François-Xavier Coudert

Researcher at CNRS

Full publication list

(updated October 27, 2017)

Full publication list

In peer-reviewed international journals

92. "Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices", G. Fraux, F.-X. Coudert, A. Boutin and A. H. Fuchs, *Chem. Soc. Rev.*, **2017**, in press.

91. "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 Mater.*, **2017**, 16, 1149–1154.

90. "Predicting the Mechanical Properties of Zeolite Frameworks by Machine Learning", J. D. Evans and F.-X. Coudert, *Chem. Mater.*, **2017**, 29, 7833–7839.

89. "Molecular Mechanism of Swing Effect in Zeolitic Imidazolate Framework ZIF-8: Continuous Deformation Upon Adsorption", F.-X. Coudert, *ChemPhysChem*, **2017**, 18, 2732–2738.

88. "Recent advances in the computational chemistry of soft porous crystals", G. Fraux and F.-X. Coudert, *Chem. Commun.*, **2017**, 53, 7211–7221.

87. "Reproducible Research in Computational Chemistry of Materials", F.-X. Coudert, *Chem. Mater.*, **2017**, 29, 2615–2617.

86. "Macroscopic Simulation of Deformation in Soft Microporous Composites", J. D. Evans and F.-X. Coudert, *J. Phys. Chem. Lett.*, **2017**, 8, 1578–1584.

85. "Molecular Insight into CO2 "Trapdoor" Adsorption in Zeolite Na-RHO", F.-X. Coudert and D. Kohen, *Chem. Mater.*, **2017**, 29, 2724–2730.

84. "Kinetic accessibility of porous materials adsorption sites studied through Lattice Boltzmann method", J.-M. Vanson, F.-X. Coudert, M. Klotz and A. Boutin, *Langmuir*, **2017**, 33, 1405–1411.

83. "Interplay between defects, disorder and flexibility in metal-organic frameworks", T. D. Bennett, A. K. Cheetham, A. H. Fuchs and F.-X. Coudert, *Nature Chem.*, **2017**, 9, 11–16.

82. "Transport and adsorption under liquid flow: the role of pore geometry", J.-M. Vanson, A. Boutin, M. Klotz and F.-X. Coudert, *Soft Matter*, **2017**, 13, 875–885.

81. "Origins of Negative Gas Adsorption", J. D. Evans, L. Bocquet and F.-X. Coudert, *Chem*, **2016**, 1, 873–886.

80. "Heterometallic Metal-Organic Frameworks of MOF-5 and UiO-66 Families: Insight from Computational Chemistry", F. Trousselet, A. Archereau, A. Boutin and F.-X. Coudert, *J. Phys. Chem. C*, **2016**, 120, 24885–24894.

79. "Computational Chemistry Methods for Nanoporous Materials", J. D. Evans, G. Fraux, R. Gaillac, D. Kohen, F. Trousselet, J.-M. Vanson and F.-X. Coudert, *Chem. Mater.*, **2017**, 29, 199–212.

78. "Modelling photophysical properties of metal-organic frameworks: a density functional theory based approach", L. Wilbraham, F.-X. Coudert and I. Ciofini, *Phys. Chem. Chem. Phys.*, **2016**, 18, 25176–25182.

77. "Microscopic Mechanism of Chiral Induction in a Metal-Organic Framework", J. D. Evans and F.-X. Coudert, *J. Am. Chem. Soc.*, **2016**, 138, 6131–6134.

76. "ELATE: An open-source online application for analysis and visualization of elastic tensors", R. Gaillac, P. Pullumbi and F.-X. Coudert, *J. Phys. Condens. Matter*, **2016**, 28, 275201.

75. "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, F.-X. Coudert and S. Kaskel, *Nature*, **2016**, 532, 348–352.

74. "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 Chem.*, **2016**, 8, 454–460.

73. "Insight into the Li2CO3-K2CO3 eutectic mixture from classical molecular dynamics: thermodynamics, structure and dynamics", D. Corradini, F.-X. Coudert and R. Vuilleumier, *J. Chem. Phys.*, **2016**, 144, 104507.

72. "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 Chem.*, **2016**, 8, 442–447.

71. "Non-interpenetrated metal-organic frameworks based on copper(II) paddlewheel and oligoparaxylene-isophthalate linkers: synthesis, structure and gas adsorption", Y. Yan, M. Juríček, F.-X. Coudert, N. A. Vermeulen, S. Grunder, A. Dailly, W. Lewis, A. J. Blake, J. F. Stoddart and M. Schröder, *J. Am. Chem. Soc.*, **2016**, 138, 3371–3381.

