

François-Xavier Coudert

Researcher at CNRS

35 years old (born June 5 1982)

Chimie ParisTech

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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

- ▶ April 2013: **Habilitation** (reviewers: professors Michele Parrinello, Gino V. Baron, Jean-Louis Barrat).
- ▶ Since 2008: **Researcher at CNRS**, in the *Molecular Simulation Group* of Chimie ParisTech (head: professor Alain Fuchs). Promoted to **first class researcher** in January 2013.
- ▶ 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. "Water and the hydrated electron under confinement: physicochemical properties and reactivity"
- ▶ 2003–2004: Master's in Molecular Physical Chemistry, Université Paris-Sud 11 (ranked: 1st).
- ▶ 2003: Six-month research project at University of Massachusetts Amherst, with prof. Scott Auerbach.
- ▶ 2001–2004: Undergraduate studies at **École normale supérieure** (Paris), Department of Chemistry.

Scientific production

- ▶ 92 publications in international peer-reviewed journals (3 273 citations, h-index = 34)
- ▶ 9 book chapters
- ▶ 20 invited talks at international conferences, 40 talks at international conferences in total
- ▶ Organizer of 5 international workshops, 14 national conferences, 4 thematic/summer schools

Awards & Honors

- ▶ 2017 & 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 8 PhD theses, 5 post-docs, 6 Master's students, 19 undergraduate students

Partnerships & contracts

- ▶ Two-week stay at Rutgers (USA), in prof. Alexander Neimark's group
- ▶ 3 grants from ANR, the French academic research funding agency (3 years each)
- ▶ Industrial collaborations with EDF, Air Liquide, Saint Gobain
- ▶ Developer of scientific apps for iPhone, iPad and Mac (500,000 downloads)

Select recent publications

- ▶ "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, in press, DOI: 10.1038/nmat4998
- ▶ "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. Senkowska, U. Stoeck, D. Wallacher, D. M. Töbrens, S. Zander, R. S. Pillai, G. Maurin, F.-X. Coudert and S. Kaskel, *Nature*, 2016, 532, 348–352
- ▶ "Carbon dioxide transport in molten calcium carbonate occurs through an oxo-Grotthuss mechanism via a pyrocarbonate anion", D. Corradini, F.-X. Coudert and R. Vuilleumier, *Nature Chemistry*, 2016, 8, 454–460
- ▶ "Encoding Complexity within Supramolecular Analogues of Frustrated Magnets", A. B. Cairns, M. J. Cliffe, J. A. M. Paddison, D. Daisenberger, M. G. Tucker, F.-X. Coudert and A. L. Goodwin, *Nature Chemistry*, 2016, 8, 442–447
- ▶ "Controlled Partial Interpenetration in Metal-Organic Frameworks", A. Ferguson, L. Liu, S. J. Tapperwijn, D. Perl, F.-X. Coudert, S. Van Cleuvenbergen, T. Verbiest, M. A. van der Veen and S. G. Telfer, *Nature Chemistry*, 2016, 8, 250–257.
- ▶ "Insulator-To-Proton-Conductor Transition in a Dense Metal-Organic Framework", S. Tominaka, F.-X. Coudert, T. D. Dao, T. Nagao and A. K. Cheetham, *J. Am. Chem. Soc.*, 2015, 137, 6428–6431.
- ▶ "Responsive Metal–Organic Frameworks and Framework Materials: Under Pressure, Taking the Heat, In the Spotlight, With Friends", F.-X. Coudert, *Chem. Mater.*, 2015, 27, 1905–1916
- ▶ "Remarkable Pressure Responses of Metal–Organic Frameworks: Proton Transfer and Linker Coiling in Zinc Alkyl Gates", A. U. Ortiz, A. Boutin, K. J. Gagnon, A. Clearfield and F.-X. Coudert, *J. Am. Chem. Soc.*, 2014, 136, 11540–11545
- ▶ "Correlated defect nanoregions in a metal–organic framework", M. J. Cliffe, W. Wan, X. Zou, P. A. Chater, A. K. Kleppe, M. G. Tucker, H. Wilhelm, N. P. Funnell, F.-X. Coudert and A. L. Goodwin, *Nature Commun.*, 2014, 5, 4176.

Full publication list at <http://coudert.name/>