benoit Coasne

(CNRS Research Director, Section 15)

A3. B. Coasne, J. P. Pikunic, R. J. M. Pellenq, K. E. Gubbins, “Comparison between Adsorption in Pores of a Simple Geometry and Realistic Models of Porous Materials”, *Mat. Res. Soc. Symp. Proc.* **790** (2003).

A2. B. Coasne, A. Grosman, C. Ortega, R. J. M. Pellenq, [Physisorption in nanopores of various sizes and shapes: A grand canonical Monte Carlo study](#), *Studies in Surface Science and Catalysis* **144**, Elsevier Science, 35 – 42 (2002).

A1. B. Coasne, A. Grosman, N. Dupont-Pavlovsky, C. Ortega, M. Simon, [Adsorption in ordered porous silicon: a reconsideration of the hysteresis phenomenon in the light of new experimental observations](#), *Mat. Res. Soc. Symp. Proc.* **651** (2000).

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).

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- 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](#), *10th International Symposium on Heat Transfer*, Beijing, China (2020). [Postponed 2022 due to COVID-19](#).
- I34. B. Coasne, [Adsorption and diffusion in porous materials](#), *8th 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).

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- 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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- I14. B. Coasne, [Molecular modeling of Amorphous Porous Materials](#), *European Research Materials Society – Fall Meeting*, Warsaw, Poland (2014).
- 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](#), *4th 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”](#). *3rd International Conference on Nanotek (Nanotek 2013)*, Las Vegas, NV, USA.
- I8. B. Coasne, [“Pressure effects in nanoconfined phases”](#). *5th Biot Conference on Poromechanics*, Vienna, Austria (2013).
- I7. B. Coasne, [“Adsorption and transport in hierarchical zeolites: the view from the nanoscale”](#). *2nd 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).
- I4. B. Coasne, [“Adsorption and dynamics of water and ions in nanopores”](#). *32nd International Conference on Solution Chemistry*, La Grande Motte, France (2011).
- I3. B. Coasne, [“Simulation moléculaire de l’adsorption et confinement de fluides dans des adsorbants microporeux et mesoporeux”](#). *26^e 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).

5. Oral communications in conferences (171)

Benoit Coasne

(CNRS Research Director, Section 15)

- O171.** A. Schlaich, D. Jin, L. Bocquet, B. Coasne, [Wetting and phase transitions of ionic liquids at metal surfaces: Elec-tronic screening using a virtual Thomas–Fermi](#), *Fundamentals of Adsorption 14*, Broomfield, CO, USA (2022).
- 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).
- O160.** I. C. Medeiros Costa, C. Laroche, J. Perez-Pellitero, B. Coasne, [Advanced characterization of hierarchical zeolites for optimal xylene separation](#), American Institute of Chemical Engineering, Pittsburgh, PA, USA (2018).
- 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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(CNRS Research Director, Section 15)

- O157.** M. Chen, B. Coasne, R. Guyer, D. Derome, J. Carmeliet, [Origin of sorption hysteresis of micro-porous polymers: an explanation based on hydrogen bonds](#), *Interpore 10th Annual Meeting*, New Orleans, LA, USA (2018).
- 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).
- O153.** I. C. Medeiros Costa, C. Laroche, J. Perez-Pellitero, B. Coasne, [Advanced characterization of hierarchical zeolites for optimal xylene separation](#), ZMPC2018 - International Symposium on Zeolites and Microporous Crystals, Yokohama, Japan (2018).
- O152.** M. Chen, B. Coasne, R. Guyer, D. Derome, J. Carmeliet, [A comparative study on sorption-induced deformation and related hysteresis of micro- and meso-porous materials](#), EMI 2018, Boston, MA, USA (2018).
- 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).
- O150.** C. Hadji, C. Latargez, B. Coasne, H. Bodiguel, B. Dollet, E. Lorenceau, [Thin liquid films for gas separation](#), EUFOAM 2018, Liege, Belgium (2018).
- O149.** P. Judeinstein, M. Maréchal, L. Noirez, B. Coasne, [Ionic liquids: the prepeak paradox](#), *Journées de la Matière Condensée 2018*, Grenoble, France (2018).
- O148.** Z. Zaafour, B. Coasne, G. Batot, C. Nieto-Draghi, D. Bauer, [Influence of adsorption on transport in flow conditions](#), *14emes Journées d'Etude des Milieux Poreux*, Nantes, France (2018).
- O147.** I. C. Medeiros Costa, C. Laroche, J. Perez-Pellitero, B. Coasne, [Advanced characterization of hierarchical zeolites for optimal xylene separation](#), American Institute of Chemical Engineers, Pittsburgh, PA, USA (2018).
- O146.** M. Chen, B. Coasne, R. Guyer, D. Derome, J. Carmeliet, [Analysis of Sorption and Mechanical Hysteresis of Nano-Porous Materials Upscaling Molecular Simulations by Dependent Domain Theory](#), *6th Biot Conference on Poromechanics*, Paris, France (2017).
- O145.** M. Lépinay, L. Broussous, C. Licitra, F. Bertin, V. Rouessac, A. Ayral, B. Coasne, [Better characterization of microporous organosilica films through combining ellipsometric porosimetry and molecular simulation](#), *11th International Symposium on the Characterization of Porous Solids*, Avignon, France (2017).
- 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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(CNRS Research Director, Section 15)

- O143.** M. Chen, K. Kulasinski, B. Coasne, Guyer, R., D. Derome, J. Carmeliet, [Multi-scale modeling of adsorption-induced deformation of micro-porous materials](#), *Engineering Mechanics Institute Conference 2016*, Nashville, TN, USA (2016).
- O142.** A. Galarneau, F. Fajula, F. Guenneau, A. Gedeon, B. Coasne, [Adsorption and transport in hierarchical microporous/mesoporous materials](#), *Fundamentals of Adsorption 12*, Lake Constance, Germany (2016).
- O141.** S. Hocine, B. Siboulet, R. Hartkamp, B. Coasne, M. Duvail, J. F. Dufreche, [Adsorption along the alkali series on silica surfaces : reversal of adsorption selectivity with pH studied with molecular dynamics](#), *5emes Journées de l'Association Française de l'Adsorption*, Paris, France (2016).
- O140.** A. Obliger, R. J. M. Pellenq, F. J. Ulm, B. Coasne, [Adsorption effects on transport of hydrocarbon mixtures in disordered nanoporous media](#), *Fundamentals of Adsorption 12*, Lake Constance, Germany (2016).
- O139.** L. Broussous, M. Lépinay, B. Coasne, C. Licitra, V. Rouessac, A. Ayral, [Molecular simulation contribution to porous low-k pore size determination after damage by etch and wet clean processes](#), *Symposium on Ultra Clean Processing of Semiconductor Surfaces*, Knokke-Heist, Belgium (2016).
- O138.** R. Pellenq, A. Obliger, B. Coasne, F. Ulm, [The texture-transport properties relation in kerogen phases](#), *Carbon 2016*, State College PA, USA (2016).
- O137.** P. Judeinstein, M. Zeghal, B. Coasne, [Nanostructured lyotropic electrolytes based on ionic liquid](#), *2016 Materials Research Society Fall Meeting*, Boston, MA, USA (2016).
- O136.** B. Coasne, [Adsorption and Transport in Hierarchical Porous Materials](#), *Workshop Rational Design for Improved Functionalities of Porous Inorganic Materials*, Cavaillon, France (2016).
- O135.** C. Bousige, F. J. Ulm, R. Pellenq, B. Coasne, [Realistic molecular model of mature and immature kerogens in organic-rich shales](#), *Engineering Mechanics Institute Conference – 2015* (EMI 2015), Stanford, CA, USA (2015).
- O134.** L. Brochard, G. Hantal, R. Pellenq, F. –J. Ulm, B. Coasne, [Upscaling molecular simulations of failure through size effects](#), *Engineering Mechanics Institute Conference – 2015* (EMI 2015), Standford, CA, USA (2015).
- O133.** T. Lee, B. Coasne, R. Pellenq, F. J. Ulm, L. Bocquet, [Retarded desorption from porous media caused by wetting/dewetting of the external surface](#), *American Physical Society APS 2015*, San Antonio, TX, USA (2015).
- O132.** L. Bocquet, T. Lee, B. Coasne, [Retarded desorption from porous media caused by wetting/dewetting of the external surface](#), *Low permeability media and nanoporous materials from characterisation to modelling*, Paris, France (2015).
- O131.** B. Coasne, K. Falk, R. Pellenq, F. J. Ulm, L. Bocquet, [Subcontinuum mass transport of condensed hydrocarbons in nanoporous media](#), *Low permeability media and nanoporous materials from characterisation to modelling*, Paris, France (2015).

Benoit Coasne

(CNRS Research Director, Section 15)

O130. L. Broussous, M. Lépinay, B. Coasne, C. Licitra, F. Bertin, V. Rouessac, A. Ayral, [Contribution of Molecular Simulation to the characterization of porous low-k materials](#), *Materials for Advanced Metallization Conference MAM2015*, Grenoble, France (2015).

O129. F. G. Alabarse, J. Rouquette, **B. Coasne**, A. Haidoux, C. Paulmann, O. Cambon, J. Haines, [Mechanism of H₂O Insertion and Chemical Bond Formation in AlPO₄-54.xH₂O at high pressure](#), *Joint AIRAPT-25 & EHPRG-53 International Conference On High Pressure Science And Technology*, Madrid, Spain (2015).

