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Full publication list

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Full publication list

In peer-reviewed international journals

129. "Structure of Metal-Organic Framework Glasses by Ab Initio Molecular Dynamics", R. Gaillac, P. Pullumbi, T. D. Bennett and F.-X. Coudert, *Chem. Mater.*, **2020**, in press.

128. "Engineering micromechanics of soft porous crystals for negative gas adsorption", S. Krause, J. D. Evans, V. Bon, I. Senkovska, S. Ehrling, P. Iacomi, D. M. Többens, D. Wallacher, M. S. Weiss, B. Zheng, P. G. Yot, G. Maurin, P. L. Llewellyn, F.-X. Coudert and S. Kaskel, *Chem. Sci.*, **2020**, in press.

127. "Machine learning approaches for the prediction of materials properties", S. Chibani and F.-X. Coudert, *APL Mater.*, **2020**, 8, 080701.

126. "Water Adsorption in Soft and Heterogeneous Nanopores", F.-X. Coudert, *Acc. Chem. Res.*, **2020**, 53, 1342–1350.

125. "Isolating the Role of the Node-Linker Bond in the Compression of UiO-66 Metal-Organic Frameworks", L. R. Redfern, M. Ducamp, M. C. Wasson, L. Robison, F. A. Son, F.-X. Coudert and O. K. Farha, *Chem. Mater.*, **2020**, 32, 5864–5871.

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23. "Structural Transitions in MIL-53 (Cr): View from Outside and Inside", A. V. Neimark, F.-X. Coudert, C. Triguero, A. Boutin, A. H. Fuchs, I. Beurroies and R. Denoyel, *Langmuir*, **2011**, 27, 4734–4741.

22. "Thermodynamic Methods and Models to Study Flexible Metal-Organic Frameworks", F.-X. Coudert, A. Boutin, M. Jeffroy, C. Mellot-Draznieks and A. H. Fuchs, *ChemPhysChem*, **2011**, 12, 247–258.

21. "Thermodynamic Analysis of the Breathing of Amino-functionalized MIL-53(Al) upon CO_2 Adsorption", A. Boutin, S. Couck, F.-X. Coudert, P. Serra-Crespo, J. Gascon, F. Kapteijn, A. H. Fuchs and J.F.M. Denayer, *Micro. Meso. Mater.*, **2011**, 140, 108–113.

20. "The Behavior of Flexible MIL-53(Al) upon CH_4 and CO_2 Adsorption", A. Boutin, F.-X. Coudert, M.-A. Springuel-Huet, A. V. Neimark, G. Férey and A. H. Fuchs, *J. Phys. Chem. C*, **2010**, 114, 22237–22244.

19. "Understanding the Effect of Confinement on the Liquid–Gas Transition: A Study of Adsorption Isotherms in a Family of Metal–Organic Frameworks", M. De Toni, P. Pullumbi, F.-X. Coudert and A. H. Fuchs, *J. Phys. Chem. C*, **2010**, 114, 21631–21637.

18. "The osmotic framework adsorbed solution theory: predicting mixture coadsorption in flexible nanoporous materials", F.-X. Coudert, *Phys. Chem. Chem. Phys.*, **2010**, 12, 10904–10913.

17. "Water adsorption in hydrophobic MOF channels", S. Paranthaman, F.-X. Coudert and A. H. Fuchs, *Phys. Chem. Chem. Phys.*, **2010**, 12, 8123–8129.

16. "Stress-Based Model for the Breathing of Metal–Organic Frameworks", A. V. Neimark, F.-X. Coudert, A. Boutin and A. H. Fuchs, *J. Phys. Chem. Lett.*, **2010**, 1, 445–449.

15. "Breathing Transitions in MIL-53(Al) Metal–Organic Framework Upon Xenon Adsorption", A. Boutin, M.-A. Springuel-Huet, A. Nossov, A. Gédéon, T. Loiseau, T. Volkringer, G. Férey, F.-X. Coudert and A. H. Fuchs, *Angew. Chem. Int. Ed.*, **2009**, 48, 8314–8317.

14. "Prediction of Breathing and Gate-Opening Transitions Upon Binary Mixture Adsorption in Metal-Organic Frameworks", F.-X. Coudert, C. Mellot-Draznieks, A. H. Fuchs and A. Boutin, *J. Am. Chem. Soc.*, **2009**, 131, 11329–11331.