70. "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 Chem.*, **2016**, 8, 250–257.

69. "Flexibility and disorder in metal-organic frameworks", T. D. Bennett, A. H. Fuchs, A. K. Cheetham and F.-X. Coudert, *Dalton Trans.*, **2016**, 45, 4058–4059.

68. "A Computational and Experimental Approach Linking Disorder, High-Pressure Behavior, and Mechanical Properties in UiO Frameworks", C. L. Hobday, R. J. Marshall, C. F. Murphie, J. Sotelo, T. Richards, D. R. Allan, T. Düren, F.-X. Coudert, R. S. Forgan, C. A. Morrison, S. A. Moggach and T. D. Bennett, *Angew. Chem. Int. Ed.*, **2016**, 55, 2401–2405.

67. "Defects in metal-organic frameworks: A compromise between adsorption and stability?", A. W. Thornton, R. Babarao, A. Jain, F. Trousselet and F.-X. Coudert, *Dalton Trans.*, **2016**, 45, 4352–4359.

66. "Multicomponent Metal-Organic Frameworks as Defect-Tolerant Materials", S. J. Lee, C. Doussot, A. Baux, L. Liu, G. B. Jameson, C. Richardson, J. J. Pak, F. Trousselet, F.-X. Coudert and S. G. Telfer, *Chem. Mater.*, **2016**, 28, 368–375.

65. "Defects and Disorder in Metal-Organic Frameworks", A. K. Cheetham, T. D. Bennett, F.-X. Coudert and A. L. Goodwin, *Dalton Trans.*, **2016**, 45, 4113–4126.

64. "Adsorption deformation of microporous composites", F.-X. Coudert, A. H. Fuchs and A. V. Neimark, *Dalton Trans.*, **2016**, 45, 4136–4140.

63. "Metal-organic frameworks: the pressure is on", F.-X. Coudert, *Acta Cryst. B*, **2015**, 71, 585–586.

62. "Mechanism of water adsorption in the large pore form of the gallium-based MIL-53 metal-organic framework", G. Weber, I. Bezverkhyy, J.-P. Bellat, A. Ballandras, G. Ortiz, G. Chaplais, J. Patarin, F.-X. Coudert, A. H. Fuchs and A. Boutin, *Micro. Meso. Mater.*, **2016**, 222, 145–152.

61. "Hydrothermal Breakdown of Flexible Metal-organic Frameworks: A Study by First-Principles Molecular Dynamics", V. Haigis, F.-X. Coudert, R. Vuilleumier, A. Boutin and A. H. Fuchs, *J. Phys. Chem. Lett.*, **2015**, 6, 4365–4370.

60. "Softening upon adsorption in microporous materials: a counter-intuitive mechanical response", F. Mouhat, D. Bousquet, A. Boutin, L. Bouëssel du Bourg, F.-X. Coudert and A. H. Fuchs, *J. Phys. Chem. Lett.*, **2015**, 6, 4265–4269.

59. "Molecular Simulation of Framework Materials", F.-X. Coudert and T. Düren, *Mol. Simul.*, **2015**, 41, 1309–1310.

58. "Computational characterization and prediction of metal-organic framework properties", F.-X. Coudert and A. H. Fuchs, *Coord. Chem. Rev.*, **2016**, 307, 211–236.

57. "Unexpected coupling between flow and adsorption in porous media", J.-M. Vanson, F.-X. Coudert, B. Rotenberg, M. Levesque, C. Tardivat, M. Klotz and A. Boutin, *Soft Matter*, **2015**, 11, 6125–6133.

56. "A systematic typology for negative Poisson's ratio materials and the prediction of complete auxeticity in pure silica zeolite JST", M. Siddorn, F.-X. Coudert, K. Evans and A. Marmier, *Phys. Chem. Chem. Phys.*, **2015**, 17, 17927–17933.

55. "Novel porous polymorphs of zinc cyanide with rich thermal and mechanical behavior", F. Trousselet, A. Boutin and F.-X. Coudert, *Chem. Mater.*, **2015**, 27, 4422–4430.

54. "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.

53. "Defect-dependent colossal negative thermal expansion in UiO-66(Hf) metal–organic framework", M. J. Cliffe, J. A. Hill, C. A. Murray, F.-X. Coudert and A. L. Goodwin, *Phys. Chem. Chem. Phys.*, **2015**, 17, 11586–11592.

52. "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.

