



### **PART A: CURRICULUM VITAE**

Benoit COASNE (Male, 45 ans, 1 child, 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: http://www-liphy.ujf-grenoble.fr/benoit-coasne

#### Research Theme

« Adsorption, phase transitions and transport in porous media »

#### 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 »

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

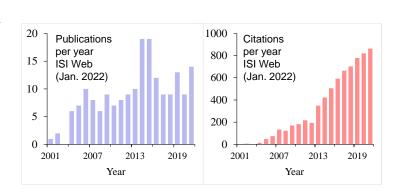
190 Articles (3 Nature Mat, 6 Nat Comm, 2 Chem Soc Rev, 2 PNAS, 2 JACS, 4 PRL., 3 J Phys Chem Lett)

45 H-index (51 Google Scholar)

**6825** Citations

44 Invited Conferences

75 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 (1 week), Adam Mickiewicz University, Poznan, Poland

(CNRS Research Director, Section 15)

#### RESPONSIBILITIES, MANAGEMENT AND SCIENTIFIC ANIMATION

#### Responsibilities

2022/	Board Member Division Chimie Physique, Société Chimique de France
2021/	(French) Chair, French/German Adsorption Cluster
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 Enginers
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	Bureau member, French Zeolite Society
2009/12	Bureau member, Local section LR of the French Chemical Society SCF

#### **Commission of Trust**

2022/24	Scientific Council Expert, IFP Energies Nouvelles
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

2018	Colloquium Chair "Matériaux poreux, granulaires, et à grande
	surface spécifique" – Conference Matériaux 2018, Strasbourg, France
2018	Symp. Chair "Soft Porous Materials" Interpore2018, N. Orleans (USA)
2010/17	Journées Annuelles Association Française de l'Adsorption (~ 70 personnes)
2011/16	Journées Annuelles Groupe Français des Zéolithes (~ 80 personnes)
2013	Ionic Liquids for Materials (~ 100 participants) ILMAT2013, Montpellier
2010	Journées SCF Grand Sud Ouest (~80 participants), Montpellier

#### Student and postdoc supervision (15 PhD, 18 postdocs, 13 undergrad)

• 16 PhD Students 1. J. Dweik, 2. C. Abrioux, 3. P. Bonnaud, 4. F. Villemot, 5. M. Lepinay (St Micro), 6. P. Billemont (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. Zaafouri (IFPEN), 14. S. Cohen (U. Maryland, Chateaubriand Fellow), 15. W. Kellouai, 16. N. Ferreira de Souza • 17 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. Billemont, 10. T. Lee, 11. A. Obliger, 12. G. Couchaux, 13. D. Mehlhorn, 14. A. Schlaich, 15. R. Manokaran, 16. A. Sam, 17. V. Prasad • 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. Tabacchioni, 12. Z. Zaafouri, 13. M. Barbagero, 14. K. Olson, 15. P. Sanchez-Moreno Royer

(CNRS Research Director, Section 15)

#### PhD and Habilitation Jurys (38 including R = Reviewer, P = President)

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. Louisfrema (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-Jamois (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)

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Contrat	Période	Organisme	Partners	Montant	Responsabilité
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 <b>€*</b>	Partner
SiMoNanoMem	2008/10	ANR	4	400 k€	Partner
Eau, Electro	2009/10	CINES	1	CPU Time	Coordin.

### Partnership with industry/Consulting

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

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# FORMATION, TEACHING, DISSEMINATION

# Teaching (> 40h/year since 2016)

2016/	Res. 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 Etonante CNRS (D. Farrusseng, B. Coasne)
2020	"Des matériaux fonctionnels à l'échelle du nanomètre (Cahier Tech-
	nique)" Usine Nouvelle (D. Farrusseng, B. Coasne)
2016	Article by P. Passebon in "Industrie & Technologies"
	https://www.industrie-techno.com/comprendre-les-gaz-de-schiste-pour-
	mieux-les-exploiter.42366
2012	"Gel de l'eau dans les mésopores du ciment" (Bonnaud, Pellenq,
	Coasne),
	Ciments, Bétons, Plâtres et Chaux 907, 64 (2012).
2012	"City texture matters" CSH MIT, Res. Profile Lett. (J. M. Sobstyl et al.)
2010	Internship 5 days L'Express.fr (French newspaper). 2 published ar-
	ticles: Bousquet/Coasne, « Nous comprenons les consommateurs d'eau
	en bouteilles » et Coasne, « 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
2000	Schillar for riight School Students off Research in France