O128. J. Haines, J. M. Thibaud, F. Alabarse, J. Rouquette, P. Hermet, O. Cambon, B. Coasne, F. Di Renzo, A. Van der Lee, D. Scelta, M. Ceppatelli, K. Dziubek, F. Gorelli, R. Bini, M. Santoro, [Use of Fourier Maps to Study High Pressure Guest Insertion and Polymerization in Zeolites](#), *2015 IUCr High-Pressure Workshop*, Campinas, Brazil (2015).

O127. P. Judeinstein, M. Zeghal, B. Coasne, [Electrolytes nanostructurés lyotropes à base de liquides ioniques](#), *Systèmes Anisotropes Auto-organisés CFCL 2015*, Autrans, France (2015).

O126. M. Zeghal, P. Judeinstein, B. Coasne, [Nanostructured lyotropic electrolytes based on ionic liquids](#), *Juelich Soft Matter Days 2015*, Juelich, Germany (2015).

O125. **B. Coasne**, [Le kérogène, un charbon poreux?](#), *Journée de réflexion « Gaz et huiles de schiste, leur exploitation : concepts fondamentaux et verrous technologiques »*, Paris, France (2014).

O124. L. Deliere, S. Topin, J.P. Fontaine, C. Daniel, Y. Schuurman, **B. Coasne**, D. Farrusseng, [Capture du xenon à l'aide de zéolithe Ag-ZSM-5](#), *2emes Journées de l'Association Française de l'Adsorption*, Paris, France (2014).

O123. M. Lépinay, **B. Coasne**, L. Broussous, K. Courouble, C. Licitra, François Bertin, Vincent Rouessac, André Ayral, [Expérience et simulation moléculaire de l'adsorption de solvants sur des surfaces de silice fonctionnalisées](#), *2emes Journées de l'Association Française de l'Adsorption*, Paris, France (2014).

O122. P. Billefont, **B. Coasne**, G. De Weireld, [Etude expérimentale et simulation moléculaire de l'adsorption du CO₂, CH₄ et de leurs mélanges dans des structures carbonées nano poreuse en présence d'eau : influence de la chimie de surface](#), *2emes Journées de l'Association Française de l'Adsorption*, Paris, France (2014).

O121. C. Bousige, **B. Coasne**, R. Pellenq, [Building realistic models of kerogen using hybrid reverse Monte Carlo simulations](#), *Carbon 2014*, Jeju Island, Korea (2014).

O120. K. I. Falk, R. Pellenq, F. J. Ulm, L. Bocquet, **B. Coasne**, [Hydrocarbon transport through porous carbons: on the validity of Darcy's law](#), *Nanoporous Materials – 7*, Niagara Falls, Canada (2014).

O119. P. Billefont, G. De Weireld, **B. Coasne**, [Adsorption of carbon dioxide, methane, and their mixture in porous carbons in the presence of water](#), *Carbon 2014*, Jeju Island, Korea (2014).

O118. K. I. Falk, R. Pellenq, F. J. Ulm, L. Bocquet, **B. Coasne**, [Hydrocarbon transport through porous carbons: on the validity of Darcy's law](#), *Carbon 2014*, Jeju Island, Korea (2014).

Benoit Coasne

(CNRS Research Director, Section 15)

O117. L. Deliere, S. Topin, J. P. Fontaine, C. Daniel, Y. Schuurman, **B. Coasne**, D. Farrusseng, [Capture du xenon dans une zeolithe Ag-ZSM-5](#), *30^e Réunion du Groupe Français des Zéolithes*, Ile de Ré, France (2014).

O116. A. Botan, F. J. Ulm, R. J. M. Pellenq, **B. Coasne**, [A bottom up model of adsorption and transport in multiscale porous media](#), *6th International Conference on Porous Media and Annual Meeting of the International Society for Porous Media*, Milwaukee, WI, USA (2014).

O115. [R. Hartkamp](#), **B. Coasne**, [Adsorption and transport of ions confined in realistic porous materials: from simple to radioactive ions](#), *Adsorption of Ions at Solid-Electrolyte Interfaces*, Leiden, The Netherlands (2014).

O114. [F. Villemot](#), A. Galarneau, **B. Coasne**, [Adsorption and Dynamics in Hierarchical Metal Organic Frameworks](#), *Nanoporous Materials – 7*, Niagara Falls, Canada (2014).

O113. [G. Ori](#), F. Villemot, L. Viau, A. Vioux, C. Massobrio, **B. Coasne**, [Hybrid Materials made up of Ionic Liquids Confined in Porous Silica and Chalcogenide](#), *Nanotech Advanced Materials and Applications*, Washington, DC, USA (2014).

O112. [F. Villemot](#), A. Galarneau, **B. Coasne**, [Adsorption and Dynamics in Hierarchical Metal Organic Frameworks](#), *Nanotech Advanced Materials and Applications*, Washington, DC, USA (2014).

O111. [G. Ori](#), M. Celino, C. Massobrio, **B. Coasne**, [Surface properties of amorphous nanoporous GeS₂](#), *Nanotech Advanced Materials and Applications*, Washington, DC, USA (2014).

O110. G. Hantal, [L. Brochard](#), R. J.-M. Pellenq, F. J. Ulm, **B. Coasne**, [Importance of the orthogonal mechanical response of interfaces: Case of organic-clay composites](#), *Multi-physics modeling of solids: International Colloquium of Mechanics*, Paris, France (2014).

O109. [G. Ori](#), C. Massobrio, **B. Coasne**, [Matériaux hybrides constitués de liquides ioniques confinés dans un chalcogénure nanoporeux](#), *Matériaux 2014*, Montpellier, France (2014).

O108. [F. Villemot](#), A. Galarneau, **B. Coasne**, [Adsorption et Transport dans des Metal Organic Frameworks Hiérarchisés](#), *Matériaux 2014*, Montpellier, France (2014).

O107. [C. Bousige](#), R. Pellenq, F.-J. Ulm, **B. Coasne**, [Reconstruction de modèles réalistes de kérogènes par simulations Hybrid Reverse Monte Carlo](#), *Matériaux 2014*, Montpellier, France (2014).

O106. [C. Bousige](#), R. Pellenq, F.-J. Ulm, **B. Coasne**, [Adsorption et transport dans des modèles réalistes de gaz de schiste](#), *Matériaux 2014*, Montpellier, France (2014).

O105. L. Ngoc Ho, D. Farrusseng, **B. Coasne**, [Effet de sursolubilité sur l'adsorption et transport de gaz dans des argiles](#), *Journées annuelles NEEDS – Milieux Poreux 2014*, Nantes, France (2014).

O104. B. Coasne, C. Weigel, A. Polian, M. Kint, J. Rouquette, J. Haines, [M. Foret](#), R. Vacher, B. Rufflé, [Poroelastic behavior of vitreous silica under rare gas compression](#), *Condensed Matter in Paris 2014 – CMD25*, Paris, France (2014).

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(CNRS Research Director, Section 15)

O103. B. Coasne, [C. Weigel](#), A. Polian, M. Kint, J. Rouquette, J. Haines, M. Foret, R. Vacher, B. Rufflé, [Poroelastic behavior of vitreous silica under rare gas compression](#), *52nd European High Pressure Research Group International Meeting – EHPRG*, Lyon, France (2014).

O102. **B. Coasne**, L. Viau, A. Vioux, [Ionogels: Understanding the structure and dynamics of ionic liquids confined in silica nanopores](#), *9th International Conference of Adsorption*, Baltimore, MD, USA (2013).

O101. [J. Haines](#), F. Alabarse, J. Rouquette, O. Cambon, **B. Coasne**, A. Van der Lee, M. Santoro, F. G. Gorelli, R. Bini, C. Paulmann, [“Zeolite host-guest systems under pressure: towards the high pressure synthesis of zeolite/polymer nanocomposites”](#), *2013 International Union of Crystallography Commission on High Pressure*, Hamburg, Germany (2013).

O100. [N. L. Ho](#), S. Clauzier, Y. Schuurman, D. Farrusseng, **B. Coasne**, [Gas oversolubility in solvents nanoconfined in porous silica: adsorption-driven versus bulk-like solubility mechanisms](#), *9th International Conference of Adsorption*, Baltimore, MD, USA (2013).

O99. [P. Billemont](#), **B. Coasne**, G. De Weireld, [Experiment and molecular simulation of adsorption of carbon dioxide, methane, and their mixture in nanoporous carbons in the presence of water](#), *9th International Conference of Adsorption*, Baltimore, MD, USA (2013).

O98. [A. Botan](#), R. J. M. Pellenq, F. J. Ulm, **B. Coasne**, [A bottom-up approach for multiscale dynamics in porous media: upscaling molecular simulation results into a fluid lattice model](#), *Concreep-9@MIT: International Conference on Creep, Shrinkage and Durability Mechanics of Concrete and Concrete Structures*, Cambridge, MA, USA (2013).

O97. [P. Billemont](#), **B. Coasne**, G. De Weireld, [Experiment and molecular simulation of adsorption of carbon dioxide, methane, and their mixture in nanoporous carbons in the presence of water](#), *Carbon 2013*, Rio, Brazil (2013).