51. "Experimental Evidence of Negative Linear Compressibility in the MIL-53 Metal-Organic Framework Family", P. Serra-Crespo, A. Dikhtiarenko, E. Stavitski, J. Juan-Alcañiz, F. Kapteijn, F.-X. Coudert and J. Gascon, *CrystEngComm*, **2015**, 17, 276–280.

50. "Thermal and mechanical stability of zeolitic imidazolate frameworks polymorphs", L. Bouëssel du Bourg, A. U. Ortiz, A. Boutin and F.-X. Coudert, *APL Mat.*, **2014**, 2, 124110.

49. "Necessary and sufficient elastic stability conditions in various crystal systems", F. Mouhat and F.-X. Coudert, *Phys. Rev. B*, **2014**, 90, 224104.

48. "Challenges in first-principles NPT molecular dynamics of soft porous crystals: A case study on MIL-53(Ga)", V. Haigis, Y. Belkhodja, F.-X. Coudert, R. Vuilleumier and A. Boutin, *J. Chem. Phys.*, **2014**, 141, 064703.

47. "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.

46. "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, *Nat. Commun.*, **2014**, 5, 4176.

45. "Prediction of Flexibility of Metal–Organic Frameworks CAU-13 and NOTT-300 by First Principles Molecular Simulations", A. U. Ortiz, A. Boutin and F.-X. Coudert, *Chem. Commun.*, **2014**, 50, 5867–5870.

44. "Water Adsorption in Flexible Gallium-Based MIL-53 Metal-Organic Framework", F.-X. Coudert, A. U. Ortiz, V. Haigis, D. Bousquet, A. H. Fuchs, A. Ballandras, G. Weber, I. Bezverkhyy, N. Geoffroy, J.-P. Bellat, G. Ortiz, G. Chaplais, J. Patarin and A. Boutin, *J. Phys. Chem. C*, **2014**, 118, 5397–5405.

43. "A Thermodynamic Description of the Adsorption Induced Structural Transitions in Flexible MIL-53 Metal-Organic Framework", F.-X. Coudert, A. Boutin and A. H. Fuchs, *Mol. Phys.*, **2014**, 112, 1257–1261.

42. "Reorientational dynamics of water confined in zeolites", A. C. Fogarty, F.-X. Coudert, A. Boutin and D. Laage, *ChemPhysChem*, **2014**, 15, 521–529.

41. "Comment on "Volume shrinkage of metal organic framework host induced by the dispersive attraction of guest gas molecules" by H. Kim, S. S. Han and J. Joo, Phys. Chem. Chem. Phys., 2013, 15, 18822", F.-X. Coudert, A. H. Fuchs and A. V. Neimark, *Phys. Chem. Chem. Phys.*, **2014**, 16, 4394–4395.

40. "Adsorption in complex porous networks with geometrical and chemical heterogeneity", Q.-T. Doan, G. Lefèvre, O. Hurisse and F.-X. Coudert, *Mol. Simul.*, **2014**, 40, 16–24.

39. "What Makes Zeolitic Imidazolate Frameworks Hydrophobic or Hydrophilic? Impact of Geometry and Functionalization on Water Adsorption", A. U. Ortiz, A. P. Freitas, A. Boutin, A. H. Fuchs and F.-X. Coudert, *Phys. Chem. Chem. Phys.*, **2014**, 16, 9940–9949.

38. "Structure and dynamics of the hydrated metal-organic framework MIL-53(Cr) by first-principles molecular dynamics", V. Haigis, F.-X. Coudert, R. Vuilleumier and A. Boutin, *Phys. Chem. Chem. Phys.*, **2013**, 15, 19049–19056.

37. "Adsorption Deformation and Structural Transitions in Metal-Organic Frameworks: From the Unit Cell to the Crystal", F.-X. Coudert, A. Boutin, A. H. Fuchs and A. V. Neimark, *J. Phys. Chem. Lett.*, **2013**, 4, 3198–3205.

36. "Systematic investigation of the mechanical properties of pure silica zeolites: stiffness, anisotropy, and negative linear compressibility", F.-X. Coudert, *Phys. Chem. Chem. Phys.*, **2013**, 15, 16012–16018.

35. "Water evaporation in silica colloidal deposits", J. Peixinho, G. Lefèvre, F.-X. Coudert and O. Hurisse, *J. Colloid Interface Sci.*, **2013**, 408, 206–211.

34. "Investigating the Pressure-Induced Amorphization of Zeolitic Imidazolate Framework ZIF-8: Mechanical Instability due to Shear Mode Softening", A. U. Ortiz, A. Boutin, A. H. Fuchs and F.-X. Coudert, *J. Phys. Chem. Lett.*, **2013**, 4, 1861–1865.