13. "Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues", D. W. Lewis, A. R. Ruiz-Salvador, A. Gomez, L. M. Rodriguez-Albelo, F.-X. Coudert, B. Slater, A. K. Cheetham and C. Mellot-Draznieks, *CrystEngComm*, **2009**, 11, 2272–2276.

12. "Double Structural Transition in Hybrid Material MIL-53 upon Hydrocarbon Adsorption: The Thermodynamics Behind the Scenes", F.-X. Coudert, C. Mellot-Draznieks, A. H. Fuchs and A. Boutin, *J. Am. Chem. Soc.*, **2009**, 131, 3442–3443.

11. "Water nanodroplets confined in zeolite pores", F.-X. Coudert, F. Cailliez, R. Vuilleumier, A. H. Fuchs and A. Boutin, *Faraday Discuss.*, **2009**, 141, 377–398.

10. "Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organic–Inorganic Frameworks", F.-X. Coudert, M. Jeffroy, A. H. Fuchs, A. Boutin and C. Mellot-Draznieks, *J. Am. Chem. Soc.*, **2008**, 130, 14294–14302.

9. "Mechanism and kinetics of hydrated electron diffusion", K. A. Tay, F.-X. Coudert and A. Boutin, *J. Chem. Phys.*, **2008**, 129, 054505.

8. "Temperature Effect on the Absorption Spectrum of the Hydrated Electron Paired with a Lithium Cation in Deuterated Water", M. Lin, Y. Kumagai, I. Lampre, F.-X. Coudert, Y. Muroya, A. Boutin, M. Mostafavi and Y. Katsumura, *J. Phys. Chem. A*, **2007**, 111, 3548–3553.

7. "Dipole Moment, Hydrogen Bonding and IR Spectrum of Confined Water", F.-X. Coudert, R. Vuilleumier and A. Boutin, *ChemPhysChem*, **2006**, 7, 2464–2467.

6. "Confinement effect on the hydrated electron behaviour", F.-X. Coudert and A. Boutin, *Chem. Phys. Lett.*, **2006**, 428, 68–72.

5. "Molecular Dynamics Simulations of Electron-Alkali Cation Pairs in Bulk Water", F.-X. Coudert, P. Archirel and A. Boutin, *J. Phys. Chem. B*, **2005**, 110, 607–615.

4. "Molecular dynamics simulations of the temperature and density dependence of the absorption spectra of hydrated electron and solvated silver atom in water", A. Boutin, R. Spezia, F.-X. Coudert and M. Mostafavi, *Chem. Phys. Lett.*, **2005**, 409, 219–223.

3. "Theoretical Study of Neutral Dipolar Atom in Water: Structure, Spectroscopy and Formation of an Excitonic State", R. Spezia, F.-X. Coudert and A. Boutin, *Mod. Phys. Lett. B*, **2004**, 18, 1327–1345.

2. "Reactivity of an Excess Electron with Monovalent Cations in Bulk Water by Mixed Quantum Classical Molecular Dynamics Simulations", R. Spezia, C. Nicolas, F.-X. Coudert, P. Archirel, R. Vuilleumier and A. Boutin, *Mol. Simul.*, **2004**, 30, 749–754.

1. "Distribution of Sodium Cations in Faujasite-Type Zeolite: A Canonical Parallel Tempering Simulation Study", C. Beauvais, X. Guerrault, F.-X. Coudert, A. Boutin and A. H. Fuchs, *J. Phys. Chem. B*, **2004**, 108, 399–404.

In conference proceedings

2. "Adsorption-Induced Breathing transitions in Metal-Organic Frameworks", A. H. Fuchs, F.-X. Coudert, C. Triguero, A. Boutin and A. V. Neimark, *Poromechanics V, Proceedings of the Fifth Biot Conference on Poromechanics*, Vienna (2013), Ed. C. Hellmich, B. Pichler, D. Adam, p. 626.

1. "Hydrothermal and Mechanical Stability of Metal–Organic Frameworks", F.-X. Coudert, A. Ortiz, M. De Toni, A. Boutin and A. H. Fuchs, *CONCREEP-9@MIT, Proceedings of the Ninth Conference on Creep, Shrinkage and Durability Mechanics of Concrete and other Quasi-Brittle Materials*, Cambridge MA (2013), Ed. H. M. Jennings, F.-J. Ulm, R. Pellenq.

