

# François-Xavier Coudert

## Researcher at CNRS

### Full publication list

(updated July 6, 2018)

#### Full publication list

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##### In peer-reviewed international journals

101. "Adsorption Contraction Mechanics: Understanding Breathing Energetics in Isoreticular Metal-Organic Frameworks", S. Krause, J. Evans, V. Bon, I. Senkovska, S. Ehrling, U Stoeck, P. Yot, P. Iacomi, P. Llewellyn, G. Maurin, F.-X. Coudert and S. Kaskel, *J. Phys. Chem. C*, **2018**, in press.
100. "Negative Hydration Expansion in ZrW<sub>2</sub>O<sub>8</sub>: Microscopic Mechanism, Spaghetti Dynamics, and Negative Thermal Expansion", M. Baise, P. M. Maffettone, F. Trousselet, N. P. Funnell, F.-X. Coudert and A. L. Goodwin, *Phys. Rev. Lett.*, **2018**, 120, 265501.
99. "Conformational chiral polymorphism in cis-bis-triphenylphosphine complexes of transition metals", N. Tshabang, G. P. Makgatle, S. A. Bourne, N. Kann, J. D. Evans, F.-X. Coudert and L. Öhrström, *CrystEngComm*, **2018**, in press.
98. "Structure and Dynamics of Water Confined in Imogolite Nanotubes", L. Scalfi, G. Fraux, A. Boutin and F.-X. Coudert, *Langmuir*, **2018**, 34, 6748–6756.
97. "Air separation with graphene mediated by nanowindow-rim concerted motion", F. Vallejos-Burgos, F.-X. Coudert and K. Kaneko, *Nature Commun.*, **2018**, 9, 1812.
96. "Structure and Dynamics of Solvated Polymers near a Silica Surface: On the Different Roles Played by Solvent", E. Perrin, M. Schoen, F.-X. Coudert and A. Boutin, *J. Phys. Chem. B*, **2018**, 122, 4573–4582.
95. "Melting of Zeolitic Imidazolate Frameworks with Different Topologies: Insight from First-Principles Molecular Dynamics", R. Gaillac, P. Pullumbi and F.-X. Coudert, *J. Phys. Chem. C*, **2018**, 122, 6730–6736.
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92. "Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices", G. Fraux, F.-X. Coudert, A. Boutin and A. H. Fuchs, *Chem. Soc. Rev.*, **2017**, 46, 7421–7437.
91. "Liquid metal-organic frameworks", R. Gaillac, P. Pullumbi, K. A. Beyer, K. W. Chapman, D. A. Keen, T. D. Bennett and F.-X. Coudert, *Nature Mater.*, **2017**, 16, 1149–1154.
90. "Predicting the Mechanical Properties of Zeolite Frameworks by Machine Learning", J. D. Evans and F.-X. Coudert, *Chem. Mater.*, **2017**, 29, 7833–7839.
89. "Molecular Mechanism of Swing Effect in Zeolitic Imidazolate Framework ZIF-8: Continuous Deformation Upon Adsorption", F.-X. Coudert, *ChemPhysChem*, **2017**, 18, 2732–2738.
88. "Recent advances in the computational chemistry of soft porous crystals", G. Fraux and F.-X. Coudert, *Chem. Commun.*, **2017**, 53, 7211–7221.
87. "Reproducible Research in Computational Chemistry of Materials", F.-X. Coudert, *Chem. Mater.*, **2017**, 29, 2615–2617.

