François-Xavier Coudert

Senior researcher at CNRS *Professeur attaché* at ENS / PSL 42 years old (born 5 June 1982)

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Research interests

Improving our understanding of the physical and chemical properties of nanoporous solids, especially stimuli-responsive materials (Soft Porous Crystals), and the adsorption of molecular fluids in their pores. To achieve this, I use and develop a large variety of theoretical methods at scales going from the atoms to the full crystal and the powder sample. Static quantum chemistry calculations, first-principles molecular dynamics, classical simulations (molecular dynamics and Monte Carlo), as well as macroscopic theoretical thermodynamic and kinetic models.

Positions and Education

- Since 2019: Senior researcher at CNRS (directeur de recherche)
- Since 2019: Professeur attaché at École normale supérieure / PSL
- April 2013: Habilitation (reviewers: profs. Michele Parrinello, Gino V. Baron, Jean-Louis Barrat).
- > 2008–2019: Researcher at CNRS (chargé de recherche), at PSL University / Chimie ParisTech.
- > 2007–2008: **Post-doctoral researcher at University College London** Chemistry Department, in prof. Richard Catlow's group (superviser: Dr. Caroline Mellot-Draznieks).
- > 2004–2007: PhD in Chemistry at Université Paris-Sud 11, under the direction of Dr. Anne Boutin.
- > 2003: MSc intern at University of Massachussetts Amherst, with prof. Scott Auerbach.
- > 2001–2004: Undergraduate studies at École normale supérieure (Paris), Department of Chemistry.

Scientific production

- ▶ 170 publications in international peer-reviewed journals (20 118 citations, *h*-index = 69)
- 9 book chapters
- > 37 invited talks at international conferences, 63 talks at international conferences in total
- > Organizer of 6 international conferences, 7 national conferences, 4 thematic/summer schools

Awards & Honors

- > 2018 : International Award for Creative Work, Japan Society of Coordination Chemistry
- > 2017 : Emerging Investigator, Chemical Communications (RSC)
- > 2016 & 2012: CNRS Scientific Excellence Award (prime d'excellence scientifique)
- > 2016: Distinguished Junior Member of the Société Chimique de France
- 2015: Young Researcher Award (prix Jeune Chercheur) of the Division de Chimie Physique (Société Chimique de France & Société Française de Physique)
- > 2009: Best Oral Contribution at the "Horizons in Hydrogen Bond Research" conference
- > 2008: Best Poster at the British Zeolite Association's conference

Teaching experience

- Statistical Physics and Molecular Simulation (giving lectures and supervising practicals) in Chimie ParisTech's engineer cursus (at Master's level) and École Normale Supérieure.
- Advanced Molecular Simulation at the graduate level.
- Supervised 16 PhD theses, 16 post-docs, 10 Master's students, 19 undergraduate students.

Partnerships & contracts

- > 5 grants from ANR, the French academic research funding agency (3 to 4 years each)
- Industrial collaborations with EDF, Air Liquide, Saint Gobain, and Orano companies
- Developer of scientific apps for iPhone, iPad and Mac (500,000 downloads)

Community involvement

- Member of the International Commission on Metal–Organic Frameworks / IZA
- Associate Editor, Communications Chemistry
- > 2016–2019: Associate Editor, Adsorption Science & Technology
- Editorial Advisory Board, C&EN (Chemical and Engineering News), American Chemical Society
- Scientific Advisory Board, chemRxiv preprint server
- > 2014–2019: Scientific Advisory Board for Chemistry at CNRS
- Guest editor for two issues, in Molecular Simulation (2015) and Dalton Transactions (2016)

Selected recent publications

- *Machine learning interatomic potentials for amorphous zeolitic imidazolate frameworks", N. Castel, D. André, C. Edwards, J. D. Evans and <u>F-X. Coudert</u>, *Digital Discovery*, 2024, 3 (2), 355–368.
- "Tunable acetylene sorption by flexible catenated metal–organic frameworks", M. Bonneau, C. Lavenn, J.-J. Zheng, A. Legrand, T. Ogawa, K. Sugimoto, <u>F.-X. Coudert</u>, R. Reau, S. Sakaki, K.-i. Otake and S. Kitagawa, *Nature Chemistry*, 2022, 14, 816–822.
- * "Best practices in machine learning for chemistry", N. Artrith, K. T. Butler, <u>F.-X. Coudert</u>, S. Han, O. Isayev, A. Jain and A. Walsh, *Nature Chemistry*, **2021**, 13, 505–508.
- "The changing state of porous materials", T. D. Bennett, <u>F.-X. Coudert</u>, S. L. James and A. I. Cooper, *Nature Materials*, 2021, 20, 1179–1187.
- "Structure and chemistry of graphene oxide in liquid water from first principles", F. Mouhat, <u>F.-X.</u> <u>Coudert</u> and M.-L. Bocquet, *Nature Commun.*, 2020, 11, 1566.
- "Air separation with graphene mediated by nanowindow-rim concerted motion", F. Vallejos-Burgos, <u>F.-X. Coudert</u> and K. Kaneko, *Nature Commun.*, 2018, 9, 1812
- "Liquid metal-organic frameworks", R. Gaillac, P. Pullumbi, K. A. Beyer, K. W. Chapman, D. A. Keen, T. D. Bennett and <u>F.-X. Coudert</u>, *Nature Materials*, 2017, 16, 1149–1154
- "Interplay between defects, disorder and flexibility in metal-organic frameworks", T. D. Bennett, A. K. Cheetham, A. H. Fuchs and <u>F.-X. Coudert</u>, *Nature Chemistry*, 2017, 9, 11–16
- *A pressure amplifying framework material with negative gas adsorption transitions", S. Krause, V. Bon, I. Senkovska, U. Stoeck, D. Wallacher, D. M. Többens, S. Zander, R. S. Pillai, G. Maurin, <u>F-X. Coudert</u> and S. Kaskel, *Nature*, 2016, 532, 348–352

Full publication list at www.coudert.name