Book chapters

9. "Modeling of zeolites: from the unit cell to the crystal", F.-X. Coudert and A. H. Fuchs, in *Verified Syntheses of Zeolitic Materials (3rd edition)*, Elsevier (2016).

8. "Thermodynamic Methods for Prediction of Gas Separation in Flexible Frameworks", F.-X. Coudert, in *Metal-Organic Frameworks, Applications from Catalysis to Gas Storage*, D. Farrusseng, Wiley-VCH (2011).

7. "Dynamique moléculaire mixte classique-quantique de l'électron hydraté", A. Boutin and F.-X. Coudert, in *Réactions ultrarapides en solution — Approches expérimentales et théoriques*, T. Gustavsson and M. Mostafavi, CNRS Éditions (2007).

1–6. *Annales des concours*, sessions 2003 à 2005, aux éditions H&K: corrigés des épreuves de chimie des concours d'entrée des grandes écoles (*book of exams with complete hints and solutions, for French schools of engineering*).

In non peer-reviewed publications (comments, etc.)

- "Charting a course for chemistry", A. Aspuru-Guzik et al, *Nature Chemistry*, **2019**, 1, 286–294.
- "Des matériaux poreux au comportement extraordinaire", F.-X. Coudert, *L'Actualité chimique*, **2019**, 438–439, 125–126.
- "D'une vision scientifique à une vision sociétale", J.-P. Djukic et al., *L'Actualité chimique*, **2019**, 436, 15–18.
- "New materials: when chemistry combines metals and organic molecules", F.-X. Coudert, *Paris Innovation Review*, **2017**.
- "Strontium's scarlet sparkles", F.-X. Coudert, *Nature Chemistry*, **2015**, 7, 940.
- "Comment etiquette", F.-X. Coudert, *Nature Chemistry*, **2015**, 7, 369.
- "Setting the record straight", F.-X. Coudert, *Chemistry World*, **2015**, March issue, page 40.
- "This Study is Intentionally Left Blank", G. Wright, F.-X. Coudert, M. Bentley, G. Steel, and S. Deville, *Annals of Improbable Research*, **2015**, 21, 14–19 (available on figshare).

In media

- "Mendeleïev, le tableau s'alourdit", F.-X. Coudert, *La Méthode Scientifique*, France Culture, 26/02/2019.
- "Les 150 ans du tableau périodique des éléments de Mendeleïev", F.-X. Coudert, *La Tête au carré*, France Inter, 14/02/2019.
- "Le tableau périodique des éléments fête ses 150 ans", F.-X. Coudert, *La Tête au carré*, France Inter, 31/01/2019.
- "CO_2 : comment lui tendre un piège ?", F.-X. Coudert, *La Méthode Scientifique*, France Culture, 02/01/2019.
- "Le règne des matériaux poreux sur mesure", F.-X. Coudert, *La Recherche*, **2018**, 532, 60–65.
- "L'eau, une histoire trouble", F.-X. Coudert, *La Méthode Scientifique*, France Culture, 23/03/2017.
- "Mendeleïev : un tableau enfin complet ?", F.-X. Coudert, *La Méthode Scientifique*, France Culture, 11/01/2017.

Oral communications

As invited speaker (28)