86. "Macroscopic Simulation of Deformation in Soft Microporous Composites", J. D. Evans and F.-X. Coudert, *J. Phys. Chem. Lett.*, **2017**, 8, 1578–1584.
85. "Molecular Insight into CO<sub>2</sub> "Trapdoor" Adsorption in Zeolite Na-RHO", F.-X. Coudert and D. Kohen, *Chem. Mater.*, **2017**, 29, 2724–2730.
84. "Kinetic accessibility of porous materials adsorption sites studied through Lattice Boltzmann method", J.-M. Vanson, F.-X. Coudert, M. Klotz and A. Boutin, *Langmuir*, **2017**, 33, 1405–1411.
83. "Interplay between defects, disorder and flexibility in metal-organic frameworks", T. D. Bennett, A. K. Cheetham, A. H. Fuchs and F.-X. Coudert, *Nature Chem.*, **2017**, 9, 11–16.
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81. "Origins of Negative Gas Adsorption", J. D. Evans, L. Bocquet and F.-X. Coudert, *Chem*, **2016**, 1, 873–886.
80. "Heterometallic Metal-Organic Frameworks of MOF-5 and UiO-66 Families: Insight from Computational Chemistry", F. Trousselet, A. Archereau, A. Boutin and F.-X. Coudert, *J. Phys. Chem. C*, **2016**, 120, 24885–24894.
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73. "Insight into the Li<sub>2</sub>CO<sub>3</sub>-K<sub>2</sub>CO<sub>3</sub> eutectic mixture from classical molecular dynamics: thermodynamics, structure and dynamics", D. Corradini, F.-X. Coudert and R. Vuilleumier, *J. Chem. Phys.*, **2016**, 144, 104507.
72. "Encoding complexity within supramolecular analogues of frustrated magnets", A. B. Cairns, M. J. Cliffe, J. A. M. Paddison, D. Daisenberger, M. G. Tucker, F.-X. Coudert and A. L. Goodwin, *Nature Chem.*, **2016**, 8, 442–447.
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66. "Multicomponent Metal-Organic Frameworks as Defect-Tolerant Materials", S. J. Lee, C. Doussot, A. Baux, L. Liu, G. B. Jameson, C. Richardson, J. J. Pak, F. Trousselet, F.-X. Coudert and S. G. Telfer, *Chem. Mater.*, **2016**, 28, 368–375.
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1. “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](#)).

## 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 (3<sup>rd</sup> 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)*.

## Oral communications

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### As invited speaker

- ▶ “Soft Porous Crystals, Molecular Insight from Computational Chemistry”, *Thermodynamics 2017*, September 5–8 2017, Edinburgh (UK).
- ▶ “Flexibility, Defects & Disorder in Soft Porous Crystals”, *7th FEZA Conference — Federation of European Zeolite Associations*, July 3–7 2017, Sofia (Bulgaria).
- ▶ “Mechanical Impact of Adsorption in Compliant Nanoporous Materials”, *Characterization of Porous Solids (COPS-XI)*, May 14–17 2017, Avignon (France).
- ▶ “Flexibility, Defects & Disorder in Soft Porous Crystals”, *Switchability in Porous Metal–Organic Frameworks*, March 13–14 2017, Dresden (Germany).
- ▶ “Coupling transport and adsorption through Lattice Boltzmann methods”, *EMN Meeting on Mesoporous Materials*, June 13–17 2016, Prague (Czech Republic).
- ▶ “Mechanical impact of adsorption in compliant microporous materials”, *12th International Conference on the Fundamentals of Adsorption*, May 30–June 3 2016, Friedrichshafen (Germany).
- ▶ “First-principles dynamics and free energy methods for flexible materials”, *CP2K-UK Conference*, February 22 2016, London (UK).
- ▶ “Computational characterization of flexibility and disorder: from the unit cell to the crystal”, *Frontiers in Materials Science, Cambridge-JNCASR Winter School*, December 7–11 2015, Bangalore (India).

- ▶ “Molecular simulation of materials flexibility and disorder”, *International workshop on Flexibility and Disorder in Metal–Organic Frameworks*, June 3–5 2015, Paris (France).
- ▶ “Polymorphism and Flexibility in Nanoporous Molecular Frameworks”, *CPM-7: 7th International Workshop on the Characterization of Porous Materials*, May 3–6 2015, Delray Beach FL (USA).
- ▶ “On the Impact of Adsorption in Compliant Nanoporous Materials”, *4th Symposium on Future Challenges for Carbon-based Nanoporous Materials*, March 16–18 2015, Nagano (Japan).
- ▶ “Interfaces and porous materials: Insight from Molecular Simulation”, *CAPZEO-2014: Fourth International Summer School on Quantum Electronic Calculations*, June 8–12 2014, Rabat (Morocco).
- ▶ “Theoretical Insight into Soft Porous Crystals”, *CFCAM meeting on simulation of systems under thermodynamic gradients*, March 25–26 2014, Paris (France).
- ▶ “Anisotropic Elastic Properties of Flexible Metal–Organic Frameworks”, *International symposium on CO<sub>2</sub> capture*, September 18–20 2013, Marne-la-Vallée (France).
- ▶ “Modeling of Soft Porous Crystals: From the Unit Cell to the Crystal”, *Gordon Research Conference Nanoporous Materials & Their Applications*, August 11–16 2013, Holderness NH (USA).
- ▶ “Structural transitions in metal–organic frameworks: thermodynamics & mechanics”, *International workshop on adsorption in compliant solids*, June 5–7 2013, Paris (France).
- ▶ “Ab Initio Investigation into the Hydration Mechanism of IRMOFs”, *CECAM/GDRi workshop on Aging of Engineering Materials*, February 8–10 2012, Zürich (Switzerland).
- ▶ “Effect of confinement on water in zeolite nanopores”, *Indo French Seminar on Diffusion in Nanoporous and Dense Media*, April 1–5 2009, Bangalore (India).
- ▶ “Water nanodroplets confined in zeolite pores”, *Faraday Discussion 141: Water, From Interfaces to Bulk*, August 27–29 2008, Edinburgh (UK).