33. "Adsorption induced transitions in soft porous crystals: An osmotic potential approach to multistability and intermediate structures", D. Bousquet, F.-X. Coudert, A. G. J. Fossati, A. V. Neimark, A. H. Fuchs and A. Boutin, *J. Chem. Phys.*, **2013**, 138, 174706.

32. "Metal-organic frameworks with wine-rack motif: What determines their flexibility and elastic properties?", A. U. Ortiz, A. Boutin, A. H. Fuchs and F.-X. Coudert, *J. Chem. Phys.*, **2013**, 138, 174703.

31. "Temperature-Induced Structural Transitions in the Gallium-Based MIL-53 Metal-Organic Framework", A. Boutin, D. Bousquet, A. U. Ortiz, F.-X. Coudert, A. H. Fuchs, A. Ballandras, G. Weber, I. Bezverkhyy, J.-P. Bellat, G. Ortiz, G. Chaplais, J.-L. Paillaud, C. Marichal, H. Nouali and J. Patarin, *J. Phys. Chem. C*, **2013**, 117, 8180–8188.

30. "Anisotropic Elastic Properties of Flexible Metal–Organic Frameworks: How Soft Are Soft Porous Crystals?", A. U. Ortiz, A. Boutin, A. H. Fuchs and F.-X. Coudert, *Phys. Rev. Lett.*, **2012**, 109, 195502.

29. "Understanding adsorption-induced structural transitions in metal-organic frameworks: From the unit cell to the crystal", C. Triguero, F.-X. Coudert, A. Boutin, A. H. Fuchs and A. V. Neimark, *J. Chem. Phys.*, **2012**, 137, 184702.

28. "Free energy landscapes for the thermodynamic understanding of adsorption-induced deformations and structural transitions in porous materials", D. Bousquet, F.-X. Coudert and A. Boutin, *J. Chem. Phys.*, **2012**, 137, 044118.

27. "How Can a Hydrophobic MOF be Water-Unstable? Insight into the Hydration Mechanism of IRMOFs", M. De Toni, R. Jonchiere, P. Pullumbi, F.-X. Coudert and A. H. Fuchs, *ChemPhysChem*, **2012**, 13, 3497–3503.

26. "Molecular Simulation of a Zn–Triazamacrocyle Metal–Organic Frameworks Family with Extraframework Anions", M. De Toni, F.-X. Coudert, S. Paranthaman, P. Pullumbi, A. Boutin and A. H. Fuchs, *J. Phys. Chem. C*, **2012**, 116, 2952–2959.

25. "Predicting Mixture Coadsorption in Soft Porous Crystals: Experimental and Theoretical Study of CO2/CH4 in MIL-53(Al)", A. U. Ortiz, M.-A. Springuel-Huet, F.-X. Coudert, A. H. Fuchs and A. Boutin, *Langmuir*, **2012**, 28, 494–498.

24. "Mechanism of Breathing Transitions in Metal-Organic Frameworks", C. Triguero, F.-X. Coudert, A. Boutin, A. H. Fuchs and A. V. Neimark, *J. Phys. Chem. Lett.*, **2011**, 2, 2033–2037.

23. "Structural Transitions in MIL-53 (Cr): View from Outside and Inside", A. V. Neimark, F.-X. Coudert, C. Triguero, A. Boutin, A. H. Fuchs, I. Beurroies and R. Denoyel, *Langmuir*, **2011**, 27, 4734–4741.

22. "Thermodynamic Methods and Models to Study Flexible Metal-Organic Frameworks", F.-X. Coudert, A. Boutin, M. Jeffroy, C. Mellot-Draznieks and A. H. Fuchs, *ChemPhysChem*, **2011**, 12, 247–258.

21. "Thermodynamic Analysis of the Breathing of Amino-functionalized MIL-53(Al) upon CO2 Adsorption", A. Boutin, S. Couck, F.-X. Coudert, P. Serra-Crespo, J. Gascon, F. Kapteijn, A. H. Fuchs and J.F.M. Denayer, *Micro. Meso. Mater.*, **2011**, 140, 108–113.

20. "The Behavior of Flexible MIL-53(Al) upon CH4 and CO2 Adsorption", A. Boutin, F.-X. Coudert, M.-A. Springuel-Huet, A. V. Neimark, G. Férey and A. H. Fuchs, *J. Phys. Chem. C*, **2010**, 114, 22237–22244.