- "Molecular simulation of soft porous crystals", *26th International Conference on Chemical Thermodynamics*, 19–23 July 2020, London (UK) — cancelled due to COVID-19.
- "The most flexible state of MOFs is the liquid!", *FlexMOF Symposium 2019*, 4–5 December 2019, Dresden (Germany).
- "Flexibility, defects and disorder in soft porous crystals", *Okinawa Colloids 2019*, 3–8 November 2019, Okinawa (Japan).
- "Soft Porous Crystals: Extraordinary Responses to Stimulation", *14th International conference on materials chemistry (MC14)*, 8–11 July 2019, Birmingham (UK).
- "Modelling Defects and Disorder in Nanoporous Materials", *MOFSIM 2019*, 10–12 April 2019, Ghent (Belgium).
- "Soft Porous Crystals: Extraordinary Responses to Stimulation", *MOF 2018*, 9–13 December 2018, Auckland (New Zealand).
- "Flexibility, defects and disorder in soft porous crystals", *SMARTER6*, 2–6 September 2018, Ljubljana (Slovenia).
- "Soft Porous Crystals: Extraordinary Responses to Stimulation", *Japanese Society of Coordination Chemistry*, 28–30 July 2018, Sendai (Japan).
- "Soft Porous Crystals: Extraordinary Responses to Stimulation", *GFZ International Congress*, 26–29 March 2018, Cabourg (France).
- "Soft Porous Crystals, Molecular Insight from Computational Chemistry", *Thermodynamics 2017*, 5–8 September 2017, Edinburgh (UK).
- "Flexibility, Defects & Disorder in Soft Porous Crystals", *7th FEZA Conference — Federation of European Zeolite Associations*, 3–7 July 2017, Sofia (Bulgaria).
- "Mechanical Impact of Adsorption in Compliant Nanoporous Materials", *Characterization of Porous Solids (COPS-XI)*, 14–17 May 2017, Avignon (France).
- "Flexibility, Defects & Disorder in Soft Porous Crystals", *Switchability in Porous Metal-Organic Frameworks*, 13-14 March 2017, Dresden (Germany).
- "Coupling transport and adsorption through Lattice Boltzmann methods", *EMN Meeting on Mesoporous Materials*, 13–17 June 2016, Prague (Czech Republic).
- "Mechanical impact of adsorption in compliant microporous materials", *12th International Conference on the Fundamentals of Adsorption*, 30 May to 3 June 2016, Friedrichshafen (Germany).
- "First-principles dynamics and free energy methods for flexible materials", *CP2K-UK Conference*, 22 February 2016, London (UK).
- "Computational characterization of flexibility and disorder: from the unit cell to the crystal", *Frontiers in Materials Science, Cambridge-JNCASR Winter School*, 7–11 December 2015, Bangalore (India).
- "Molecular simulation of materials flexibility and disorder", *International workshop on Flexibility and Disorder in Metal–Organic Frameworks*, 3–5 June 2015, Paris (France).
- "Polymorphism and Flexibility in Nanoporous Molecular Frameworks", *CPM-7: 7th International Workshop on the Characterization of Porous Materials*, 3–6 May 2015, Delray Beach FL (USA).
- "On the Impact of Adsorption in Compliant Nanoporous Materials", *4th Symposium on Future Challenges for Carbon-based Nanoporous Materials*, 16–18 March 2015, Nagano (Japan).
- "Interfaces and porous materials: Insight from Molecular Simulation", *CAPZEO-2014: Fourth International Summer School on Quantum Electronic Calculations*, 8–12 June 2014, Rabat (Morroco).
- "Theoretical Insight into Soft Porous Crystals", *CFCAM meeting on simulation of systems under thermodynamic gradients*, 25–26 March 2014, Paris (France).
- "Anisotropic Elastic Properties of Flexible Metal–Organic Frameworks", *International symposium on CO_2 capture*, 18–20 September 2013, Marne-la-Vallée (France).
- "Modeling of Soft Porous Crystals: From the Unit Cell to the Crystal", Gordon Research Conference *Nanoporous Materials & Their Applications*, 11–16 August 2013, Holderness NH (USA).
- "Structural transitions in metal–organic frameworks: thermodynamics & mechanics", *International workshop on adsorption in compliant solids*, 5–7 June 2013, Paris (France).

- "Ab Initio Investigation into the Hydration Mechanism of IRMOFs", CECAM/GDRi workshop on *Aging of Engineering Materials*, 8–10 February 2012, Zürich (Switzerland).
- "Effect of confinement on water in zeolite nanopores", *Indo French Seminar on Diffusion in Nanoporous and Dense Media*, 1–5 April 2009, Bangalore (India).
- "Water nanodroplets confined in zeolite pores", Faraday Discussion 141: *Water, From Interfaces to Bulk*, 27–29 August 2008, Edinburgh (UK).