#### In international conferences

- ▶ “Flexibility, Defects & Disorder in Soft Porous Crystals: Molecular Insight from Computational Chemistry”, *12th International Conference on the Fundamentals of Adsorption*, May 30–June 3 2016, Friedrichshafen (Germany).
- ▶ “Assessing and predicting flexibility in MOFs with molecular simulation”, *EUROMOF 2015, 1st European Conference on Metal Organic Frameworks and Porous Polymers*, October 11–14 2015, Potsdam (Germany).
- ▶ “Molecular simulation of stimuli-responsive framework materials”, *12th International Conference on Materials Chemistry (MC12)*, July 20–23 2015, York (UK).
- ▶ “Polymorphism in nanoporous materials: assessing mechanical, thermal stability, and experimental feasibility”, *249th ACS National Meeting (PHYS division)*, March 22–26 2015, Denver CO (USA).
- ▶ “Assessing and predicting flexibility in framework materials with molecular simulation”, *249th ACS National Meeting (COMP division)*, March 22–26 2015, Denver CO (USA).
- ▶ “Remarkable Pressure Responses of MOFs: Proton Transfer, Linker Coiling, Order-to-Disorder Transitions”, *249th ACS National Meeting (PMSE division)*, March 22–26 2015, Denver CO (USA).
- ▶ “Fluids in Soft Porous Crystals: Coupling Adsorption and Deformation”, *RSC/IOP Joint Meeting on Computer Simulation of Confined Fluids*, December 8 2014, London (UK).
- ▶ “Assessing and predicting flexibility in MOFs with molecular simulation”, *IUCr 2014 — 23rd Congress and general assembly*, August 5–12 2014, Montreal (Canada).
- ▶ “Mechanical Stability of Metal-Organic Frameworks: Insight from Molecular Simulation”, *CONCREEP-9@MIT*, September 22–25 2013, Cambridge MA (USA).
- ▶ “Anisotropic Elastic Properties of Flexible Metal–Organic Frameworks”, *EUROMAT 2013*, September 8–13 2013, Sevilla (France).
- ▶ “Understanding Stimuli-Induced Structural Transitions in MOFs”, *17th International Zeolite Conference*, July 7–12 2013, Moscow (Russia).
- ▶ “Ab Initio Investigation into the Hydration Mechanism of IRMOFs”, *FOA11: 11th International Conference on the Fundamentals of Adsorption*, May 19–24 2013, Baltimore MD (USA).
- ▶ “Ab Initio Investigation into the Hydration Mechanism of MOFs”, *Characterization of Porous Media 6*, April 30–May 2 2012, Delray Beach FL (USA).



- ▶ “Water in Metal–Organic Frameworks”, *Transient Chemical Structures in Dense Media*, November 30 2010, Paris (France).
- ▶ “Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organic–Inorganic Frameworks”, International Zeolite Conference 16, July 5–9 2010, Sorrento (Italy).
- ▶ “Adsorption of Water in Metal–Organic Frameworks: Insight From Molecular Simulation”, *Fundamentals of Adsorption 10*, May 24–30 2010, Awaji (Japan).
- ▶ “Water Intrusion in Hydrophobic Zeolites”, *Fundamentals of Adsorption 10*, May 24–30 2010, Awaji (Japan).
- ▶ “Effect of confinement on water in zeolite nanopores”, XVIII International Conference on *Horizons in Hydrogen Bond Research*, September 14–18 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*, May 15–18 2006, Lyon (France).
- ▶ “Elemental Femtochemistry of a Confined Hydrated Electron”, Workshop on *Ab initio dynamical simulations in condensed matter*, April 19 2006, Paris (France).