O96. [K. I. Falk](#), **B. Coasne**, R. J. M. Pellenq, F. J. Ulm, [Alkane adsorption in realistic models of disordered porous carbons: application to oil and gas extraction from shale](#), *Carbon 2013*, Rio, Brazil (2013).

O95. [G. Ori](#), M. Celino, C. Massobrio, **B. Coasne**, [Structural and Dynamical Insights into Ionic Liquids Confined in Porous Chalcogenides: a Molecular Simulation Study](#), *Material Research Society Spring Meeting*, San Francisco, CA, USA (2013)

O94. [G. Ori](#), M. Celino, C. Massobrio, **B. Coasne**, [Ionic Liquids Confined in Porous Chalcogenides: a Molecular Simulation Study](#), *Material Research Society Spring Meeting*, San Francisco, CA, USA (2013).

O93. [G. Ori](#), M. Celino, C. Massobrio, **B. Coasne**, [Structural and Dynamical Insights into Ionic Liquids Confined in Porous Chalcogenides: a Molecular Simulation Study](#), *10th Pacific Rim Conference on Ceramic and Glass Technology*, San Diego, CA, USA (2013).

O92. [G. Ori](#), M. Celino, C. Massobrio, **B. Coasne**, [Ionic Liquids Confined in Porous Chalcogenides: a Molecular Simulation Study](#), *10th Pacific Rim Conference on Ceramic and Glass Technology*, San Diego, CA, USA (2013).

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O91. L. Ngoc Ho, S. Clauzier, Y. Schuurman, D. Farrusseng, **B. Coasne**, [Gas over-solubility in solvents nanoconfined in mesoporous silica: adsorption-driven versus bulk-like solubility mechanisms](#), *2emes Journées de l'Association Française de l'Adsorption*, Paris, France (2013).

O90. F. Villemot, **B. Coasne**, A. Galarneau, [Adsorption et dynamique dans des solides hiérarchisés à base de MOF](#), *2emes Journées de l'Association Française de l'Adsorption*, Paris, France (2013).

O89. C. Daniel, Y. Schuurman, D. Farrusseng, M. A. Springuel-Huet, A. Nossov, L. Deliere, S. Topin, J. P. Fontaine, **B. Coasne**, [Characterization of very strong xenon adsorption on silver-exchanged zeolites](#), *2emes Journées de l'Association Française de l'Adsorption*, Paris, France (2013).

O88. M. Barboiu, A. Gilles, Y. Le Duc, P. A. Cazade, M. Michau, Y. M. Legrand, A. Van der Lee, **B. Coasne**, J. Post, T. Fyles, [Artificial water channels: a primitive mimic of Gramicidin-A channel](#), *2013 North American Membrane Society Meeting*, Boise, ID, USA (2013).

O87. A. Botan, R. J. M. Pellenq, F. J. Ulm, **B. Coasne**, [Lattice model of fluid dynamics in porous media: application to kerogen in gas shale](#), *5th International Conference Porous Media*, Prague, Czech Republic (2013).

O86. P. Billefont, **B. Coasne**, G. De Weireld, [Adsorption of carbon dioxide, methane, and their mixture in porous carbons: effect of surface chemistry, water content and pore disorder](#), *5th International Conference on Coal Science & Technology 2013*, State College, PA, USA (2013).

O85. L. Ngoc Ho, D. Farrusseng, Y. Schuurman, **B. Coasne**, [Effets de sursolubilité sur les propriétés de confinement et de transport des milieux poreux](#), *Journées annuelles NEEDS – Milieux Poreux 2013*, Paris, France (2013).

O84. **B. Coasne**, R. Chal, C. Gerardin, A. Galarneau, [Molecular simulation of the adsorption and dynamics of molecules in hierarchical nanoporous materials](#), *International Conference on Multiscale Approaches for Process Innovation*, Lyon, France (2012).

O83. E. Secret, C. C. Wu, P. Gonzales, D. Cot, M. J. Sailor, A. Galarneau, **B. Coasne**, F. Cunin, [Columnar mesoporous silicon: a textural study](#), *Porous Semiconductors – Science and Technology*, Malaga, Spain (2012).

O82. **B. Coasne**, L. Viau, A. Vioux, [Ionogels for energy applications: Understanding the structure and dynamics of ionic liquids confined in silica nanopores](#), *6th Pacific Basin Conference on Adsorption Science and Technology*, Taipei, Taiwan (2012).

O81. **B. Coasne**, F. Villemot, R. Chal, A. Galarneau, C. Gerardin, F. Fajula, [Molecular simulation of adsorption and dynamics in hierarchical nanoporous materials](#), *6th Pacific Basin Conference on Adsorption Science and Technology*, Taipei, Taiwan (2012).

O80. **B. Coasne**, J. S. Bender, X. He, J. Fourkas, [Adsorption and dynamics of benzene confined in silica nanopores](#), *6th Pacific Basin Conference on Adsorption Science and Technology*, Taipei, Taiwan (2012).

Benoit Coasne

(CNRS Research Director, Section 15)

O79. B. Coasne, J. Haines, C. Levelut, O. Cambon, M. Santoro, F. Gorelli, G. Garbarino, [Enhanced mechanical strength of zeolites by adsorption of guest molecules](#), *6th Pacific Basin Conference on Adsorption Science and Technology*, Taipei, Taiwan (2012).

O78. P. Billemon, **B. Coasne**, G. De Weireld, [Adsorption of carbon dioxide and methane in porous carbons in the presence of water](#), *6th Pacific Basin Conference on Adsorption Science and Technology*, Taipei, Taiwan (2012).

O77. K. Gubbins, Y. Long, J. Palmer, **B. Coasne**, M. Sliwinska-Bartkowiak, [High pressure effect and material deformation due to adsorption](#), *6th Pacific Basin Conference on Adsorption Science and Technology*, Taipei, Taiwan (2012).

O76. P. Billemon, **B. Coasne**, G. De Weireld, [Etude expérimentale et théorique de l'adsorption du dioxyde de carbone et du méthane en présence d'eau dans des matériaux carbonés nanoporeux](#), *1^{eres} Journées de l'Association Française de l'Adsorption*, Paris, France (2012).

O75. S. Clauzier, L. Ho, A. El-Bahraoui, M. Pera-Titus, **B. Coasne**, D. Farrusseng, [Sursolubilité de l'hydrogène dans un solvant confiné dans une matrice poreuse de silice : expérience et simulation moléculaire](#), *1^{eres} Journées de l'Association Française de l'Adsorption*, Paris, France (2012).

O74. B. Coasne, L. Viau, A. Vioux, [Understanding the physical and chemical properties of ionogels: Dynamics of ionic liquids entrapped in nanoporous silica](#), *Second International Conference on Multifunctional, Hybrid and Nanomaterials*, Strasbourg, France (2011).

O73. B. Coasne, J. Nigon, R. Chal, A. Galarneau, C. Gerardin, [Molecular simulation of the adsorption and dynamics of molecules in hierarchical nanoporous materials](#), *Second International Conference on Multifunctional, Hybrid and Nanomaterials*, Strasbourg, France (2011).

O72. P. Bonnaud, Q. Ji, **B. Coasne**, R. J. M. Pellenq, K. J. Van Vliet, [Thermodynamics, Mechanics, and Dynamics Properties of Water and Ions Confined in Nanopores: Application to Cement Hydrates](#), *Material Research Society Fall Meeting*, Boston, MA, USA (2011).

O71. B. Coasne, J. Haines, O. Cambon, C. Levelut, [Renforcement mécanique des zéolithes par insertion de molécules étrangères](#), *Journée Hautes Pressions*, Montpellier, France (2011).

O70. B. Coasne, [Modélisation moléculaire des Matériaux](#), *Journée d'échange scientifique St Gobain – Pôle Balard*, Montpellier, France (2011).

O69. B. Coasne, L. Viau, A. Vioux, [Structure and dynamics of ionic liquids entrapped in nanoporous silica](#), *Ionic Liquids derived Materials*, Vienna, Austria (2011).

O68. J. Haines, O. Cambon, F. Alabarse, **B. Coasne**, C. Levelut, M. Santoro, F. Gorelli, D. Keen, S. Kohara, [Amorphization, insertion and reactions in microporous materials at high pressure](#), *XXII Congress of the International Union of Crystallography*, Madrid, Spain (2011).

O67. P. Billemon, **B. Coasne**, G. De Weireld, [An experimental and molecular simulation study of the adsorption of carbon dioxide and methane in nanoporous carbons in](#)

Benoit Coasne

(CNRS Research Director, Section 15)

the presence of water: Development of a disordered pore model. *XXII Carbon for Energy Storage/Conversion and Environment Protection*, Vichy, France (2011).

O66. Y. Long, J. C. Palmer, **B. Coasne**, M. Sliwinska-Bartkowiak, K. E. Gubbins, "High pressure effects in nanopores", *AIChE Annual Meeting (American Institute of Chemical Engineers)*, Minneapolis, Minnesota, USA (2011).

O65. **B. Coasne**, L. Viau, A. Vioux, "Tonic liquids confined in nanoporous silica". *4th International Workshop on Dynamics in Confinement*, Grenoble, France (2010).