19. "Understanding the Effect of Confinement on the Liquid–Gas Transition: A Study of Adsorption Isotherms in a Family of Metal–Organic Frameworks", M. De Toni, P. Pullumbi, F.-X. Coudert and A. H. Fuchs, *J. Phys. Chem. C*, **2010**, 114, 21631–21637.

18. "The osmotic framework adsorbed solution theory: predicting mixture coadsorption in flexible nanoporous materials", F.-X. Coudert, *Phys. Chem. Chem. Phys.*, **2010**, 12, 10904–10913.

17. "Water adsorption in hydrophobic MOF channels", S. Paranthaman, F.-X. Coudert and A. H. Fuchs, *Phys. Chem. Chem. Phys.*, **2010**, 12, 8123–8129.

16. "Stress-Based Model for the Breathing of Metal–Organic Frameworks", A. V. Neimark, F.-X. Coudert, A. Boutin and A. H. Fuchs, *J. Phys. Chem. Lett.*, **2010**, 1, 445–449.

15. "Breathing Transitions in MIL-53(Al) Metal–Organic Framework Upon Xenon Adsorption", A. Boutin, M.-A. Springuel-Huet, A. Nossov, A. Gédéon, T. Loiseau, T. Volkringer, G. Férey, F.-X. Coudert and A. H. Fuchs, *Angew. Chem. Int. Ed.*, **2009**, 48, 8314–8317.

14. "Prediction of Breathing and Gate-Opening Transitions Upon Binary Mixture Adsorption in Metal-Organic Frameworks", F.-X. Coudert, C. Mellot-Draznieks, A. H. Fuchs and A. Boutin, *J. Am. Chem. Soc.*, **2009**, 131, 11329–11331.

13. "Zeolitic imidazole frameworks; structural and energetics trends compared with their zeolite analogues", D. W. Lewis, A. R. Ruiz-Salvador, A. Gomez, L. M. Rodriguez-Albelo, F.-X. Coudert, B. Slater, A. K. Cheetham and C. Mellot-Draznieks, *CrystEngComm*, **2009**, 11, 2272–2276.

12. "Double Structural Transition in Hybrid Material MIL-53 upon Hydrocarbon Adsorption: The Thermodynamics Behind the Scenes", F.-X. Coudert, C. Mellot-Draznieks, A. H. Fuchs and A. Boutin, *J. Am. Chem. Soc.*, **2009**, 131, 3442–3443.

11. "Water nanodroplets confined in zeolite pores", F.-X. Coudert, F. Cailliez, R. Vuilleumier, A. H. Fuchs and A. Boutin, *Faraday Discuss.*, **2009**, 141, 377–398.

10. "Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organic–Inorganic Frameworks", F.-X. Coudert, M. Jeffroy, A. H. Fuchs, A. Boutin and C. Mellot-Draznieks, *J. Am. Chem. Soc.*, **2008**, 130, 14294–14302.

9. "Mechanism and kinetics of hydrated electron diffusion", K. A. Tay, F.-X. Coudert and A. Boutin, *J. Chem. Phys.*, **2008**, 129, 054505.

8. "Temperature Effect on the Absorption Spectrum of the Hydrated Electron Paired with a Lithium Cation in Deuterated Water", M. Lin, Y. Kumagai, I. Lampre, F.-X. Coudert, Y. Muroya, A. Boutin, M. Mostafavi and Y. Katsumura, *J. Phys. Chem. A*, **2007**, 111, 3548–3553.

7. "Dipole Moment, Hydrogen Bonding and IR Spectrum of Confined Water", F.-X. Coudert, R. Vuilleumier and A. Boutin, *ChemPhysChem*, **2006**, 7, 2464–2467.

6. "Confinement effect on the hydrated electron behaviour", F.-X. Coudert and A. Boutin, *Chem. Phys. Lett.*, **2006**, 428, 68–72.

5. "Molecular Dynamics Simulations of Electron-Alkali Cation Pairs in Bulk Water", F.-X. Coudert, P. Archirel and A. Boutin, *J. Phys. Chem. B*, **2005**, 110, 607–615.

4. "Molecular dynamics simulations of the temperature and density dependence of the absorption spectra of hydrated electron and solvated silver atom in water", A. Boutin, R. Spezia, F.-X. Coudert and M. Mostafavi, *Chem. Phys. Lett.*, **2005**, 409, 219–223.