In international conferences (20)

- "Flexibility, Defects & Disorder in Soft Porous Crystals: Molecular Insight from Computational Chemistry", *12th International Conference on the Fundamentals of Adsorption*, 30 May – 3 June 2016, Friedrichshafen (Germany).
- "Assessing and predicting flexibility in MOFs with molecular simulation", *EUROMOF 2015, 1st European Conference on Metal Organic Frameworks and Porous Polymers*, 11–14 October 2015, Potsdam (Germany).
- "Molecular simulation of stimuli-responsive framework materials", *12th International Conference on Materials Chemistry (MC12)*, 20–23 July 2015, York (UK).
- "Polymorphism in nanoporous materials: assessing mechanical, thermal stability, and experimental feasibility", *249th ACS National Meeting* (PHYS division), 22–26 March 2015, Denver CO (USA).
- "Assessing and predicting flexibility in framework materials with molecular simulation", *249th ACS National Meeting* (COMP division), 22–26 March 2015, Denver CO (USA).
- "Remarkable Pressure Responses of MOFs: Proton Transfer, Linker Coiling, Order-to-Disorder Transitions", *249th ACS National Meeting* (PMSE division), 22–26 March 2015, Denver CO (USA).
- "Fluids in Soft Porous Crystals: Coupling Adsorption and Deformation", *RSC/IOP Joint Meeting on Computer Simulation of Confined Fluids*, 8 December 2014, London (UK).
- "Assessing and predicting flexibility in MOFs with molecular simulation", *IUCr 2014 — 23rd Congress and general assembly*, 5–12 August 2014, Montreal (Canada).
- "Mechanical Stability of Metal-Organic Frameworks: Insight from Molecular Simulation", *CONCREEP-9@MIT*, 22–25 September 2013, Cambridge MA (USA).
- "Anisotropic Elastic Properties of Flexible Metal–Organic Frameworks", *EUROMAT 2013*, 8–13 September 2013, Sevilla (France).
- "Understanding Stimuli-Induced Structural Transitions in MOFs", *17th International Zeolite Conference*, 7–12 July 2013, Moscow (Russia).
- "Ab Initio Investigation into the Hydration Mechanism of IRMOFs", *FOA11: 11th International Conference on the Fundamentals of Adsorption*, 19–24 May 2013, Baltimore MD (USA).
- "Ab Initio Investigation into the Hydration Mechanism of MOFs", *Characterization of Porous Media 6*, 30 April – 2 May 2012, Delray Beach FL (USA).
- "Water in Metal–Organic Frameworks", *Transient Chemical Structures in Dense Media*, 30 November 2010, Paris (France).
- "Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organic–Inorganic Frameworks", International Zeolite Conference 16, 5–9 July 2010, Sorrento (Italy).
- "Adsorption of Water in Metal–Organic Frameworks: Insight From Molecular Simulation", *Fundamentals of Adsorption 10*, 24–30 May 2010, Awaji (Japan).
- "Water Intrusion in Hydrophobic Zeolites", *Fundamentals of Adsorption 10*, 24–30 May 2010, Awaji (Japan).
- "Effect of confinement on water in zeolite nanopores", XVIII International Conference on *Horizons in Hydrogen Bond Research*, 14–18 September 2009, Paris (France).
- "Water confined in nanopores : structure, dipole, IR and more", CECAM workshop on *New developments for first principles molecular dynamics simulations in condensed matter and molecular physics*, 15–18 May 2006, Lyon (France).
- "Elemental Femtochemistry of a Confined Hydrated Electron", Workshop on *Ab initio dynamical simulations in condensed matter*, 19 April 2006, Paris (France).

In national conferences (17)

- "Crystals with extraordinary behavior under stimulation", *GECOM CONCOORD*, 19–24 May 2019, Erquy (France).