O64. N. L. Ho, F. Porcheron, **B. Coasne**, R. J. M. Pellenq, "Enhanced CO₂ solubility in solvents confined within porous solid materials". *10th International Conference on Fundamentals of Adsorption*, Awaji Hyogo, Japan (2010).

O63. **B. Coasne**, K. E. Gubbins, M. Sliwinska-Bartkowiak "Freezing of simple fluids in regular and disordered carbon nanotubes". *10th International Conference on Fundamentals of Adsorption*, Awaji Hyogo, Japan (2010).

O62. C. Alba-Simionesco, G. Dosseh, F. Audonnet, N. Brodie-Linder, M. Schoeffel, J. Deschamps, J. Teixeira, D. Morineau, **B. Coasne**, "Confining a liquid down to the nanoscale: more of the same or new phenomena", *CECAM Workshop on Complex Dynamics of Fluids in Disordered and Crowded Environments*, Lyon, France (2010).

O61. P. Bonnaud, **B. Coasne**, R. J. M. Pellenq, "Freezing of an electrolyte film on a mesopore surface", *CECAM Workshop on Aqueous Solvation of Ions*, ETHZ, Zurich, Switzerland (2010).

O60. P. Bonnaud, **B. Coasne**, R. J. M. Pellenq, "Gel d'un électrolyte dans des mésopores chargés", *12e Journées de la Matière Condensée*, Troyes, France (2010).

O59. Y. Long, J. C. Palmer, **B. Coasne**, M. Sliwinska-Bartkowiak, K. E. Gubbins, "Under pressure: quasi-high pressure effects in nanopores", *US-Poland Workshop on Nanoscale Phenomena in Materials and at Interfaces*, Poznan, Poland (2010).

O58. Y. Long, J. C. Palmer, **B. Coasne**, M. Sliwinska-Bartkowiak, K. E. Gubbins, "Under pressure: quasi-high pressure effects in nanopores", *8th Liblice Conference on the Statistical Mechanics of Liquids*, Brno, Czech Republic (2010).

O57. Y. Long, J. C. Palmer, **B. Coasne**, M. Sliwinska-Bartkowiak, K. E. Gubbins, "Quasi-high pressure effects in nanopores", *AIChE Annual Meeting (American Institute of Chemical Engineers)*, Salt Lake City, Utah, USA (2010).

O56. **B. Coasne**, C. Alba-Simionesco, F. Audonnet, G. Dosseh, K. E. Gubbins, "Adsorption and Freezing of Benzene on Silica Surfaces and Nanopores". *5th Pacific Basin Conference on Adsorption Science and Technology*, Singapore (2009).

O55. **B. Coasne**, J. Czwartowski, M. Sliwinska-Bartkowiak, K. E. Gubbins, "Effect of Pressure on Freezing of Pure Fluids and Mixtures Confined in Nanopores". *5th Pacific Basin Conference on Adsorption Science and Technology*, Singapore (2009).

O54. **B. Coasne**, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, "Intrusion and Retraction of Fluids in Ordered and Disordered Nanopores". *5th Pacific Basin Conference on Adsorption Science and Technology*, Singapore (2009).

Benoit Coasne

(CNRS Research Director, Section 15)

O53. P. A. Cazade, J. Dweik, **B. Coasne**, F. Henn, J. Palmeri, "[Confinement de solutions électrolytiques dans des nanopores](#)". *Journées simulation numérique*, Paris, France (2009).

O52. P. Bonnaud, R. J. M. Pellenq, **B. Coasne**, "[Gel d'un film moléculaire ou électrolytique à la surface d'un mésopore](#)". *Journées simulation numérique*, Paris, France (2009).

O51. P. Bonnaud, R. J. M. Pellenq, **B. Coasne**, "[Freezing of a molecular or electrolyte film at a mesopore surface](#)". *7th International Symposium Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids*, Kazimierz Dolny, Poland (2009).

O50. P. A. Cazade, J. Dweik, **B. Coasne**, F. Henn, J. Palmeri, "[Dynamics of electrolyte solutions confined in nanopores](#)". *7th International Symposium Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids*, Kazimierz Dolny, Poland (2009).

O49. **B. Coasne**, J. Czwartos, M. Sliwinska-Bartkowiak, K. E. Gubbins, "[Effect of Pressure on Freezing of Pure Fluids and Mixtures Confined in Nanopores](#)". *7th International Symposium Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids*, Kazimierz Dolny, Poland (2009).

O48. J. Dweik, **B. Coasne**, F. Henn, J. Palmeri, "[Study of ion transport across nanoporous membranes](#)". *Euromembrane 2009*, Montpellier, France (2009).

O47. C. Abrioux, S. Balme, **B. Coasne**, S. Devautour-Vinot, M. Kharroubi, G. Maurin, F. Henn, "[Ion dynamics in confined geometry and related effects of water adsorption](#)". *3rd International Conference on Physics of Solid State Ionics*, Kumamoto, Japan (2009).

O46. R. J. M. Pellenq, **B. Coasne**, "[A unifying approach to capillary condensation and evaporation in nanopores](#)", *Material Research Society Fall Meeting*, Boston, MA, USA (2009).

O45. R. J. M. Pellenq, **B. Coasne**, "[A unifying approach to capillary condensation and evaporation in nanopores](#)". *International Workshop on the Recent Advances in the Understanding of Confined Fluids*, Abingdon, Oxon, United Kingdom (2008).

O44. A. Mezzy, **B. Coasne**, R. J. M. Pellenq, D. Ravot, J. C. Tedenac, "[Thermodynamical Stability of ZnO Nanostructures obtained within porous materials: Experiment and molecular simulation](#)". *JEEP XXXIV: Journées d'études des équilibres entre phases*, Marrakech, Maroc (2008).

O43. C. Abrioux, A. Nicolas, **B. Coasne**, S. Devautour-Vinot, G. Maurin, J. C. Giuntini, F. Henn, A. Boutin, A. Di Lella, C. Nieto-Draghi, A. H. Fuchs, "[Cation redistribution in Faujasite zeolites upon adsorption of small dipolar molecules: Molecular simulation and dielectric relaxation spectroscopy](#)". *8th international symposium on the characterization of porous solids*, Edinburgh, Scotland (2008).

O42. J. Dweik, **B. Coasne**, F. Henn, J. Palmeri, "[Molecular dynamics study of ion partitioning and transport in nanoporous membranes](#)". *Engineering with Membranes 2008*, Algarve, Portugal (2008).

O41. **B. Coasne**, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, "[Adsorption and Intrusion of Fluids in Regular and Defective Nanopores](#)". *7th Liquid Matter Conference*, Lund, Sweden (2008).

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(CNRS Research Director, Section 15)

O40. B. Coasne, C. Alba-Simionesco, F. Audonnet, G. Dosseh, K. E. Gubbins, “[Adsorption and Freezing of Benzene on Silica Surfaces and Nanopores](#)”. *11èmes Journées de la Matière Condensée*, Strasbourg, France (2008).

O39. B. Coasne, J. Czwartos, M. Sliwinska-Bartkowiak, K. E. Gubbins, “[Effect of pressure on Freezing of pure fluids and mixtures confined in nanopores](#)”. *Inorganic Materials Conference*, Dresden, Germany (2008).

O38. K. E. Gubbins, S. Bhattacharya, C. Bichara, **B. Coasne**, F. R. Hung, S. K. Jain, R. J. M. Pellenq, T. Roussel, “[Modeling Micelle-Templated Porous Silicas and Carbon Replicas](#)”. *CECAM Workshop on Surfactant Templated Porous Materials: Synthesis and Characterisation*, Zurich, Switzerland (2008).

O37. B. Coasne, S. K. Jain, K. E. Gubbins, “[Phase transitions of simple fluids confined in nanoporous carbons](#)”. *JEEP XXXIII: Journées d'études des équilibres entre phases*, Lyon, France (2007).

O36. B. Coasne, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, “[Molecular simulation of gas adsorption and porosimetry in nanopores](#)”. *9th International Conference on Fundamentals of Adsorption*, Giardini Naxos, Sicily – Italy (2007).

O35. J. Czwartos, M. Sliwinska-Bartkowiak, **B. Coasne**, K. E. Gubbins, “[Confinement effect on freezing of azeotropic mixtures: Experiment and molecular simulation](#)”. *9th International Conference on Fundamentals of Adsorption*, Giardini Naxos, Sicily – Italy (2007).

O34. C. Abrioux, **B. Coasne**, G. Maurin, A. Boutin, J. C. Giuntini, A. H. Fuchs, F. Henn, C. Nieto, “[Influence of the cation/zeolite interatomic potentials on the cation distribution in faujasites](#)”. *9th International Conference on Fundamentals of Adsorption*, Giardini Naxos, Sicily – Italy (2007).

O33. B. Coasne, C. Alba-Simionesco, G. Dosseh, K. E. Gubbins, “[Molecular simulation of the adsorption and structure of benzène confined in mesoporous silicas](#)”. *9th International Conference on Fundamentals of Adsorption*, Giardini Naxos, Sicily – Italy (2007).

O32. B. Coasne, F. Di Renzo, A. Galarneau, R. J. M. Pellenq, “[Adsorption et intrusion de fluides dans des silices nanoporeuses présentant des défauts morphologiques](#)”. *23^e Réunion du Groupe Français des Zéolithes*, La Grande Motte, France (2007).