(CNRS Research Director, Section 15)

#### **PART B: SCIENTIFIC PRODUCTION**

Publications in peer-reviewed journals (172)
including 4 invited review articles (titles in red)
 Communication/press releases are indicated in green

# In Preparation

**P179.** 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, To be submitted (2022).

**P178.** 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, To be submitted (2022).

# **Submitted**

- **P177.** Z. Zaafouri, G. Batot, C. Nieto-Draghi, B. Rotenberg, **B. Coasne**, D. Bauer, Impact of adsorption kinetics on pollutant dispersion in water flowing through porous media, To be submitted (2022).
- **P176.** 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, Submitted (2022).
- **P175.** V. Wernert, K. L. Nguyen, P. Levitz, **B. Coasne**, R. Denoyel, Impact of surface diffusion on transport through porous materials, To be submitted (2022).
- **P174.** J. W. M. Osterrieth et al., How reproducible are surface areas calculated from the BET equation?, Submitted (2022).
- **P173.** I. C. Medeiros-Costa, C. Laroche, **B. Coasne**, J. Pérez-Pellitero, Xylene Selectivity at the External Surface of Hierarchical Zeolites: Experiment and Molecular Modeling, *Langmuir*, Submitted (2022).

- (CNRS Research Director, Section 15)
- **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.*, in press (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.*, in press (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.** 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).
- **P168.** 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*, in press (2021).
- + CNRS communication: https://www.inp.cnrs.fr/index.php/fr/cnrsinfo/un-fluide-virtuel-pour-simuler-des-liquides-charges-confines
- **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 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, Hygrome-chanical mechanisms of wood cell wall revealed by molecular modeling and mixture rule analysis: Role of components, interphases and hydrogen bonding, *Sci. Adv.* **7**, eabi8919 (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).

- (CNRS Research Director, Section 15)
- **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).

- **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).

- (CNRS Research Director, Section 15)
- **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).

- **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).
- **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), *Microp. Mesop. Mater.* **287**, 167 (2019).
- **P141. B. Coasne**, D. Farrusseng, Gas oversolubility in nanoconfined liquids: Review and perspectives (invited review paper), *Microp. 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, Woodmoisture relationships studied with molecular dynamics methodological guidelines, *Forests* **10**, 628 (2019).

- (CNRS Research Director, Section 15)
- **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).

# 2001 - 2018

- **P134.** M. Bah, E. D. Manga, H. Blasco, P. Da Costa, M. Drobek, **B. Coasne**, A. Ayral, 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).
- **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
- $+ CNRS \quad communication: \quad https://inp.cnrs.fr/fr/cnrsinfo/pourquoi-le-gonflement-de-lacellulose-lors-de-son-hydratation-est-irreversible$
- **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).
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- **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).
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- **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).

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- **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).
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- **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).
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- **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).
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- **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. 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).

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- **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 (19)

- **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 Enginers), 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 Enginers), 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 Enginers), 14-19 (2017).
- **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 Enginers) (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).

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- **A10.** N. Fekkar-Nemmiche, 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).
- **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).

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- **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 (44)

- **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 Universita 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 Conference on Engineering Mechanics and Physics of Porous Materials, Northwestern University, Chicago, USA (2021). Visioconference.
- **I36. B. Coasne**, Fluid adsorption and diffusion in nanoporous materials, *APS March Meeting*, USA (2021). Visioconference.
- **I35. B. Coasne**, Adsorption and diffusion in porous materials, 10<sup>b</sup> 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).

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- **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).
- **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'), *Materiaux 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 Enginers, 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, 6<sup>th</sup> International Symposium "Advanced microporous and mesoporous materials", Black Sea Coast, Bulgaria (2015).

