Franois Xavier Coudert

List of Publications by Citations

147 papers	9,763 citations	52 h-index	96 g-index
235 ext. papers	11,760 ext. citations	8.8 avg, IF	7.08 L-index

#	Paper	IF	Citations
147	Necessary and sufficient elastic stability conditions in various crystal systems. *Physical Review B*, **2014**, 90,	3.3	1370
146	Correlated defect nanoregions in a metal-organic framework. *Nature Communications*, **2014**, 5, 4176	17.4	420
145	A pressure-amplifying framework material with negative gas adsorption transitions. *Nature*, **2016**, 532, 348-52	50.4	380
144	Responsive Metal□Organic Frameworks and Framework Materials: Under Pressure, Taking the Heat, in the Spotlight, with Friends. *Chemistry of Materials*, **2015**, 27, 1905-1916	9.6	370
143	ELATE: an open-source online application for analysis and visualization of elastic tensors. *Journal of Physics Condensed Matter*, **2016**, 28, 275201	1.8	307
142	Mixed-metal metal-organic frameworks. *Chemical Society Reviews*, **2019**, 48, 2535-2565	58.5	292
141	Thermodynamics of guest-induced structural transitions in hybrid organic-inorganic frameworks. *Journal of the American Chemical Society*, **2008**, 130, 14294-302	16.4	259
140	Interplay between defects, disorder and flexibility in metal-organic frameworks. *Nature Chemistry*, **2016**, 9, 11-16	17.6	256
139	Anisotropic elastic properties of flexible metal-organic frameworks: how soft are soft porous crystals?. *Physical Review Letters*, **2012**, 109, 195502	7.4	222
138	Liquid metal-organic frameworks. *Nature Materials*, **2017**, 16, 1149-1154	27	207
137	Stress-Based Model for the Breathing of Metal-Organic Frameworks. *Journal of Physical Chemistry Letters*, **2010**, 1, 445-9	6.4	187
136	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. *CrystEngComm*, **2009**, 11, 2272	3.3	181
135	The Behavior of Flexible MIL-53(Al) upon CH4 and CO2 Adsorption. *Journal of Physical Chemistry C*, **2010**, 114, 22237-22244	3.8	171
134	Computational characterization and prediction of metal□organic framework properties. *Coordination Chemistry Reviews*, **2016**, 307, 211-236	23.2	162
133	Breathing transitions in MIL-53(Al) metal-organic framework upon xenon adsorption. *Angewandte Chemie - International Edition*, **2009**, 48, 8314-7	16.4	161
132	Prediction of breathing and gate-opening transitions upon binary mixture adsorption in metal-organic frameworks. *Journal of the American Chemical Society*, **2009**, 131, 11329-31	16.4	133
131	Defects and disorder in metal organic frameworks. *Dalton Transactions*, **2016**, 45, 4113-26	4.3	125

