François-Xavier Coudert
Researcher at CNRS

Full publication list
(updated November 2, 2018)

Full publication list
In peer-reviewed international journals


In conference proceedings


Book chapters


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


In media


Oral communications

As invited speaker

- “Flexibility, defects and disorder in soft porous crystals”, SMARTER6, September 2–6 2018, Ljubljana (Slovenia).


“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).


“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).


“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).


**In international conferences**


“Assessing and predicting flexibility in MOFs with molecular simulation”, IUCr 2014 — 23rd Congress and general assembly, August 5–12 2014, Montreal (Canada).


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


In national conferences

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


“Isothermes de type V de H2O et CO2 dans les MOF”, Groupe Français des Zéolithes, March 31—May 2 2010, Giens (France).


Invited seminars in research groups

- Ruhr-Universität Bochum, April 26 2018, Bochum (Germany).
- Ghent University, April 25 2017, Ghent (Belgium).
- Université de Rennes, February 16 2018, Rennes (France).
- 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).
- 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

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

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\textsubscript{2} capture, September 18–20 2013, Marne-la-Vallée (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).

Students and post-doc supervised

- **6 post-doctoral researchers**
  - Siwar Chebbi, starting June 2018.
  - Jack Evans, from September 2015 to September 2017.
  - Fabien Trousselet, 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**
  - David Bousquet, co-advisor (50%): 2010–2014. Now at CEA.
  - Jean-Mathieu Vanson, co-advisor (60%): 2014–2017.
  - Guillaume Fraux, advisor (100%): 2015–2019.

- **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.
- Henri Hay (supervisor: Guillaume Ferlat), September 2016.
- Laura Ronchi (supervisor: Jean Daou), October 2017.