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- **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).
- **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, 4<sup>th</sup> International Workshop on Crystallization in Porous Media, Amsterdam, Netherlands (2014).
- **I10. B. Coasne**, Chemistry of interfaces between inorganic minerals and porous carbons: implications for the mechanical properties of gas shale, *Society of Engineering Science* and American Society of Mechanical Engineering Annual Meetings, Providence, RI, USA (2013).
- **19**. **B. Coasne**, "Adsorption, intrusion, and freezing in porous silica: the view from the nanoscale". 3<sup>rd</sup> International Conference on Nanotek (Nanotek 2013), Las Vegas, NV, USA.
- **I8**. **B. Coasne**, "Pressure effects in nanoconfined phases". 5<sup>th</sup> Biot Conference on Poromechanics, Vienna, Austria (2013).
- **I7**. **B. Coasne**, "Adsorption and transport in hierarchical zeolites: the view from the nanoscale". 2<sup>nd</sup> Worskshop 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". 32<sup>nd</sup> 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". *26e Réunion du Groupe Français des Zéolithes*, Presqu'ile 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).
- II. B. Coasne, "Transition de phase dans des matériaux nanoporeux". Matériaux Hybrides Organisés Multifonctionnels (HMOM), La Grande Motte, France (2006).

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#### 5. Oral communications in conferences (170)

- **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 Hierachical Porous Materials, *INTERPORE* 2019, Valencia, Spain (2019).
- **O166.** M. Bah, E. D. Manga, P. da Costa, M. Drobek, A. Ayral, G. Despaux, 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 Asdorption 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.** <u>B. Coasne</u>, 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. Despaux, P. Da Costa, A. Ayral, B. Coasne, <u>A. Julbe</u>, 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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- **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. Zaafouri, 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, <u>A. Ayral</u>, 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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- **O43.** C. Abrioux, A. Nicolas, <u>B. Coasne</u>, 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 partioning and transport in nanoporous membranes". *Engineering with Membranes 2008*, Algarve, Portugal (2008).
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- **O40.** <u>B. Coasne</u>, 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).
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- **O36.** <u>B. Coasne</u>, 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).
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- **O32.** <u>B. Coasne</u>, F. Di Renzo, A. Galarneau, R. J. M. Pellenq, "Adsorption et intrusion de fluides dans des silices nanoporeuses présentant des défauts morphologiques". 23<sup>e</sup> Réunion du Groupe Français des Zéolithes, La Grande Motte, France (2007).
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- **O28.** <u>B. Coasne</u>, S. K. Jain, K. E. Gubbins, "Freezing of argon in a disordered nanoporous structure". *3<sup>rd</sup> International Workshop on Dynamics in Confinement*, Grenoble, France (2006).
- **O27.** <u>B. Coasne</u>, 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).
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- **O25.** S. Bhattacharya, <u>K. E. Gubbins</u>, **B. Coasne**, F. R. Hung, "Molecular simulation of gas adsorption in mesoporous silica SBA-15". 4<sup>th</sup> 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.** <u>B. Coasne</u>, S. K. Jain, K. E. Gubbins, "Freezing and melting in ordered and disordered porous carbons". 7<sup>th</sup> 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.** <u>B. Coasne</u>, S. K. Jain, K. E. Gubbins, "Freezing of fluids confined in ordered and disordered porous carbons". 6<sup>th</sup> 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<sup>e</sup> 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, <u>B. Coasne</u>, 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).

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- **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)*, Cincinnatti, 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)*, Cincinnatti, 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.** <u>B. Coasne</u>, 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.** <u>B. Coasne</u>, 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.** <u>B. Coasne</u>, 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).

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- **O4.** <u>B. Coasne</u>, 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". 6<sup>th</sup> international symposium on the characterization of porous solids, Alicante, Spain (2002).
- **O3.** <u>B. Coasne</u>, 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<sup>eme</sup> édition des Journées simulation numérique, Matière condensée et Désordre Interface simulation/expérience, Paris, France (2002).
- **O2. B. Coasne**, <u>A. Grosman</u>, 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.** <u>B. Coasne</u>, 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).

