François-Xavier Coudert
Senior Researcher at CNRS

Full publication list
(updated 25th November 2021)

In peer-reviewed international journals


In conference proceedings


Book chapters


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

- “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.
- “CO₂ : comment lui tendre un piège ?”, F.-X. Coudert, La Méthode Scientifique, France Culture, 02/01/2019.
- “L’eau, une histoire trouble”, F.-X. Coudert, La Méthode Scientifique, France Culture, 23/03/2017.
Oral communications

As invited speaker (31)

- “Preprints in the chemistry community”, ACS Fall 2021, 22–26 August 2021, Atlanta (US) — held online.
- “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.
- “The most flexible state of MOFs is the liquid!”, FlexMOF Symposium 2019, 4–5 December 2019, Dresden (Germany).
- “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).
- “Flexibility, defects and disorder in soft porous crystals”, SMARTER6, 2–6 September 2018, Ljubljana (Slovenia).
- “Mechanical impact of adsorption in compliant microporous materials”, 12th International Conference on the Fundamentals of Adsorption, 30 May to 3 June 2016, Friedrichshafen (Germany).
- “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).

“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).


“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).


**In international conferences (21)**


“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 MOFs”, *Characterization of Porous Media 6*, 30 April – 2 May 2012, Delray Beach FL (USA).


In national conferences (18)


“Computational Chemistry of MOFs”, *First French Congress on MOFs, COFs and Porous Polymers*, 16–17 May 2018, 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).


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).


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 Symposium on CO₂ capture, 18–20 September 2013, Marne-la-Vallée (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).
Students and post-doc supervised

- 13 post-doctoral researchers
  - Dario Corradini, 2014–2015.

- 12 PhD students
  - Jean-Mathieu Vanson, co-advisor (60%): 2014–2017.
  - David Bousquet, co-advisor (50%): 2010–2014. Now at CEA.

- 10 Master’s students

- 19 undergrad students

Habilitation (HDR) committees

Vincent Dahirel (Sorbonne Université), December 2020.

PhD thesis committees

Benjamin Helfrecht (supervisor: Michele Ceriotti), June 2021.
Adrian Gonzalez Nelson (supervisor: Élisabeth Charlaix), May 2021.
Valentin Gérard (supervisor: Élisabeth Charlaix), November 2020.
Tung Doan (supervisor: Quy-Dong To), February 2020.
Boushra Mortada (supervisor: Claire Marichal), November 2019.
Johannes P. Dürholt (supervisor: Rochus Schmid), September 2019.
Sven Rogge (supervisor: Veronique Van Speybroeck), May 2018.
Laura Ronchi (supervisor: Jean Daou), October 2017.
Henri Hay (supervisor: Guillaume Ferlat), September 2016.
Louis Vanduyfhuys (supervisor: Veronique Van Speybroeck), September 2015.
François Vilemot (supervisor: Benoit Coasne), November 2014.
Ines Collings (supervisor: Andrew Goodwin), June 2014.
Benoit Carrier (supervisor: Henri Van Damme), December 2013.
Nicolas Ferrando (supervisor: Anne Boutin), June 2011.