130	Structural transitions in MIL-53 (Cr): view from outside and inside. *Langmuir*, **2011**, 27, 4734-41	4	125
129	Metal-organic frameworks with wine-rack motif: what determines their flexibility and elastic properties?. *Journal of Chemical Physics*, **2013**, 138, 174703	3.9	124
128	Adsorption Deformation and Structural Transitions in Metal□Organic Frameworks: From the Unit Cell to the Crystal. *Journal of Physical Chemistry Letters*, **2013**, 4, 3198-3205	6.4	121
127	Defects in metal-organic frameworks: a compromise between adsorption and stability?. *Dalton Transactions*, **2016**, 45, 4352-9	4.3	114
126	Investigating the Pressure-Induced Amorphization of Zeolitic Imidazolate Framework ZIF-8: Mechanical Instability Due to Shear Mode Softening. *Journal of Physical Chemistry Letters*, **2013**, 4, 1861-5	6.4	110
125	What makes zeolitic imidazolate frameworks hydrophobic or hydrophilic? The impact of geometry and functionalization on water adsorption. *Physical Chemistry Chemical Physics*, **2014**, 16, 9940-9	3.6	106
124	Thermodynamic methods and models to study flexible metal-organic frameworks. *ChemPhysChem*, **2011**, 12, 247-58	3.2	100
123	Defect-dependent colossal negative thermal expansion in UiO-66(Hf) metal-organic framework. *Physical Chemistry Chemical Physics*, **2015**, 17, 11586-92	3.6	99
122	Experimental Evidence of Negative Linear Compressibility in the MIL-53 Metal-Organic Framework Family. *CrystEngComm*, **2015**, 17, 276-280	3.3	99
121	How can a hydrophobic MOF be water-unstable? Insight into the hydration mechanism of IRMOFs. *ChemPhysChem*, **2012**, 13, 3497-503	3.2	99
120	Predicting the Mechanical Properties of Zeolite Frameworks by Machine Learning. *Chemistry of Materials*, **2017**, 29, 7833-7839	9.6	95
119	Non-Interpenetrated Metal-Organic Frameworks Based on Copper(II) Paddlewheel and Oligoparaxylene-Isophthalate Linkers: Synthesis, Structure, and Gas Adsorption. *Journal of the American Chemical Society*, **2016**, 138, 3371-81	16.4	91
118	Controlled partial interpenetration in metal-organic frameworks. *Nature Chemistry*, **2016**, 8, 250-7	17.6	87
117	Thermal and mechanical stability of zeolitic imidazolate frameworks polymorphs. *APL Materials*, **2014**, 2, 124110	5.7	83
116	Dipole moment, hydrogen bonding and IR spectrum of confined water. *ChemPhysChem*, **2006**, 7, 2464-7	3.2	82
115	A Computational and Experimental Approach Linking Disorder, High-Pressure Behavior, and Mechanical Properties in UiO Frameworks. *Angewandte Chemie - International Edition*, **2016**, 55, 2401-5	16.4	80
114	Pressure promoted low-temperature melting of metal-organic frameworks. *Nature Materials*, **2019**, 18, 370-376	27	74
113	Thermodynamic analysis of the breathing of amino-functionalized MIL-53(Al) upon CO2 adsorption. *Microporous and Mesoporous Materials*, **2011**, 140, 108-113	5.3	72

112	Double structural transition in hybrid material MIL-53 upon hydrocarbon adsorption: the thermodynamics behind the scenes. *Journal of the American Chemical Society*, **2009**, 131, 3442-3	16.4	69
111	Structure and chemistry of graphene oxide in liquid water from first principles. *Nature Communications*, **2020**, 11, 1566	17.4	68
110	Origins of Negative Gas Adsorption. *CheM*, **2016**, 1, 873-886	16.2	68
109	Adsorption induced transitions in soft porous crystals: an osmotic potential approach to multistability and intermediate structures. *Journal of Chemical Physics*, **2013**, 138, 174706	3.9	67
108	Remarkable pressure responses of metal-organic frameworks: proton transfer and linker coiling in zinc alkyl gates. *Journal of the American Chemical Society*, **2014**, 136, 11540-5	16.4	66
107	The osmotic framework adsorbed solution theory: predicting mixture coadsorption in flexible nanoporous materials. *Physical Chemistry Chemical Physics*, **2010**, 12, 10904-13	3.6	66
106	Water adsorption in hydrophobic MOF channels. *Physical Chemistry Chemical Physics*, **2010**, 12, 8123-9	3.6	66
105	Distribution of Sodium Cations in Faujasite-Type Zeolite: A Canonical Parallel Tempering Simulation Study. *Journal of Physical Chemistry B*, **2004**, 108, 399-404	3.4	66
104	Mechanism of Breathing Transitions in Metal□Organic Frameworks. *Journal of Physical Chemistry Letters*, **2011**, 2, 2033-2037	6.4	63
103	Insulator-to-Proton-Conductor Transition in a Dense Metal-Organic Framework. *Journal of the American Chemical Society*, **2015**, 137, 6428-31	16.4	61
102	Water nanodroplets confined in zeolite pores. *Faraday Discussions*, **2009**, 141, 377-98; discussion 443-65	3.6	61
101	Best practices in machine learning for chemistry. *Nature Chemistry*, **2021**, 13, 505-508	17.6	61
100	Computational Chemistry Methods for Nanoporous Materials. *Chemistry of Materials*, **2017**, 29, 199-212	9.6	54
99	Molecular Mechanism of Swing Effect in Zeolitic Imidazolate Framework ZIF-8: Continuous Deformation upon Adsorption. *ChemPhysChem*, **2017**, 18, 2732-2738	3.2	53
98	Rotational Dynamics of Linkers in Metal?Organic Frameworks. *Nanomaterials*, **2019**, 9,	5.4	52
97	Systematic investigation of the mechanical properties of pure silica zeolites: stiffness, anisotropy, and negative linear compressibility. *Physical Chemistry Chemical Physics*, **2013**, 15, 16012-8	3.6	52
96	Temperature-Induced Structural Transitions in the Gallium-Based MIL-53 Metal□Organic Framework. *Journal of Physical Chemistry C*, **2013**, 117, 8180-8188	3.8	52
95	Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices. *Chemical Society Reviews*, **2017**, 46, 7421-7437	58.5	50

