

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 (supervisor: 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 Massachusetts Amherst, with prof. Scott Auerbach.
- ▶ 2001–2004: Undergraduate studies at **École normale supérieure** (Paris), Department of Chemistry.

Scientific production

- ▶ 163 publications in international peer-reviewed journals (16 892 citations, *h*-index = 66)
- ▶ 9 book chapters
- ▶ 36 invited talks at international conferences, 59 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 14 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

- ▶ 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

- ▶ “Tunable acetylene sorption by flexible catenated metal–organic frameworks”, M. Bonneau, C. Lavenn, J.-J. Zheng, A. Legrand, T. Ogawa, K. Sugimoto, F.-X. Coudert, 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, F.-X. Coudert, S. Han, O. Isayev, A. Jain and A. Walsh, ***Nature Chemistry*, 2021**, 13, 505–508.
- ▶ “The changing state of porous materials”, T. D. Bennett, F.-X. Coudert, 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, F.-X. Coudert and M.-L. Bocquet, ***Nature Commun.*, 2020**, 11, 1566.
- ▶ “Air separation with graphene mediated by nanowindow-rim concerted motion”, F. Vallejos-Burgos, F.-X. Coudert 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 F.-X. Coudert, ***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 F.-X. Coudert, ***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. Többers, S. Zander, R. S. Pillai, G. Maurin, F.-X. Coudert and S. Kaskel, ***Nature*, 2016**, 532, 348–352

Full publication list at www.coudert.name