- "Computational Chemistry of MOFs", *First French Congress on MOFs, COFs and Porous Polymers*, 16–17 May 2018, Paris (France).
- "Évolution de la communication scientifique", *Innométriques 2017*, 30 November 2017, Paris (France).
- "Dynamique moléculaire et méthode de Monte–Carlo", *DynaMol summer school*, 23–27 May 2016, Paris (France).
- "Matériaux intelligents et réactifs : comprendre et prédire leur comportement", *Journées francophones des jeunes physico-chimistes*, 19–23 October 2015, Girona (Spain).
- "Introduction to Molecular Dynamics and Monte Carlo simulations", *MeMoSim2015: Méthodes De Modélisation Et Simulation Multiéchelles*, 30 March – 2 April 2015, Lyon (France).
- "Des cristaux… mous et troués, mais intelligents !", *Journée Cristallographie à Chimie ParisTech* (dans le cadre de l'Année Internationale de la Cristallographie), 11 December 2014, Paris (France).
- "Theoretical insight into Soft Porous Crystals: Problems and tools to solve them", *Journées francophones des jeunes physico-chimistes*, 13–17 October 2014, Dammarie-les-Lys (France).
- "Anisotropic Elastic Properties of Flexible Metal-Organic Frameworks", Colloque Société Française de Physique, division *Physique Atomique, Moléculaire et Optique*, *Journées de Spectroscopie Moléculaire*, 7–10 July 2014, Reims (France).
- "Structure des Phases Adsorbées : Apports de la Simulation Moléculaire", *Journées École de l'Association Française de l'Adsorption*, 10 February 2014, Paris (France).
- "Ab Initio Investigation into the Hydration Mechanism of MOFs", *Journées 2013 de l'Association Française de l'Adsorption*, 14–15 February 2013, Paris (France).
- "Ab Initio Investigation into Hydrothermal Stability and Mechanical Properties of Soft Porous Crystals", *Atelier Simulation des Matériaux Désordonnés*, 12–13 December 2012, Marseille (France).
- "Adsorption & effets de confinement: Outils théoriques, simulation moléculaire", *GdR Thermodynamique Moléculaire et des Procédés*, 11 December 2012, Paris (France).
- "Modèles thermodynamiques et mécaniques pour la description des matériaux poreux flexibles", *Journées 2012 de l'Association Française de l'Adsorption*, 24–25 May 2012, Paris (France).
- "Adsorption & effets de confinement — Outils théoriques et simulation moléculaire", *Groupe Français d'Adsorption et des Surfaces Hétérogènes*, 2 July 2010, Paris (France).
- "Isothermes de type V de H2O et CO2 dans les MOF", *Groupe Français des Zéolithes*, 31 March – 2 May 2010, Giens (France).
- "Adsorption dans les matériaux nanoporeux flexibles", *Journées Modélisation à Paris*, 15–16 June 2009, Paris (France).

Invited seminars in research groups (24)

- University of Cambridge, 5 May 2020, online.
- University of Kyoto, 22 October 2019, Kyoto (Japan).
- Université Paris Diderot, 27 September 2019, Paris (France).
- Ruhr-Universität Bochum, 23 September 2019, Bochum (Germany).
- *Nature* publishing group, 8 July 2019, London (UK).
- Ruhr-Universität Bochum, 26 April 2018, Bochum (Germany).
- Ghent University, 25 April 2018, Ghent (Belgium).
- Université de Rennes, 16 February 2018, Rennes (France).
- Université de Haute Alsace, 16 October 2017, Mulhouse (France).
- iCeMS, University of Kyoto, 18 April 2017, Kyoto (Japan).
- Air Liquide, Delaware Research And Technology Center, 9 March 2017, Newark DE (USA).
- Université de Strasbourg, 11 October 2016, Strasbourg (France).
- Université Grenoble Alpes, 9 May 2016, Grenoble (France).
- Ghent University, 6 October 2015, Ghent (Belgium).
- Technische Universität Dresden, 8 July 2015, Dresden (Germany).
- Saint-Gobain/CNRS research lab, 18 March 2015, Cavaillon (France).

- École Normale Supérieure, 14 October 2014, Paris (France).
- University of Bath, 28 July 2014, Bath (UK).
- University of Oxford, 25 June 2014, Oxford (UK).
- Université de Bourgogne, 10 March 2014, Dijon (France).
- ENSICAEN / Université de Caen, 3 February 2014, Caen (France).
- Université de Strasbourg, 20 June 2013, Strasbourg (France).
- Université Paris Est, 18 January 2013, Paris (France).
- Universités d'Aix-Marseille, 15 June 2010, Marseille (France).

Community involvement

Editorial responsibilities

- Associate Editor of *Adsorption Science & Technology*
- Editorial Board member for *Communications Chemistry*
- Editorial Advisory Board, *C&EN (Chemical and Engineering News)*, American Chemical Society
- Scientific advisory board, chemRxiv

Guest editor of journal special issues

- Special issue on "Simulation of framework materials" in *Molecular Simulation* (Spring 2015).
- Special issue on "Flexibility and Disorder in Metal–Organic Frameworks" in *Dalton Transactions* (Early 2016).