94	Free energy landscapes for the thermodynamic understanding of adsorption-induced deformations and structural transitions in porous materials. *Journal of Chemical Physics*, **2012**, 137, 044118	3.9	50
93	Metal-organic framework crystal-glass composites. *Nature Communications*, **2019**, 10, 2580	17.4	49
92	Towards general network architecture design criteria for negative gas adsorption transitions in ultraporous frameworks. *Nature Communications*, **2019**, 10, 3632	17.4	46
91	Machine learning approaches for the prediction of materials properties. *APL Materials*, **2020**, 8, 080701	5.7	46
90	Investigation of structure and dynamics of the hydrated metal-organic framework MIL-53(Cr) using first-principles molecular dynamics. *Physical Chemistry Chemical Physics*, **2013**, 15, 19049-56	3.6	45
89	Carbon dioxide transport in molten calcium carbonate occurs through an oxo-Grotthuss mechanism via a pyrocarbonate anion. *Nature Chemistry*, **2016**, 8, 454-60	17.6	44
88	Water Adsorption in Flexible Gallium-Based MIL-53 Metal□Organic Framework. *Journal of Physical Chemistry C*, **2014**, 118, 5397-5405	3.8	44
87	Molecular Insight into CO2 □Trapdoor□Adsorption in Zeolite Na-RHO. *Chemistry of Materials*, **2017**, 29, 2724-2730	9.6	43
86	Multicomponent Metal□Organic Frameworks as Defect-Tolerant Materials. *Chemistry of Materials*, **2016**, 28, 368-375	9.6	43
85	Predicting mixture coadsorption in soft porous crystals: experimental and theoretical Study of CO2/CH4 in MIL-53(Al). *Langmuir*, **2012**, 28, 494-8	4	43
84	Air separation with graphene mediated by nanowindow-rim concerted motion. *Nature Communications*, **2018**, 9, 1812	17.4	42
83	Adsorption Contraction Mechanics: Understanding Breathing Energetics in Isoreticular Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2018**, 122, 19171-19179	3.8	39
82	Reorientational dynamics of water confined in zeolites. *ChemPhysChem*, **2014**, 15, 521-9	3.2	37
81	Rich Polymorphism of a Metal-Organic Framework in Pressure-Temperature Space. *Journal of the American Chemical Society*, **2019**, 141, 9330-9337	16.4	35
80	Prediction of flexibility of metal-organic frameworks CAU-13 and NOTT-300 by first principles molecular simulations. *Chemical Communications*, **2014**, 50, 5867-70	5.8	35
79	Polycatenated 2D Hydrogen-Bonded Binary Supramolecular Organic Frameworks (SOFs) with Enhanced Gas Adsorption and Selectivity. *Crystal Growth and Design*, **2018**, 18, 2555-2562	3.5	33
78	Melting of Zeolitic Imidazolate Frameworks with Different Topologies: Insight from First-Principles Molecular Dynamics. *Journal of Physical Chemistry C*, **2018**, 122, 6730-6736	3.8	33
77	Nanoscale metamaterials: Meta-MOFs and framework materials with anomalous behavior. *Coordination Chemistry Reviews*, **2019**, 388, 48-62	23.2	31