3. "Theoretical Study of Neutral Dipolar Atom in Water: Structure, Spectroscopy and Formation of an Excitonic State", R. Spezia, F.-X. Coudert and A. Boutin, *Mod. Phys. Lett. B*, **2004**, 18, 1327–1345.

2. "Reactivity of an Excess Electron with Monovalent Cations in Bulk Water by Mixed Quantum Classical Molecular Dynamics Simulations", R. Spezia, C. Nicolas, F.-X. Coudert, P. Archirel, R. Vuilleumier and A. Boutin, *Mol. Simul.*, **2004**, 30, 749–754.

1. "Distribution of Sodium Cations in Faujasite-Type Zeolite: A Canonical Parallel Tempering Simulation Study", C. Beauvais, X. Guerrault, F.-X. Coudert, A. Boutin and A. H. Fuchs, *J. Phys. Chem. B*, **2004**, 108, 399–404.

In conference proceedings

2. "Adsorption-Induced Breathing transitions in Metal-Organic Frameworks", A. H. Fuchs, F.-X. Coudert, C. Triguero, A. Boutin and A. V. Neimark, *Poromechanics V, Proceedings of the Fifth Biot Conference on Poromechanics*, Vienna (2013), Ed. C. Hellmich, B. Pichler, D. Adam, p. 626.

1. "Hydrothermal and Mechanical Stability of Metal–Organic Frameworks", F.-X. Coudert, A. Ortiz, M. De Toni, A. Boutin and A. H. Fuchs, *CONCREEP-9@MIT, Proceedings of the Ninth Conference on Creep, Shrinkage and Durability Mechanics of Concrete and other Quasi-Brittle Materials*, Cambridge MA (2013), Ed. H. M. Jennings, F.-J. Ulm, R. Pellenq.

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

3. "Comment etiquette", F.-X. Coudert, *Nature Chemistry*, **2015**, 7, 369.

2. "Setting the record straight", F.-X. Coudert, *Chemistry World*, **2015**, March issue, page 40.

1. "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).

Book chapters

9. "Modeling of zeolites: from the unit cell to the crystal", F.-X. Coudert and A. H. Fuchs, in *Verified Syntheses of Zeolitic Materials (3rd edition)*, Elsevier (2016).

8. "Thermodynamic Methods for Prediction of Gas Separation in Flexible Frameworks", F.-X. Coudert, in *Metal-Organic Frameworks, Applications from Catalysis to Gas Storage*, D. Farrusseng, Wiley-VCH (2011).

7. "Dynamique moléculaire mixte classique-quantique de l'électron hydraté", A. Boutin and F.-X. Coudert, in *Réactions ultrarapides en solution — Approches expérimentales et théoriques*, T. Gustavsson and M. Mostafavi, CNRS Éditions (2007).

1–6. *Annales des concours*, sessions 2003 à 2005, aux éditions H&K: corrigés des épreuves de chimie des concours d'entrée des grandes écoles (*book of exams with complete hints and solutions, for French schools of engineering*).

Oral communications

As invited speaker

- "Soft Porous Crystals, Molecular Insight from Computational Chemistry", *Thermodynamics 2017*, September 5–8 2017, Edinburgh (UK).
- "Flexibility, Defects & Disorder in Soft Porous Crystals", *7th FEZA Conference — Federation of European Zeolite Associations*, July 3–7 2017, Sofia (Bulgaria).
- "Mechanical Impact of Adsorption in Compliant Nanoporous Materials", *Characterization of Porous Solids (COPS-XI)*, May 14–17 2017, Avignon (France).
- "Flexibility, Defects & Disorder in Soft Porous Crystals", *Switchability in Porous Metal-Organic Frameworks*, March 13-14 2017, Dresden (Germany).
- "Coupling transport and adsorption through Lattice Boltzmann methods", *EMN Meeting on Mesoporous Materials*, June 13–17 2016, Prague (Czech Republic).
- "Mechanical impact of adsorption in compliant microporous materials", *12th International Conference on the Fundamentals of Adsorption*, May 30–June 3 2016, Friedrichshafen (Germany).
- "First-principles dynamics and free energy methods for flexible materials", *CP2K-UK Conference*, February 22 2016, London (UK).
- "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).