O31. C. Abrioux, **B. Coasne**, G. Maurin, F. Henn, A. Boutin, A. Di Lella, C. Nieto-Draghi, A. H. Fuchs, “[A molecular simulation study of the distribution of cation in zeolite](#)”. *Thermodynamics 2007*, Rueil-Malmaison, France (2007).

O30. B. Coasne, C. Alba-Simionesco, G. Dosseh, K. E. Gubbins, “[Molecular simulation of the adsorption and structure of benzène confined in mesoporous silicas](#)”. *Thermodynamics 2007*, Rueil-Malmaison, France (2007).

O29. F. R. Hung, S. Bhattacharya, **B. Coasne**, M. Thommes, K. E. Gubbins, “[A Monte Carlo study of gas adsorption on atomistic models of templated mesoporous silicas](#)”. *AIChE Annual Meeting (American Institute of Chemical Engineers)*, Salt Lake City, Utah, USA (2007).

Benoit Coasne

(CNRS Research Director, Section 15)

O28. B. Coasne, S. K. Jain, K. E. Gubbins, "Freezing of argon in a disordered nanoporous structure". *3rd International Workshop on Dynamics in Confinement*, Grenoble, France (2006).

O27. B. Coasne, S. K. Jain, K. E. Gubbins, R. J. –M. Pellenq, "Solidification d'argon dans un carbone poreux désordonné". *Journées scientifiques du Groupe Français d'Etude des Carbones*, Presqu'îles de Giens, France (2006).

O26. B. Coasne, "Adsorption et condensation de fluides dans des silices mésoporeuses". *Réunion du GDR Verres*, Montpellier, France (2006).

O25. S. Bhattacharya, K. E. Gubbins, **B. Coasne**, F. R. Hung, "Molecular simulation of gas adsorption in mesoporous silica SBA-15". *4th Pacific Basin Conference on Adsorption Science and Technology*, Tianjin, China (2006).

O24. R. J. –M. Pellenq, B. Coasne, "Testing the validity of small – angle and adsorption – based characterization techniques by atomic – scale simulation". *NSTI Nanotech2006*, Boston, MA, USA (2006).

O23. B. Coasne, S. K. Jain, K. E. Gubbins, "Freezing and melting in ordered and disordered porous carbons". *7th Liblice Conference on Statistical Mechanics of Liquids*, Lednice, Czech Republic (2006).

O22. R. J. M. Pellenq, B. Coasne, R. O. Denoyel, J. Puibasset, "A theoretical and molecular simulation study on the effect of pore morphology and topology on capillary condensation in nanopores". *7th Liblice Conference on Statistical Mechanics of Liquids*, Lednice, Czech Republic (2006).

O21. B. Coasne, S. K. Jain, K. E. Gubbins, "Freezing of fluids confined in ordered and disordered porous carbons". *6th International Symposium Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids*, Zakopane, Poland (2006).

O20. A. Mezy, J. C. Tedenac, T. Bretagnon, B. Coasne, C. Gérardin, P. Lefebvre, B. Pichon, D. Ravot, S. Suwanboon, D. Tichit, "Synthèse de Nanofils de ZnO dans des Matériaux Poreux Ordonnés : Expérience et Simulation Moléculaire". *Matériaux 2006: 2^e conférence pluridisciplinaire sur les matériaux*, Dijon, France (2006).

O19. R. J. M. Pellenq, B. Coasne, R. O. Denoyel, J. Puibasset, "Effect of Pore Morphology and Topology on Adsorption and Capillary Condensation in Nanopores: A Theoretical and Molecular Simulation Study" (Keynote Lecture). *7th international symposium on the characterization of porous solids*, Aix-en-Provence, France (2005).

O18. F. R. Hung, B. Coasne, K. E. Gubbins, F. R. Siperstein, M. Sliwinska-Bartkowiak, "A Monte Carlo Study of Capillary Condensation and Freezing Within Realistic Models of MCM-41 Materials". *7th international symposium on the characterization of porous solids*, Aix-en-Provence, France (2005).

O17. M. Sliwinska-Bartkowiak, M. Jazdzewska, B. Coasne, F. R. Hung, K. E. Gubbins, "Freezing of simple fluids within carbon and silica nanotubes: a combined experimental and simulation approach". *European - Material Research Society Fall Meeting*, Warsaw, Poland (2005).

Benoit Coasne

(CNRS Research Director, Section 15)

- O16.** B. Coasne, F. R. Hung, K. E. Gubbins, "[Development of realistic models of MCM-41 materials for gas adsorption studies](#)". *AICHE Annual Meeting (American Institute of Chemical Engineers)*, Cincinnati, OH, USA (2005).
- O15.** F. R. Hung, **B. Coasne**, K. E. Gubbins, "[A Monte Carlo study of capillary condensation and freezing of krypton within realistic models of MCM-41 materials](#)". *AICHE Annual Meeting (American Institute of Chemical Engineers)*, Cincinnati, OH, USA (2005).
- O14.** S. Bhattacharya, **B. Coasne**, F. R. Hung, K. E. Gubbins, "[Molecular models of MCF and SBA-15 and gas adsorption: A molecular simulation study](#)". *AICHE Annual Meeting (American Institute of Chemical Engineers)*, Cincinnati, OH, USA (2005).
- O13.** R. J. M. Pellenq, **B. Coasne**, K. E. Gubbins, "[A Monte Carlo study of capillary condensation in mesoporous media: from a single regular pore to a disordered porous matrix](#)". *8th International Conference on Fundamentals of Adsorption*, Sedona, AZ, USA (2004).
- O12.** **B. Coasne**, K. E. Gubbins, F. R. Hung, E. E. Santiso, M. Sliwinska-Bartkowiak, "[Phase transitions and chemical reactions at the nano-scale: Effects of confinement](#)" (Invited talk). *227th ACS National Meeting*, Anaheim, USA (2004).
- O11.** B. Coasne, J. Czwartos, F. R. Hung, K. E. Gubbins, M. Sliwinska-Bartkowiak, "[Freezing/Melting of binary mixtures confined in nanopores](#)". *8th International Conference on Fundamentals of Adsorption*, Sedona, AZ, USA (2004).
- O10.** F. R. Hung, **B. Coasne**, K. E. Gubbins, G. Dudziak, M. Sliwinska-Bartkowiak, "[Effect of Confinement and Adsorbate-Wall Interactions on Freezing/Melting within Cylindrical Pores: Experiment and Molecular Simulation](#)". *AICHE Annual Meeting (American Institute of Chemical Engineers)*, Austin, TX, USA (2004).
- O9.** F. R. Hung, E. E. Santiso, **B. Coasne**, K. E. Gubbins, G. Dudziak, M. Sliwinska-Bartkowiak, "[Solid-Fluid Phase Transitions in Confinement within Multi-Walled Carbon Nanotubes](#)". *AICHE Annual Meeting (American Institute of Chemical Engineers)*, Austin, TX, USA (2004).
- O8.** B. Coasne, J. Czwartos, F. R. Hung, K. E. Gubbins, M. Sliwinska-Bartkowiak, "[Solid - Liquid Phase Diagram of Mixtures Confined in Nanopores](#)". *AICHE Annual Meeting (American Institute of Chemical Engineers)*, Austin, TX, USA (2004).
- O7.** F. R. Hung, **B. Coasne** and K. E. Gubbins, G. Dudziak, M. Sliwinska-Bartkowiak, "[Solid-Fluid Phase Behavior of Fluids Confined in Cylindrical Pores: Simulation and Experimental Studies](#)". *AICHE Annual Meeting (American Institute of Chemical Engineers)*, San Francisco, CA, USA (2003).
- O6.** B. Coasne, J. Czwartos, F. R. Hung, K. E. Gubbins, M. Sliwinska-Bartkowiak, "[Freezing/Melting of binary mixtures confined in nanopores](#)". *AICHE Annual Meeting (American Institute of Chemical Engineers)*, San Francisco, CA, USA (2003).
- O5.** R. J. M. Pellenq, **B. Coasne**, "[Grand Canonical Monte-Carlo Study of Adsorption and Condensation in Nanopores: From Simple Pore geometry to Disordered Matrix](#)". *Material Research Society Fall Meeting*, Boston, MA, USA (2003).

Benoit Coasne

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O4. B. Coasne, A. Grosman, C. Ortega, R. J. M. Pellenq, "Study of adsorption in mesoscopic pores by means of Monte Carlo simulation in the grand canonical ensemble". *6th international symposium on the characterization of porous solids*, Alicante, Spain (2002).

O3. B. Coasne, A. Grosman, C. Ortega, R. J. M. Pellenq, "Etude de la physisorption/condensation de gaz dans un matériau mésoporeux par simulation Monte Carlo dans l'ensemble grand canonique". *8^{eme} édition des Journées simulation numérique, Matière condensée et Désordre - Interface simulation/expérience*, Paris, France (2002).

O2. B. Coasne, A. Grosman, C. Ortega, M. Simon, "A reconsideration of the origin of the hysteresis phenomenon in the light of new experimental observations" (Invited contribution). *CECAM/ESF workshop on phase transitions in complex confined systems*, Lyon, France (2001).

O1. B. Coasne, A. Grosman, N. Dupont-Pavlovsky, C. Ortega, M. Simon, "Adsorption in ordered porous silicon: a reconsideration of the hysteresis phenomenon in the light of new experimental observations". *Material Research Society Fall Meeting*, Boston, MA, USA (2000).