76	Microscopic Mechanism of Chiral Induction in a Metal-Organic Framework. *Journal of the American Chemical Society*, **2016**, 138, 6131-4	16.4	31
75	Recent advances in the computational chemistry of soft porous crystals. *Chemical Communications*, **2017**, 53, 7211-7221	5.8	30
74	Heterometallic Metal–Organic Frameworks of MOF-5 and UiO-66 Families: Insight from Computational Chemistry. *Journal of Physical Chemistry C*, **2016**, 120, 24885-24894	3.8	28
73	Impacts of the Imidazolate Linker Substitution (CH3, Cl, or Br) on the Structural and Adsorptive Properties of ZIF-8. *Journal of Physical Chemistry C*, **2018**, 122, 26945-26955	3.8	28
72	Understanding adsorption-induced structural transitions in metal-organic frameworks: from the unit cell to the crystal. *Journal of Chemical Physics*, **2012**, 137, 184702	3.9	27
71	Transport and adsorption under liquid flow: the role of pore geometry. *Soft Matter*, **2017**, 13, 875-885	3.6	25
70	Ab Initio Derived Force Fields for Zeolitic Imidazolate Frameworks: MOF-FF for ZIFs. *Journal of Chemical Theory and Computation*, **2019**, 15, 2420-2432	6.4	24
69	Unexpected coupling between flow and adsorption in porous media. *Soft Matter*, **2015**, 11, 6125-33	3.6	23
68	Challenges in first-principles NPT molecular dynamics of soft porous crystals: a case study on MIL-53(Ga). *Journal of Chemical Physics*, **2014**, 141, 064703	3.9	23
67	Breathing Transitions in MIL-53(Al) Metal–Organic Framework Upon Xenon Adsorption. *Angewandte Chemie*, **2009**, 121, 8464-8467	3.6	23
66	Insight into the Li2CO3-K2CO3 eutectic mixture from classical molecular dynamics: Thermodynamics, structure, and dynamics. *Journal of Chemical Physics*, **2016**, 144, 104507	3.9	23
65	Encoding complexity within supramolecular analogues of frustrated magnets. *Nature Chemistry*, **2016**, 8, 442-7	17.6	22
64	Understanding the Effect of Confinement on the Liquid–Gas Transition: A Study of Adsorption Isotherms in a Family of Metal–Organic Frameworks. *Journal of Physical Chemistry C*, **2010**, 114, 21631-21637	3.8	22
63	On the use of the IAST method for gas separation studies in porous materials with gate-opening behavior. *Adsorption*, **2018**, 24, 233-241	2.6	20
62	Modelling photophysical properties of metal-organic frameworks: a density functional theory based approach. *Physical Chemistry Chemical Physics*, **2016**, 18, 25176-25182	3.6	20
61	A Computational and Experimental Approach Linking Disorder, High-Pressure Behavior, and Mechanical Properties in UiO Frameworks. *Angewandte Chemie*, **2016**, 128, 2447-2451	3.6	20
60	A systematic typology for negative Poisson's ratio materials and the prediction of complete auxeticity in pure silica zeolite JST. *Physical Chemistry Chemical Physics*, **2015**, 17, 17927-33	3.6	19
59	Melting of hybrid organic-inorganic perovskites. *Nature Chemistry*, **2021**, 13, 778-785	17.6	19

