François-Xavier Coudert
Senior Researcher at CNRS

Full publication list

(updated 17th January 2023)

Full publication list

In peer-reviewed international journals

154. "Rapid Adsorption Enthalpy Surface Sampling (RAESS) to Characterize Nanoporous Materials", E. Ren and F.-X. Coudert, *Chem. Sci.*, **2023**, in press.

153. "Alchemical Osmostat for Monte Carlo Simulation: Sampling Aqueous Electrolyte Solution in Open Systems", A. De Izarra, F.-X. Coudert, A. H. Fuchs and A. Boutin, *J. Phys. Chem. B*, **2023**, in press.

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- "Responsive and disordered porous frameworks: connecting microscopic and macroscopic worlds", *MOF2020: 7th International Conference on Metal-Organic Frameworks and Open Framework Compounds*, 20–23 September 2020, Dresden (Germany) — held online.
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- "Interfaces and porous materials: Insight from Molecular Simulation", *CAPZEO-2014: Fourth International Summer School on Quantum Electronic Calculations*, 8–12 June 2014, Rabat (Morroco).
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- "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 (25)

- Saint-Gobain Recherche, 3 February 2021, Paris (France).
- 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

- Editorial Board member (External Editor) for *Communications Chemistry* (since 2018)
- Scientific advisory board, ChemRxiv (since 2018)
- Editorial Advisory Board, *C&EN (Chemical and Engineering News)*, American Chemical Society (since 2016)
- Editorial Advisory Board, *Accounts of Materials Research* (since 2020)
- Editorial Board member for *Adsorption Science & Technology* (since 2019), former Associate Editor (2016–2019)

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

- October 2020: co-chair of the Faraday Discussion on "Cooperative phenomena in framework materials" (planned in Sapporo, Japan; held online)
- 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.

PhD students supervised (14)

- Dune André, advisor: 2022–2025.
- Lionel Zoubritzky, advisor: 2021–2024.
- Emmanuel Ren, advisor: 2020–2023.
- Nicolas Castel, advisor: 2020–2023.
- Maxime Ducamp, advisor, 2019–2022. "Materials with targeted responsive behaviour"
- Wenke Li, advisor, 2018–2021. "Computational simulation of CdSe quantum dots doped glasses"
- Guillaume Fraux, advisor: 2015–2019. "Molecular simulation of fluid adsorption in flexible nanoporous materials at multiple scales"
- Romain Gaillac, advisor, 2015–2018. "Molecular modelling of physics-chemical properties in microporous solids"
- Elsa Perrin, co-advisor (50%), 2015–2018. "Investigating silica nanoparticles / polymer composites: a coarse-grained molecular dynamics study"
- Liam Wilbraham, co-advisor (50%), 2014–2017. "Theoretical study of excited-state processes in the condensed phase"
- Jean-Mathieu Vanson, co-advisor (60%), 2014–2017. Interdépendence entre géométrie, adsorption et transport dans les matériaux à porosité hiérachique
- Aurélie Ortiz, co-advisor (80%), 2011–2014. "Étude par simulation moléculaire de la flexibilité des matériaux nanoporeux : propriétés structurales, mécaniques et thermodynamiques"
- David Bousquet, co-advisor (50%), 2010–2014. "Modélisation de l'adsorption dans les matériaux nanoporeux flexibles"
- Marta De Toni, co-advisor (80%), 2009–2012. "Simulation moléculaire de l'interaction de molécules polaires avec des matériaux de la famille des MOFs"

Post-doctoral researchers supervised (15)

- Luca Brugnoli, 2022–2023.
- Ambroise De Izarra, 2021–2023.
- Clément Wespiser, 2021.
- Thibaud Dreher, 2019–2020.
- Félix Mouhat, 2018–2020.
- Siwar Chibani, 2018–2020.
- Antoine Carof, 2018–2019.
- Jack Evans, 2015–2017.
- Clarisse Péan, 2015–2017.
- Fabien Trousselet, 2014–2016.
- Dario Corradini, 2014–2015.
- Quang-Tri Doan, 2012–2013.
- Jorge Peixinho, 2010–2011.
- Carlos Triguero, 2010–2012.
- Selvarengan Paranthaman, 2009–2010.

Habilitation (HDR) committees

- Vincent Dahirel (Sorbonne Université), December 2020.

PhD thesis committees (17)

- Maxime Langevin (supervisors: Rodolphe Vuilleumier & Marc Bianciotto), November 2022. "Generating drug-like molecules with artifical intelligence"
- Qing Wang (supervisors: Didier Tichit & Hazar Guesmi), October 2021. "Multi-Scale Theoretical Modeling of Pt- and Au-Based Catalysts Under Reactive Media"
- Benjamin Helfrecht (supervisor: Michele Ceriotti), June 2021. "Structure–Property Relationships in Complex Materials by Combining Supervised and Unsupervised Machine Learning"
- Adrian Gonzalez Nelson (supervisor: Freek Kapteijn & Monique A. van der Veen), May 2021. "Emergent rotational dynamics and optical properties of metal-organic frameworks"
- Valentin Gérard (supervisor: Élisabeth Charlaix), November 2020. "Technique d'intrusiométrie rapide pour l'étude du mouillage dynamique et du transport de soluté dans des pores hydrophobes nanométriques"
- Cyrille Takoukam Takoundjou (supervisor: Emeric Bourasseau), October 2020. "Étude du diagramme de phases du combustible MOX par simulation moléculaire de type Monte Carlo"
- Tung Doan (supervisor: Quy-Dong To), February 2020. "Homogenization of 2D nanoporous materials by combining micromechanics and molecular dynamics approaches"
- Boushra Mortada (supervisor: Claire Marichal), November 2019. "Synthesis of metal-organic frameworks for energetic applications"
- Johannes P. Dürholt (supervisor: Rochus Schmid), September 2019. "Force Field based Multiscale Simulations of Metal-Organic Frameworks"
- Sven Rogge (supervisor: Veronique Van Speybroeck), May 2018. "Derivation and Application of a Reliable Procedure to Computationally Model the Mechanical Stability of Rigid and Flexible Metal–Organic Frameworks"
- Laura Ronchi (supervisor: Jean Daou), October 2017. "Synthesis of hydrophobic zeolites for energetic applications"
- Henri Hay (supervisor: Guillaume Ferlat), September 2016. "Étude de la structure et des propriétés des polymorphes de SiO_2 et B_2O_3 par méthodes ab initio"
- Louis Vanduyfhuys (supervisor: Veronique Van Speybroeck), September 2015. "Insights in the Behaviour of Metal-Organic Frameworks through Molecular Modeling: from Force Field Derivation to Thermodynamic Analysis"
- François Villemot (supervisor: Benoit Coasne), November 2014. "Adsorption et transport dans des solides poreux hiérarchisés"
- Ines Collings (supervisor: Andrew Goodwin), June 2014. "Structure-property relationships in framework materials: anomalous mechanics by design"
- Benoît Carrier (supervisor: Henri Van Damme), December 2013. "Effet de l'eau sur les propriétés mécaniques à court et long termes des argiles gonflantes : expériences sur films autoporteurs et simulations moléculaires"
- Nicolas Ferrando (supervisor: Anne Boutin), June 2011. "Potentiels intermoléculaires et algorithmes de Monte Carlo : application à l'étude des composés oxygénés"