Organization of conferences, workshops and tutorials

- Since May 2009: co-organizer of the meeting "Molecular modeling in Paris", a two-day national conference every Spring.
- Co-organizer of the International CECAM Workshop on Multi-scale modelling of flexible and disordered porous materials, 11–13 June 2018, Paris (France).
- Co-organizer of the International Workshop on "Flexibility and Disorder in Metal–Organic Frameworks", 3–5 June 2015, Paris (France).
- Co-organizer of the International Symposium on CO_2 capture, 18–20 September 2013, Marne-la-Vallée (France).
- Co-organizer of the International Workshop on "Adsorption in Compliant Solids", 5–7 June 2013, Paris (France).
- Co-organizer of the International Workshop on "Adsorption in Compliant Solids: Theory, Simulation, and Experiments", 9–11 June 2011, Paris (France).
- Co-organizer of a one-week tutorial on "Ab initio molecular dynamics with CPMD & CP2K", 6–9 April 2010, Paris (France).
- Organizing practicals at the "Quantum Simulation of Liquids and Solids" CECAM tutorial, 2006.

Peer-review and proposal review

- Reviewer of project proposals for the NSF and the French ANR (Agence Nationale de la Recherche).
- Reviewer for many journals, including: *Nature*, *Science*, *Nature Chemistry*, *Nature Materials*, *Phys. Rev. Lett.*, *J. Am. Chem. Soc.*, *Angewandte Chemie*, *Chem. Rev.*, *Chem. Soc. Rev.*, *Acc. Chem. Rev.*, *J. Phys. Chem.* (and *J. Phys. Chem. Lett.*), *PCCP*, *J. Mater. Chem.*, *Langmuir*, *Adsorption*, *Mol. Simulat.*, etc.

Students and post-doc supervised

- 12 post-doctoral researchers
  Thibaud Dreher, starting February 2019.
  Félix Mouhat, starting October 2018.
  Siwar Chebbi, starting June 2018.
  Antoine Carof, starting June 2018.
  Jack Evans, from September 2015 to September 2017.
  Clarisse Péan, 2015–2017.
  Fabien Trousselet, from September 2014 to September 2016.
  Dario Corradini, 2014–2015.
  Quang-Tri Doan, from July 2012 to July 2013.
  Jorge Peixinho, from December 2010 to December 2011.
  Carlos Triguero, from February 2010 to February 2012.
  Selvarengan Paranthaman, January–November 2009.
- 10 PhD students
  Marta De Toni, co-advisor (80%): 2009–2012. Now at Sanofi.
  David Bousquet, co-advisor (50%): 2010–2014. Now at CEA.
  Aurélie Ortiz, co-advisor (80%): 2011–2014. Now at Saint-Gobain.
  Jean-Mathieu Vanson, co-advisor (60%): 2014–2017.
  Liam Wilbraham, co-advisor (50%): 2014–2017.
  Romain Gaillac, advisor: 2015–2018.
  Elsa Perrin, co-advisor (50%): 2015–2018.
  Guillaume Fraux, advisor: 2015–2019.
  Wenke Li, advisor: 2018–2021.
  Maxime Ducamp, advisor: 2019–2022.
- 10 Master's students
- 19 undergrad students

PhD thesis committees

Nicolas Ferrando (supervisor: Anne Boutin), June 2011.
Benoît Carrier (supervisor: Henri Van Damme), December 2013.
Ines Collings (supervisor: Andrew Goodwin), June 2014.
François Villemot (supervisor: Benoit Coasne), November 2014.
Louis Vanduyfhuys (supervisor: Veronique Van Speybroeck), September 2015.
Henri Hay (supervisor: Guillaume Ferlat), September 2016.
Laura Ronchi (supervisor: Jean Daou), October 2017.
Sven Rogge (supervisor: Veronique Van Speybroeck), May 2018.
Johannes P. Dürholt (supervisor: Rochus Schmid), September 2019.
Boushra Mortada (supervisor: Claire Marichal), November 2019.
Tung Doan (supervisor: Quy-Dong To), February 2020.