6. Poster communications in conferences (103)

- C103.** I. C. Medeiros-Costa, C. Laroche, J. Perez-Pellitero, B. Coasne, [Advanced characterization of hierarchical zeolites for optimal xylene separation](#), *1st International Meeting of the Group Francais des Zeolithes*, Cabourg, France (2018).
- C102.** L. Ho, D. Farrusseng, B. Coasne, [Oversolubility Effects on Confinement and Transport in Porous Media](#), *Interpore 10th Annual Meeting*, New Orleans, LA, USA (2018).
- C101.** Z. Zaafour, B. Coasne, G. Batot, C. Nieto-Draghi, D. Bauer, [Adsorption in flow conditions](#), *Solid-Liquid Interfaces: Challenging Molecular Aspects for Industrial Applications*, Rueil-Malmaison, France (2018).
- C100.** D. Jin, B. Coasne, [Theory and Molecular Simulation of Methane Hydrate in Porous Media](#), *Interpore 10th Annual Meeting*, New Orleans, LA, USA (2018).
- C99.** I. Medeiros-Costa, C. Laroche, J. Perez-Pellitero, B. Coasne, [Characterization of hierarchical X-zeolites for xylene separation](#), *11th International Symposium on the Characterization of Porous Solids*, Avignon, France (2017).
- C98.** M. Bah, E. D. Manga, M. Drobek, E. Le Clezio, G. Despau, Philippe Da Costa, B. Coasne, A. Ayrat, A. Julbe, [Acoustic emission: toward a real-time diagnosis tool for studying gas permeation through porous ceramic membranes](#), *11th International Symposium on the Characterization of Porous Solids*, Avignon, France (2017).
- C97.** I. Deroche, T. J. Daou, B. Coasne, [Phase diagram for adsorption in pure silica zeolites](#), *11th International Symposium on the Characterization of Porous Solids*, Avignon, France (2017).
- C96.** R. Bey, C. Picard, E. Charlaix, B. Coasne, [Confined interfaces at the nanoscale: continuous thermodynamics and line tension](#), *10th Liquid Matter Conference*, Ljubljana, Slovenia (2017).
- C95.** P. Judeinstein, M. Zeghal, B. Coasne, [Anisotropic ionic liquid materials](#), *10th Liquid Matter Conference*, Ljubljana, Slovenia (2017).
- C94.** L. Deliere, B. Coasne, S. Topin, C. Greau, C. Moulin, D. Farrusseng, [Break-through in Xenon Capture and Purification Using Adsorbent-Supported Silver Nanoparticles](#), *Fundamentals of Adsorption 12*, Lake Constance, Germany (2016).
- C93.** B. Siboulet, S. Hocine, B. Coasne, M. Duvail, P. Turq, J. F. Dufreche, [Ionic specificity of adsorption in silicas studied with molecular dynamics and potential of mean force](#), *Low permeability media and nanoporous materials from characterisation to modelling*, Paris, France (2015).
- C92.** J. Bender, S. R. Cohen, B. Coasne, J. T. Fourkas, [Structure and Low-Frequency Dynamics of Benzene Confined in Amorphous Silica Nanopores](#), *Gordon Research Conference on Chemistry & Physics of Liquids*, Holderness, NH, USA (2015).

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- C91.** D. Farrusseng, C. Daniel, **B. Coasne**, [Mapping of water adsorption properties in Metal-Organic Frameworks](#), *3emes Journées de l'Association Française de l'Adsorption*, Paris, France (2014).
- C90.** A. Galarneau, F. Villemot, J. Rodriguez, F. Fajula, **B. Coasne**, [Validité de la méthode t-plot pour déterminer la microporosité dans des solides poreux hiérarchisés](#), *3emes Journées de l'Association Française de l'Adsorption*, Paris, France (2014).
- C89.** L. Deliere, S. Topin, J.P. Fontaine, C. Daniel, Y. Schuurman, **B. Coasne**, D. Farrusseng, [Enhanced xenon capture using silver exchanged-zeolite: role of metal nanoparticles](#), *10th international symposium on the characterization of porous solids*, Granada, Spain (2014).
- C88.** A. Boutin, **B. Coasne**, A. H. Fuchs, A. Galarneau, F. Di Renzo, [Experiment and Theory of Low Pressure Nitrogen Adsorption in Organic Layers Supported or Grafted on Inorganic Adsorbents: Towards a Tool to Characterize Surfaces of Hybrid Organic/Inorganic Systems](#), *30^e Réunion du Groupe Français des Zéolithes*, Ile de Ré, France (2014).
- C87.** F. Villemot, A. Galarneau, J. Rodriguez, F. Di Renzo, F. Fajula, **B. Coasne**, [Validity of the t-plot Method to Assess Microporosity in Hierarchical Micro/Mesoporous Materials](#), *Nanoporous Materials – 7*, Niagara Falls, Canada (2014).
- C86.** F. Villemot, A. Galarneau, J. Rodriguez, F. Di Renzo, F. Fajula, **B. Coasne**, [Assessing the pore network of hierarchical micro/mesoporous materials](#), *Nanotech Advanced Materials and Applications*, Washington, DC, USA (2014).
- C85.** L. Deliere, S. Topin, J. P. Fontaine, D. Farrusseng, C. Daniel, Y. Schuurman, **B. Coasne**, [Enhanced xenon capture using silver exchanged-zeolite: Evidence of the role of metal nanoparticles](#), *Nanoporous Materials – 7*, Niagara Falls, Canada (2014).
- C84.** R. Hartkamp, R. J. M. Pellenq, **B. Coasne**, [Adsorption and transport of ions confined in realistic porous materials: from simple to radioactive ions](#), *9th Liquid Matter Conference*, Lisboa, Portugal (2014).
- C83.** L. Deliere, S. Topin, J. P. Fontaine, D. Farrusseng, C. Daniel, Y. Schuurman, **B. Coasne**, [Enhanced xenon capture using silver exchanged-zeolite: Evidence of the role of metal nanoparticles](#), *6th International FEZA Conference*, Leipzig, Germany (2014).
- C82.** A. Galarneau, F. Villemot, J. Rodriguez, F. Di Renzo, F. Fajula, **B. Coasne**, [Validity of the t-plot method to assess microporosity in hierarchical micro/mesoporous materials](#), *6th International FEZA Conference*, Leipzig, Germany (2014).
- C81.** A. Botan, L. Brochard, R. Pellenq, F. J. Ulm, **B. Coasne**, [From microscopic dynamics to mesoscale transport in porous materials: application to kerogen in gas shale](#), *9th International Conference of Adsorption*, Baltimore, MD, USA (2013).
- C80.** **B. Coasne**, P. Ugliengo, [Ab-initio model of micelle-templated mesoporous silicas: structural, morphological and adsorption properties](#), *9th International Conference of Adsorption*, Baltimore, MD, USA (2013).
- C79.** F. Villemot, **B. Coasne**, A. Galarneau, [Adsorption and dynamics in MOF-based hierarchical solids](#), *9th International Conference of Adsorption*, Baltimore, MD, USA (2013).

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C78. J. S. Bender, X. X. He, **B. Coasne**, J. T. Fourkas, [Probing density effects within nanoconfined benzene with molecular dynamics simulations of the optical Kerr effect](#), *9th International Conference of Adsorption*, Baltimore, MD, USA (2013).

C77. L. Deliere, S. Topin, J. P. Fontaine, Y. Schuurman, D. Farrusseng, **B. Coasne**, [Very strong adsorption sites of Ag-ZSM-5 for xenon capture from atmosphere: experimental and molecular modeling](#), *17th International Zeolite Conference*, Moscow, Russia (2013).

C76. G. Ori, M. Celino, C. Massobrio, **B. Coasne**, [Ionic Liquids Confined in Porous Chalcogenides: a Molecular Simulation Study](#), *6th Congress on Ionic Liquids*, Algarve, Portugal (2013).

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](#), *6th Congress on Ionic Liquids*, Algarve, Portugal (2013).

C74. G. Ori, L. Viau, A. Vioux, **B. Coasne**, [Loading-Controlled Stiffening and Pressure effects in Ionic Liquids Confined in Nanoporous Silica](#), *6th Congress on Ionic Liquids*, Algarve, Portugal (2013).

C73. G. Ori, C. Massobrio, **B. Coasne**, [Molecular simulation of ionic liquid confined in porous chalcogenides](#), *Multifunctional Hybrid Materials 2013*, Sorrento, Italy (2013).

C72. F. Villemot, A. Galarneau, **B. Coasne**, [Adsorption and diffusion of adsorbates in hierarchical microporous-mesoporous MOF: The view from the nanoscale](#), *Multifunctional Hybrid Materials 2013*, Sorrento, Italy (2013).

C71. L. Deliere, S. Topin, J. P. Fontaine, D. Farrusseng, Y. Schuurman, **B. Coasne**, [Etude de l'adsorption du xenon sur une zéolithe MFI dopée à l'argent: identification des sites d'adsorption](#), *2^{emes} Journées de l'Association Française de l'Adsorption*, Paris, France (2013).

C70. G. Hantal, L. Brochard, **B. Coasne**, F. J. Ulm, R. J. M. Pellenq, [Chemistry of interfaces between inorganic minerals and porous carbons: implications for the mechanical properties of gas shale](#), *Carbon 2013*, Rio, Brazil (2013).