### In national conferences

- ▶ “Dynamique moléculaire et méthode de Monte–Carlo”, *DynaMol summer school*, May 23–27 2016, Paris (France).
- ▶ “Matériaux intelligents et réactifs : comprendre et prédire leur comportement”, *Journées francophones des jeunes physico-chimistes*, October 19–23 2015, Girona (Spain).
- ▶ “Introduction to Molecular Dynamics and Monte Carlo simulations”, *MeMoSim2015: Méthodes De Modélisation Et Simulation Multiéchelles*, March 30–April 2 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), December 11 2014, Paris (France).
- ▶ “Theoretical insight into Soft Porous Crystals: Problems and tools to solve them”, *Journées francophones des jeunes physico-chimistes*, October 13–17 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*, July 7–10 2014, Reims (France).
- ▶ “Structure des Phases Adsorbées : Apports de la Simulation Moléculaire”, *Journées École de l’Association Française de l’Adsorption*, February 10 2014, Paris (France).
- ▶ “Ab Initio Investigation into the Hydration Mechanism of MOFs”, *Journées 2013 de l’Association Française de l’Adsorption*, February 14–15 2013, Paris (France).
- ▶ “Ab Initio Investigation into Hydrothermal Stability and Mechanical Properties of Soft Porous Crystals”, *Atelier Simulation des Matériaux Désordonnés*, December 12–13 2012, Marseille (France).
- ▶ “Adsorption & effets de confinement: Outils théoriques, simulation moléculaire”, *GdR Thermodynamique Moléculaire et des Procédés*, December 11 2012, Paris (France).
- ▶ “Modèles thermodynamiques et mécaniques pour la description des matériaux poreux flexibles”, *Journées 2012 de l’Association Française de l’Adsorption*, May 24–25 2012, Paris (France).
- ▶ “Adsorption & effets de confinement — Outils théoriques et simulation moléculaire”, *Groupe Français d’Adsorption et des Surfaces Hétérogènes*, July 2 2010, Paris (France).
- ▶ “Isothermes de type V de H<sub>2</sub>O et CO<sub>2</sub> dans les MOF”, *Groupe Français des Zéolithes*, March 31–May 2 2010, Giens (France).
- ▶ “Adsorption dans les matériaux nanoporeux flexibles”, *Journées Modélisation à Paris*, June 15–16 2009, Paris (France).

### Invited seminars in research groups

- ▶ Université de Haute Alsace, October 16 2017, Mulhouse (France).
- ▶ iCeMS, University of Kyoto, April 18 2017, Kyoto (Japan).
- ▶ Air Liquide, Delaware Research And Technology Center, March 9 2017, Newark DE (USA).
- ▶ Université de Strasbourg, October 11 2016, Strasbourg (France).
- ▶ Université Grenoble Alpes, May 9 2016, Grenoble (France).

- ▶ Ghent University, October 6 2015, Ghent (Belgium).
- ▶ Technische Universität Dresden, July 8 2015, Dresden (Germany).
- ▶ Saint-Gobain/CNRS research lab, March 18 2015, Cavaillon (France).
- ▶ École Normale Supérieure, October 14 2014, Paris (France).
- ▶ University of Bath, July 28 2014, Bath (UK).
- ▶ University of Oxford, June 25 2014, Oxford (UK).
- ▶ Université de Bourgogne, March 10 2014, Dijon (France).
- ▶ ENSICAEN / Université de Caen, February 3 2014, Caen (France).
- ▶ Université de Strasbourg, June 20 2013, Strasbourg (France).
- ▶ Université Paris Est, January 18 2013, Paris (France).
- ▶ Universités d'Aix-Marseille, June 15 2010, Marseille (France).

## Community involvement

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### 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 Workshop on “Flexibility and Disorder in Metal–Organic Frameworks”, June 3–5 2015, Paris (France).
- ▶ Co-organizer of the International Symposium on CO<sub>2</sub> capture, September 18–20 2013, Marne-la-Vallée (France).
- ▶ Co-organizer of the International Workshop on “Adsorption in Compliant Solids”, June 5–7 2013, Paris (France).
- ▶ Co-organizer of the International Workshop on “Adsorption in Compliant Solids: Theory, Simulation, and Experiments”, June 9–11 2011, Paris (France).
- ▶ Co-organizer of a one-week tutorial on “Ab initio molecular dynamics with CPMD & CP2K”, April 6–9 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*, *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

### ▶ 6 post-doctoral researchers

Jack Evans, from September 2015 to September 2017.  
Fabien Trouselet, from September 2014 to September 2016.  
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.

### ▶ 8 PhD students

Marta De Toni, co-advisor (80%): 2009–2012. Now at Sanofi.  
David Bousquet, co-advisor (50%): 2010–2014. Now at CEA.  
Aurélié 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 (100%):2015–2018.  
Guillaume Fraux, advisor (100%):2015–2018.  
Elsa Perrin, advisor (50%):2015–2018.

### ▶ 6 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.