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- C103. I. C. Medeiros-Costa, C. Laroche, J. Perez-Pellitero, B. Coasne, Advanced characterization of hierarchical zeolites for optimal xylene separation, 1<sup>st</sup> International Meeting of the Group Français 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. Zaafouri, 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. Despaux, Philippe Da Costa, B. Coasne, A. Ayral, 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, Breakthrough 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, 10<sup>th</sup> 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<sup>e</sup> 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).
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- **C84.** R. Hartkamp, R. J. M. Pellenq, **B. Coasne**, Adsorption and transport of ions confined in realistic porous materials: from simple to radioactive ions, 9<sup>th</sup> Liquid Matter Conference, Lisboa, Portugal (2014).
- **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, 6<sup>th</sup> 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, 6<sup>th</sup> 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, *2emes 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, 5<sup>th</sup> Biot Conference on Poromechanics, Vienna, Austria (2013).
- **C68.** L. Ngoc Ho, S. Clauzier, Y. Schuurman, D. Farrusseng, **B. Coasne**, Gas oversolubility in solvents nanoconfined in mesoporous silica: adsorption-driven versus bulk-like solubility mechanisms, 29<sup>e</sup> 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<sup>e</sup> 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<sup>e</sup> 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<sup>e</sup> 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, 2<sup>nd</sup> 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, 2<sup>nd</sup> 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<sup>e</sup> 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<sup>e</sup> 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<sup>eres</sup> 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<sup>e</sup> Reunion du Groupe Français des Zeolites, Areches, France (2011).
- **C54.** M. Manko, W. Makowski, **B. Coasne**, A. Galarneau, Thermodesorption as a new tool to characterize hierarchical micro/mesoporous materials, 27<sup>e</sup> Reunion du Groupe Français des Zeolites, Areches, France (2011).
- **C53.** M. Manko, W. Makowski, **B. Coasne**, A. Galarneau, Thermodesorption as a new tool to characterize hierarchical micro/mesoporous materials, 5<sup>th</sup> international FEZA conference, Valencia, Spain (2011).

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- **C52.** Y. Long, J. C. Palmer, B. Coasne, M. Sliwinska-Bartkowiak, K. E. Gubbins, Under pressure: quasi-high pressure effects in nanopores, 9<sup>th</sup> 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, 4<sup>h</sup> 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. Billemont, 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<sup>e</sup>* 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).

- (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". 8<sup>th</sup> 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". 8<sup>th</sup> 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". 8<sup>th</sup> 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". 8<sup>th</sup> 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". 8<sup>th</sup> 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". *11e 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).

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- **C25.** N. Fekkar-Nemmiche, 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". *23º Réunion du Groupe Français des Zéolithes*, La Grande Motte, France (2007).
- **C22.** N. Bibent, N. Fekkar-Nemmiche, S. Devautour-Vinot, G. Silly, P. Gaveau, **B. Coasne**, F. Henn, R. Mouawia, A. Mehdi, C. Reye, R. J. P. Corriu, "Mobilité des charges ioniques dans des silices mésoporeuses fonctionnalisées sous l'influence d'adsorption d'eau". *23<sup>e</sup>* Réunion du Groupe Français des Zéolithes, La Grande Motte, France (2007).
- **C21.** A. Mezy, **B. Coasne**, F. Henn, R. J. M. Pellenq, D. Ravot, J. C. Tedenac, "Nanostructures ZnO obtenues dans des matériaux nanoporeux: Expérience et simulation moléculaire". *23<sup>e</sup>* 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-Nemmiche, 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<sup>e</sup> 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<sup>e</sup> 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 Specroscopy to probe adsorption and confinement effect in functionalised mesoporous silica". *3<sup>rd</sup> 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". 7<sup>th</sup> 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 CCl<sub>4</sub> 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).

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- **C2. B. Coasne**, A. Grosman, C. Ortega, "Study of capillary condensation hysteresis in mesoscopic pores: Comparison between adsorption in P + type porous silicon and adsorption in SBA". 6<sup>th</sup> international symposium on the characterization of porous solids, Alicante, Spain (2002).
- **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 (75)

- **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 Universitat*, 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).
- **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).

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- **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).
- **\$55.** "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), Universite 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 Strasbroug, France (Oct. 03, 2014).
- **\$50.** "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).
- **S42.** "High pressure effects in nanoconfined phases", Laboratoire Charles Coulomb (L<sub>2</sub>C), 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).

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- **S40.** "Simulation et modélisation de la dynamique et du transport dans des nanomembranes", Journées Avenir de la fillière 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 Strasbroug, 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).
- **\$35.** "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.** "Modelisation moleculaire 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)
- **\$30.** "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)
- **\$29.** "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).
- **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 Gerhart Montpellier*, Montpellier, France (2009).

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- **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, Tecknische Universitat Berlin, Berlin, Germany (December 11, 2007).
- **\$16.** "Transitions de phase de fluides confinés dans des matériaux nanoporeux", Laboratoire de Chimie Physique, CNRS Université de Paris-Sud Orsay (January 13, 2006).
- **\$15.** "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).
- **\$13.** "Transitions de phase de fluides confinés dans des matériaux nanoporeux", Laboratoire des Colloides, 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).
- **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).

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- **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 MADI-REL, 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).
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(CNRS Research Director, Section 15)

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