C69. A. Botan, R. Pellenq, F.J. Ulm, **B. Coasne**, [Lattice model of fluid dynamics in porous media: Application to Kerogen in Gas Shale](#), *5th Biot Conference on Poromechanics*, Vienna, Austria (2013).

C68. L. Ngoc Ho, S. Clauzier, Y. Schuurman, D. Farrusseng, **B. Coasne**, [Gas over-solubility in solvents nanoconfined in mesoporous silica: adsorption-driven versus bulk-like solubility mechanisms](#), *29^e Réunion du Groupe Français des Zéolithes*, Sémur-en-Auxois (Dijon), France (2013).

C67. F. Villemot, A. Galarneau, **B. Coasne**, [Adsorption and diffusion of adsorbates in hierarchical microporous-mesoporous MOF: The view from the nanoscale](#), *29^e Réunion du Groupe Français des Zéolithes*, Sémur-en-Auxois (Dijon), France (2013).

C66. L. Deliere, S. Topin, J. P. Fontaine, D. Farrusseng, Y. Schuurman, **B. Coasne**, [Etude de l'adsorption du xenon sur une zéolithe MFI dopée à l'argent: identification](#)

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des sites d'adsorption, 29^e Réunion du Groupe Français des Zéolithes, Sémur-en-Auxois (Dijon), France (2013).

C65. A. Boutin, **B. Coasne**, A. H. Fuchs, A. Galarneau, F. Di Renzo, Experiment and Theory of Low Pressure Nitrogen Adsorption in Organic Layers Supported or Grafted on Inorganic Adsorbents: Towards a Tool to Characterize Surfaces of Hybrid Organic/Inorganic Systems, 29^e Réunion du Groupe Français des Zéolithes, Sémur-en-Auxois (Dijon), France (2013).

C64. **B. Coasne**, Freezing in ordered and disordered porous carbons: surface-induced versus homogeneous crystallization, *Carbon* 2013, Rio, Brazil (2013).

C63. A. Botan, R. J. M. Pellenq, F. J. Ulm, **B. Coasne**, Lattice model of fluid dynamics in porous media: application to kerogen in gas shale, *Carbon* 2013, Rio, Brazil (2013).

C62. X. He, J. S. Bender, **B. Coasne**, J. T. Fourkas, Density effects on the dynamics of benzene under nanoconfinement, *Gordon Research Conference: Chemistry and Physics of Liquids*, Holderness, NH, USA (2013).

C61. G. Ori, F. Villemot, L. Viau, A. Vioux, **B. Coasne**, Influence of the Size of Hydroxylated Silica Nanopores on the Structural and Order Properties of Confined Ionic Liquids, 2nd European Workshop of Ionic Liquids for Materials, Montpellier, France (2013).

C60. G. Ori, M. Celino, C. Massobrio, **B. Coasne**, Exploring the Application Scenarios of Bare and Hybrid Chalcogels by a Computational Approach, 2nd European Workshop of Ionic Liquids for Materials, Montpellier, France (2013).

C59. **B. Coasne**, J. Haines, C. Levelut, O. Cambon, M. Santoro, F. Gorelli, G. Gabarino, Enhanced mechanical strength of zeolites by adsorption of guest molecules, 28^e Réunion du Groupe Français des Zéolithes, Mittelwihr, France (2012).

C58. F. Villemot, A. Galarneau, **B. Coasne**, Simulation moléculaire de l'adsorption et de la diffusion dans des milieux poreux hiérarchisés, 28^e Réunion du Groupe Français des Zéolithes, Mittelwihr, France (2012).

C57. F. Villemot, A. Galarneau, **B. Coasne**, Simulation moléculaire de l'adsorption et de la diffusion dans des milieux poreux hiérarchisés, 1^{eres} Journées de l'Association Française de l'Adsorption, Paris, France (2012).

C56. B. Siboulet, **B. Coasne**, J. F. Dufreche, P. Turq, Modeling the effects of irradiation on normal and parallel water diffusion in confined silica, 4th International Atalante Conference on Nuclear Chemistry for Sustainable Fuel Cycles, Montpellier, France (2012).

C55. **B. Coasne**, R. Chal, A. Galarneau, C. Gerardin, Molecular simulation of the adsorption and dynamics of molecules in hierarchical nanoporous materials, 27^e Reunion du Groupe Francais des Zeolites, Arches, France (2011).

C54. M. Manko, W. Makowski, **B. Coasne**, A. Galarneau, Thermodesorption as a new tool to characterize hierarchical micro/mesoporous materials, 27^e Reunion du Groupe Francais des Zeolites, Arches, France (2011).

C53. M. Manko, W. Makowski, **B. Coasne**, A. Galarneau, Thermodesorption as a new tool to characterize hierarchical micro/mesoporous materials, 5th international FEZA conference, Valencia, Spain (2011).

Benoit Coasne

(CNRS Research Director, Section 15)

- C52.** Y. Long, J. C. Palmer, B. Coasne, M. Sliwinska-Bartkowiak, K. E. Gubbins, [Under pressure: quasi-high pressure effects in nanopores](#), *9th international symposium on the characterization of porous solids*, Dresden, Germany (2011).
- C51.** B. Coasne, L. Viau, A. Vioux, [Structure and dynamics of ionic liquids entrapped in nanoporous silica](#), *4th Congress on Ionic Liquids (COIL)*, Washington DC, USA (2011).
- C50.** P. Bonnaud, B. Coasne, P. Levitz, R. J. M. Pellenq, [Dynamics of water in hydroxylated and calcium silica nanopores](#). *4th International Workshop on Dynamics in Confinement*, Grenoble, France (2010).
- C49.** P. A. Cazade, J. Dweik, B. Coasne, F. Henn, J. Palmeri, [Structure and dynamics of electrolyte solution in nanopores](#). *4th International Workshop on Dynamics in Confinement*, Grenoble, France (2010).
- C48.** B. Coasne, L. Viau, A. Vioux, [Ionic liquids confined in nanoporous silica](#). *8th Liblice Conference on the Statistical Mechanics of Liquids*, Brno, Czech Republic (2010).
- C47.** P. Bonnaud, P. A. Cazade, B. Coasne, P. Levitz, R. J. M. Pellenq, [Dynamics of water and electrolytes in hydrophilic and hydrophobic pores](#). *8th Liblice Conference on the Statistical Mechanics of Liquids*, Brno, Czech Republic (2010).
- C46.** I. Aydogdu, B. Coasne, A. Galarneau, R. J. M. Pellenq, F. Di Renzo, [Mercury intrusion in ordered and disordered porous silicas](#). *10th International Conference on Fundamentals of Adsorption*, Awaji Hyogo, Japan (2010).
- C45.** P. Bonnaud, B. Coasne, R. J. M. Pellenq, [Freezing of a molecular or electrolyte film on a mesopore surface](#). *10th International Conference on Fundamentals of Adsorption*, Awaji Hyogo, Japan (2010).
- C44.** P. Billefont, B. Coasne, G. De Weireld, [Confinement of CO₂ and CH₄ in nanoporous carbons in presence of water](#). *10th International Conference on Fundamentals of Adsorption*, Awaji Hyogo, Japan (2010).
- C43.** C. Abrioux, B. Coasne, F. Henn, G. Maurin, [Dynamique de l'eau et des cations dans des Faujasites](#). *25^e Réunion du Groupe Français des Zéolithes*, La Porte des Isles, France (2009).
- C42.** B. Coasne, A. Mezy, R. J. M. Pellenq, D. Ravot, J. C. Tedenac, [Zinc Oxide Nanostructures Confined in Porous Silicas](#). *5th Pacific Basin Conference on Adsorption Science and Technology*, Singapore (2009).
- C41.** B. Coasne, C. Alba-Simionesco, F. Audonnet, G. Dosseh, K. E. Gubbins, [Adsorption and Freezing of Benzène on Silica Surfaces and Nanopores](#). *7th International Symposium Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids*, Kazimierz Dolny, Poland (2009).
- C40.** B. Coasne, D. Horlait, A. Mezy, D. Ravot, J. C. Tedenac, [Molecular Modeling of Semiconductor Nanostructures Obtained Within Carbon Nanotubes](#). *Carbon'09: The Annual World Conference on Carbon*, Biarritz, France (2009).
- 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).

Benoit Coasne

(CNRS Research Director, Section 15)

C38. B. Coasne, K. E. Gubbins, "A simple Microscopic Model to Predict the Phase Diagram of Materials Confined in Nanopores". *JEEP XXXIV: Journées d'études des équilibres entre phases*, Marrakech, Maroc (2008).

C37. C. Abrioux, B. Coasne, G. Maurin, F. Henn, "Self-diffusivity of water in Faujasites NaY56 and NaX96: A molecular Dynamics study". *8th international symposium on the characterization of porous solids*, Edinburgh, Scotland (2008).

C36. B. Coasne, C. Alba-Simionesco, F. Audonnet, G. Dosseh, K. E. Gubbins, "Adsorption and freezing of benzene on silica surfaces and nanopores". *8th international symposium on the characterization of porous solids*, Edinburgh, Scotland (2008).

C35. R. J. M. Pellenq, B. Coasne, "A unifying approach to capillary condensation and evaporation in nanopores". *8th international symposium on the characterization of porous solids*, Edinburgh, Scotland (2008).