- "Molecular simulation of materials flexibility and disorder", *International workshop on Flexibility and Disorder in Metal–Organic Frameworks*, June 3–5 2015, Paris (France).
- "Polymorphism and Flexibility in Nanoporous Molecular Frameworks", *CPM-7: 7th International Workshop on the Characterization of Porous Materials*, May 3–6 2015, Delray Beach FL (USA).
- "On the Impact of Adsorption in Compliant Nanoporous Materials", *4th Symposium on Future Challenges for Carbon-based Nanoporous Materials*, March 16–18 2015, Nagano (Japan).
- "Interfaces and porous materials: Insight from Molecular Simulation", *CAPZEO-2014: Fourth International Summer School on Quantum Electronic Calculations*, June 8–12 2014, Rabat (Morroco).
- "Theoretical Insight into Soft Porous Crystals", *CFCAM meeting on simulation of systems under thermodynamic gradients*, March 25–26 2014, Paris (France).
- "Anisotropic Elastic Properties of Flexible Metal–Organic Frameworks", *International symposium on CO_2 capture*, September 18–20 2013, Marne-la-Vallée (France).
- "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).
- "Structural transitions in metal–organic frameworks: thermodynamics & mechanics", *International workshop on adsorption in compliant solids*, June 5–7 2013, Paris (France).
- "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).
- "Water nanodroplets confined in zeolite pores", Faraday Discussion 141: *Water, From Interfaces to Bulk*, August 27–29 2008, Edinburgh (UK).

In international conferences

- "Flexibility, Defects & Disorder in Soft Porous Crystals: Molecular Insight from Computational Chemistry", *12th International Conference on the Fundamentals of Adsorption*, May 30–June 3 2016, Friedrichshafen (Germany).
- "Assessing and predicting flexibility in MOFs with molecular simulation", *EUROMOF 2015, 1st European Conference on Metal Organic Frameworks and Porous Polymers*, October 11–14 2015, Potsdam (Germany).
- "Molecular simulation of stimuli-responsive framework materials", *12th International Conference on Materials Chemistry (MC12)*, July 20–23 2015, York (UK).
- "Polymorphism in nanoporous materials: assessing mechanical, thermal stability, and experimental feasibility", *249th ACS National Meeting* (PHYS division), March 22–26 2015, Denver CO (USA).
- "Assessing and predicting flexibility in framework materials with molecular simulation", *249th ACS National Meeting* (COMP division), March 22–26 2015, Denver CO (USA).
- "Remarkable Pressure Responses of MOFs: Proton Transfer, Linker Coiling, Order-to-Disorder Transitions", *249th ACS National Meeting* (PMSE division), March 22–26 2015, Denver CO (USA).
- "Fluids in Soft Porous Crystals: Coupling Adsorption and Deformation", *RSC/IOP Joint Meeting on Computer Simulation of Confined Fluids*, December 8 2014, London (UK).
- "Assessing and predicting flexibility in MOFs with molecular simulation", *IUCr 2014 — 23rd Congress and general assembly*, August 5–12 2014, Montreal (Canada).
- "Mechanical Stability of Metal-Organic Frameworks: Insight from Molecular Simulation", *CONCREEP-9@MIT*, September 22–25 2013, Cambridge MA (USA).
- "Anisotropic Elastic Properties of Flexible Metal–Organic Frameworks", *EUROMAT 2013*, September 8–13 2013, Sevilla (France).
- "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 IRMOFs", *FOA11: 11th International Conference on the Fundamentals of Adsorption*, May 19–24 2013, Baltimore MD (USA).
- "Ab Initio Investigation into the Hydration Mechanism of MOFs", *Characterization of Porous Media 6*, April 30—May 2 2012, Delray Beach FL (USA).

- "Water in Metal–Organic Frameworks", *Transient Chemical Structures in Dense Media*, November 30 2010, Paris (France).
- "Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organic–Inorganic Frameworks", International Zeolite Conference 16, July 5—9 2010, Sorrento (Italy).
- "Adsorption of Water in Metal–Organic Frameworks: Insight From Molecular Simulation", *Fundamentals of Adsorption 10*, May 24—30 2010, Awaji (Japan).
- "Water Intrusion in Hydrophobic Zeolites", *Fundamentals of Adsorption 10*, May 24—30 2010, Awaji (Japan).
- "Effect of confinement on water in zeolite nanopores", XVIII International Conference on *Horizons in Hydrogen Bond Research*, September 14-18 2009, Paris (France).
- "Water confined in nanopores : structure, dipole, IR and more", CECAM workshop on *New developments for first principles molecular dynamics simulations in condensed matter and molecular physics*, May 15–18 2006, Lyon (France).
- "Elemental Femtochemistry of a Confined Hydrated Electron", Workshop on *Ab initio dynamical simulations in condensed matter*, April 19 2006, Paris (France).