C34. B. Coasne, A. Galarneau, F. Di Renzo, R. J. M. Pellenq, "Adsorption and intrusion of fluids in regular and defective nanopores". *8th international symposium on the characterization of porous solids*, Edinburgh, Scotland (2008).

C33. J. Czwartos, M. Sliwinska-Bartkowiak, B. Coasne, K. E. Gubbins, "Freezing of mixtures confined in silica nanopores: Experiment and molecular simulation". *8th international symposium on the characterization of porous solids*, Edinburgh, Scotland (2008).

C32. J. Dweik, B. Coasne, F. Henn, J. Palmeri, "Ion transport at the water/air and water/nanopore interfaces". *7th Liquid Matter Conference*, Lund, Sweden (2008).

C31. B. Coasne, C. Alba-Simionesco, F. Audonnet, G. Dosseh, K. E. Gubbins, "Adsorption and Freezing of Benzene on Silica Surfaces and Nanopores". *7th Liquid Matter Conference*, Lund, Sweden (2008).

C30. C. Abrioux, A. Nicolas, B. Coasne, S. Devautour, F. Henn, G. Maurin, A. Boutin, A. Di Lella, C. Nieto-Draghi, A. H. Fuchs, "Molecular simulation and experiment of cations in zeolite upon water adsorption". *4th FEZA Conference*, Paris, France (2008).

C29. J. Czwartos, M. Sliwinska-Bartkowiak, B. Coasne, K. E. Gubbins, "Confinement effect on melting of mixtures in activated carbon fibers and silica glasses: Experiment and molecular simulation". *E-MRS 2008 Spring meeting*, Strasbourg, France (2008).

C28. B. Coasne, A. Mezy, R. J. M. Pellenq, D. Ravot, J. C. Tedenac, "Molecular modeling of the thermodynamic stability of ZnO nanostructures obtained within porous materials". *Inorganic Materials Conference*, Dresden, Germany (2008).

C27. C. Abrioux, A. Nicolas, B. Coasne, S. Devautour, F. Henn, G. Maurin, A. Boutin, A. Di Lella, C. Nieto-Draghi, A. H. Fuchs, "Molecular simulation and experiment of cations in zeolite upon water adsorption". *11^e Journées de la Matière Condensée*, Strasbourg, France (2008).

C26. A. Mezy, B. Coasne, F. Henn, R. J. M. Pellenq, D. Ravot, J. C. Tedenac, "Thermodynamical stability of ZnO nanostructures obtained within porous materials : Experiment and molecular simulation". *JEEP XXXIII: Journées d'études des équilibres entre phases*, Lyon, France (2007).

Benoit Coasne

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- C25.** N. Fekkar-Nemliche, S. Devautour-Vinot, P. Gaveau, G. Silly, **B. Coasne**, F. Henn, A. Mehdi, C. Reye, R. Corriu, "[Adsorption of water in functionalized SBA-15 probed by NMR and conductivity measurements](#)". *9th International Conference on Fundamentals of Adsorption*, Giardini Naxos, Sicily – Italy (2007).
- C24.** F. R. Hung, **B. Coasne**, S. Bhattacharya, M. Thommes, K. E. Gubbins, "[Krypton adsorption on mesoporous silica: A combined simulation and experimental approach](#)". *9th International Conference on Fundamentals of Adsorption*, Giardini Naxos, Sicily – Italy (2007).
- C23.** C. Abrioux, **B. Coasne**, G. Maurin, J. C. Giuntini, F. Henn, A. Boutin, A. H. Fuchs, C. Nieto-Draghi, "[Influence du potentiel interatomique sur la distribution cationique dans les zéolithes de type Faujasite](#)". *23^e Réunion du Groupe Français des Zéolithes*, La Grande Motte, France (2007).
- 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^e Réunion du Groupe Français des Zéolithes*, La Grande Motte, France (2007).
- C21.** A. Mezy, **B. Coasne**, F. Henn, R. J. M. Pellenq, D. Ravot, J. C. Tedenac, "[Nanostuctures ZnO obtenues dans des matériaux nanoporeux : Expérience et simulation moléculaire](#)". *23^e Réunion du Groupe Français des Zéolithes*, La Grande Motte, France (2007).
- C20.** **B. Coasne**, A. Mezy, F. Henn, R. J. M. Pellenq, D. Ravot, J. C. Tedenac, "[Atomistic simulation of ZnO nanostructures prepared in mesoporous materials](#)". *15th International Zeolite Conference*, Beijing, China (2007).
- C19.** N. Fekkar-Nemliche, S. Devautour-Vinot, G. Silly, **B. Coasne**, F. Henn, A. Mehdi, C. Reye, R. Corriu, "[Water confined in functionalized SBA-15 probed by NMR and conductivity measurements](#)". *15th International Zeolite Conference*, Beijing, China (2007).
- C18.** C. Abrioux, **B. Coasne**, G. Maurin, A. Boutin, J. C. Giuntini, A. H. Fuchs, F. Henn, P. Ungerer, "[Influence of the cation/zeolite interatomic potentials on the cation distribution in faujasites](#)". *15th International Zeolite Conference*, Beijing, China (2007).
- C17.** R. J. M. Pellenq, **B. Coasne**, "[Effect of pore morphology and topology on adsorption and capillary condensation in nanopores](#)". *Thermodynamics 2007*, Rueil-Malmaison, France (2007).
- C16.** **B. Coasne**, F. Di Renzo, A. Galarneau, "[Adsorption et Condensation dans des silices mésoporeuses MCM-41, MCM-48 et SBA-15](#)". *22^e Réunion du Groupe Français des Zéolithes*, La Rochelle, France (2006).
- C15.** A. Galarneau, B. Lefèvre, H. Cambon, **B. Coasne**, S. Valange, Z. Gabelica, J. P. Bellat, F. Di Renzo, "[La Taille des pores des silices mésoporeuses par adsorption d'azote et pénétration de mercure](#)". *22^e Réunion du Groupe Français des Zéolithes*, La Rochelle, France (2006).

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- C14.** S. Devautour-Vinot, **B. Coasne**, N. Fekkar-Nemmiche, F. Henn, A. Mehdi, C. Reye, R. Corriu, "Dielectric Spectroscopy to probe adsorption and confinement effect in functionalised mesoporous silica". *3rd International Workshop on Dynamics in Confinement*, Grenoble, France (2006).
- C13.** R. J. –M. Pellenq, **B. Coasne**, R. O. Denoyel, J. Puibasset, "A theoretical and molecular simulation study on the effect of pore morphology and topology on capillary condensation in nanopores". *3rd International Workshop on Dynamics in Confinement*, Grenoble, France (2006).
- C12.** S. Bhattacharya, **B. Coasne**, F. R. Hung, K. E. Gubbins, "A molecular simulation study of gas adsorption in nanoporous silica". *7th Liblice Conference on Statistical Mechanics of Liquids*, Lednice, Czech Republic (2006).
- C11.** **B. Coasne**, K. E. Gubbins, F. R. Hung, R. J. –M. Pellenq, "Capillary condensation within MCM-41 materials: The role of surface disorder". *7th Liblice Conference on Statistical Mechanics of Liquids*, Lednice, Czech Republic (2006).
- 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". *9th International Conference on Dielectric and Related Phenomena*, Poznan, Poland (2006).
- C9.** B. Ratajczak, M. Sliwinska-Bartkowiak, **B. Coasne**, K. E. Gubbins, "Apparent critical point in binary mixtures: Experimental and simulation study". *US – Poland Workshop on Nanoscience and Nano-Structured Materials*, Poznan, Poland (2006).
- C8.** B. Ratajczak, **B. Coasne**, M. Sliwinska-Bartkowiak, "Apparent critical point in binary mixtures m-nitrotoluene with n-alkanes: Experimental and simulation study". *9th International Conference on Dielectric and Related Phenomena*, Poznan, Poland (2006).
- C7.** M. Sliwinska-Bartkowiak, M. Jazdzewska, F. R. Hung, **B. Coasne**, K. E. Gubbins, "Freezing of CCl₄ within carbon nanotubes: a combined experimental and simulation approach". *Thermodynamics 2005*, Sesimbra, Portugal (2005).
- C6.** **B. Coasne**, J. Czwartos, K. E. Gubbins, F. R. Hung, M. Sliwinska-Bartkowiak, "Confinement Effect on Freezing of Binary Mixtures". *7th international symposium on the characterization of porous solids*, Aix-en-Provence, France (2005).
- C5.** S. Bhattacharya, **B. Coasne**, F. R. Hung, K. E. Gubbins, "Modeling and Characterization of Triblock Surfactant Templated Mesoporous Silicas". *7th 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". *8th International Conference on Fundamentals of Adsorption*, Sedona, USA (2004).

Benoit Coasne

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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](#)". *6th international symposium on the characterization of porous solids*, Alicante, Spain (2002).

C1. B. Coasne, A. Grosman, N. Dupont-Pavlovsky, C. Ortega, M. Simon, "[Adsorption in an ordered and non-interconnected mesoporous material: Single crystal silicon](#)". *International discussion meeting on Physical Chemistry in Confining Geometries*, Berlin, Germany (2000).

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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).

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- 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).

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- 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).

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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).

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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

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