In national conferences

- "Dynamique moléculaire et méthode de Monte–Carlo", *DynaMol summer school*, May 23–27 2016, Paris (France).
- "Matériaux intelligents et réactifs : comprendre et prédire leur comportement", *Journées francophones des jeunes physico-chimistes*, October 19–23 2015, Girona (Spain).
- "Introduction to Molecular Dynamics and Monte Carlo simulations", *MeMoSim2015: Méthodes De Modélisation Et Simulation Multiéchelles*, March 30–April 2 2015, Lyon (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).
- "Theoretical insight into Soft Porous Crystals: Problems and tools to solve them", *Journées francophones des jeunes physico-chimistes*, October 13–17 2014, Dammarie-les-Lys (France).
- "Anisotropic Elastic Properties of Flexible Metal-Organic Frameworks", Colloque Société Française de Physique, division *Physique Atomique, Moléculaire et Optique*, *Journées de Spectroscopie Moléculaire*, July 7–10 2014, Reims (France).
- "Structure des Phases Adsorbées : Apports de la Simulation Moléculaire", *Journées École de l'Association Française de l'Adsorption*, February 10 2014, Paris (France).
- "Ab Initio Investigation into the Hydration Mechanism of MOFs", *Journées 2013 de l'Association Française de l'Adsorption*, February 14–15 2013, Paris (France).
- "Ab Initio Investigation into Hydrothermal Stability and Mechanical Properties of Soft Porous Crystals", *Atelier Simulation des Matériaux Désordonnés*, December 12–13 2012, Marseille (France).
- "Adsorption & effets de confinement: Outils théoriques, simulation moléculaire", *GdR Thermodynamique Moléculaire et des Procédés*, December 11 2012, Paris (France).
- "Modèles thermodynamiques et mécaniques pour la description des matériaux poreux flexibles", *Journées 2012 de l'Association Française de l'Adsorption*, May 24–25 2012, Paris (France).
- "Adsorption & effets de confinement — Outils théoriques et simulation moléculaire", *Groupe Français d'Adsorption et des Surfaces Hétérogènes*, July 2 2010, Paris (France).
- "Isothermes de type V de H2O et CO2 dans les MOF", *Groupe Français des Zéolithes*, March 31—May 2 2010, Giens (France).
- "Adsorption dans les matériaux nanoporeux flexibles", *Journées Modélisation à Paris*, June 15–16 2009, Paris (France).

Invited seminars in research groups

- 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).
- University of Oxford, June 25 2014, Oxford (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

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_2 capture, September 18–20 2013, Marne-la-Vallée (France).
- Co-organizer of the International Workshop on "Adsorption in Compliant Solids", June 5–7 2013, Paris (France).
- Co-organizer of the International Workshop on "Adsorption in Compliant Solids: Theory, Simulation, and Experiments", June 9–11 2011, Paris (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).
- Reviewer for many journals, including: *Nature*, *Phys. Rev. Lett.*, *J. Am. Chem. Soc.*, *Angewandte Chemie*, *Chem. Rev.*, *Chem. Soc. Rev.*, *Acc. Chem. Rev.*, *J. Phys. Chem.* (and *J. Phys. Chem. Lett.*), *PCCP*, *J. Mater. Chem.*, *Langmuir*, *Adsorption*, *Mol. Simulat.*, etc.

Students and post-doc supervised

- 5 post-doctoral researchers
  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
  Marta De Toni, co-advisor (80%): 2009–2012. Now at Sanofi.
  David Bousquet, co-advisor (50%): 2010–2014. Now at CEA.
  Aurélie Ortiz, co-advisor (80%): 2011–2014. Now at Saint-Gobain.
  Jean-Mathieu Vanson, co-advisor (60%): 2014–2017.
  Liam Wilbraham, co-advisor (50%): 2014–2017.
  Romain Gaillac, advisor (100%):2015–2018. Guillaume Fraux, advisor (100%):2015–2018. Elsa Perrin, advisor (50%):2015–2018.
- 5 Master's students
- 10 undergrad students

PhD thesis committees

Nicolas Ferrando (supervisor: Anne Boutin), June 15 2011.
Marta De Toni (supervisors: Alain Fuchs and FXC), July 13 2012.
David Bousquet (supervisors: Anne Boutin and FXC), October 24 2013.
Benoît Carrier (supervisor: Henri Van Damme), December 6 2013.
Ines Collings (supervisor: Andrew Goodwin), June 26 2014.
Aurélie Ortiz (supervisors: Anne Boutin and FXC), July 11 2014.
François Villemot (supervisor: Benoit Coasne), November 25 2014.