58	Hydrothermal Breakdown of Flexible Metal-Organic Frameworks: A Study by First-Principles Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2015**, 6, 4365-70	6.4	18
57	The changing state of porous materials. *Nature Materials*, **2021**, 20, 1179-1187	27	18
56	Engineering micromechanics of soft porous crystals for negative gas adsorption. *Chemical Science*, **2020**, 11, 9468-9479	9.4	16
55	Structure and Dynamics of Water Confined in Imogolite Nanotubes. *Langmuir*, **2018**, 34, 6748-6756	4	16
54	Negative Hydration Expansion in ZrW_{2}O_{8}: Microscopic Mechanism, Spaghetti Dynamics, and Negative Thermal Expansion. *Physical Review Letters*, **2018**, 120, 265501	7.4	16
53	Speeding Up Discovery of Auxetic Zeolite Frameworks by Machine Learning. *Chemistry of Materials*, **2020**, 32, 2653-2663	9.6	15
52	Systematic exploration of the mechanical properties of 13 621 inorganic compounds. *Chemical Science*, **2019**, 10, 8589-8599	9.4	15
51	A thermodynamic description of the adsorption-induced structural transitions in flexible MIL-53 metal-organic framework. *Molecular Physics*, **2014**, 112, 1257-1261	1.7	15
50	Molecular dynamics simulations of electron-alkali cation pairs in bulk water. *Journal of Physical Chemistry B*, **2006**, 110, 607-15	3.4	14
49	Molecular dynamics simulations of the temperature and density dependence of the absorption spectra of hydrated electron and solvated silver atom in water. *Chemical Physics Letters*, **2005**, 409, 219-223	2.5	14
48	The role of temperature and adsorbate on negative gas adsorption transitions of the mesoporous metal-organic framework DUT-49. *Faraday Discussions*, **2021**, 225, 168-183	3.6	13
47	Kinetic Accessibility of Porous Material Adsorption Sites Studied through the Lattice Boltzmann Method. *Langmuir*, **2017**, 33, 1405-1411	4	12
46	Softening upon Adsorption in Microporous Materials: A Counterintuitive Mechanical Response. *Journal of Physical Chemistry Letters*, **2015**, 6, 4265-9	6.4	12
45	Isolating the Role of the Node-Linker Bond in the Compression of UiO-66 Metal Organic Frameworks. *Chemistry of Materials*, **2020**, 32, 5864-5871	9.6	12
44	Mechanism of water adsorption in the large pore form of the gallium-based MIL-53 metal-organic framework. *Microporous and Mesoporous Materials*, **2016**, 222, 145-152	5.3	12
43	Macroscopic Simulation of Deformation in Soft Microporous Composites. *Journal of Physical Chemistry Letters*, **2017**, 8, 1578-1584	6.4	11
42	Adsorption deformation of microporous composites. *Dalton Transactions*, **2016**, 45, 4136-40	4.3	11
41	Materials Databases: The Need for Open, Interoperable Databases with Standardized Data and Rich Metadata. *Advanced Theory and Simulations*, **2019**, 2, 1900131	3.5	11

40	Temperature effect on the absorption spectrum of the hydrated electron paired with a lithium cation in deuterated water. *Journal of Physical Chemistry A*, **2007**, 111, 3548-53	2.8	11
39	Novel Porous Polymorphs of Zinc Cyanide with Rich Thermal and Mechanical Behavior. *Chemistry of Materials*, **2015**, 27, 4422-4430	9.6	10
38	Emissive Azobenzenes Delivered on a Silver Coordination Polymer. *Inorganic Chemistry*, **2018**, 57, 15009-15022	4.8	10
37	Structure, Dynamics, and Thermodynamics of Intruded Electrolytes in ZIF-8. *Journal of Physical Chemistry C*, **2019**, 123, 15589-15598	3.8	9
36	Modelling of framework materials at multiple scales: current practices and open questions. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2019**, 377, 20180220	3	9
35	Water evaporation in silica colloidal deposits. *Journal of Colloid and Interface Science*, **2013**, 408, 206-11	9.3	9
34	Mechanism and kinetics of hydrated electron diffusion. *Journal of Chemical Physics*, **2008**, 129, 054505	3.9	9
33	Structure of Metal–Organic Framework Glasses by Ab Initio Molecular Dynamics. *Chemistry of Materials*, **2020**, 32, 8004-8011	9.6	9
32	Transient Catenation in a Zirconium-Based Metal-Organic Framework and Its Effect on Mechanical Stability and Sorption Properties. *Journal of the American Chemical Society*, **2021**, 143, 1503-1512	16.4	9
31	Water Adsorption in Soft and Heterogeneous Nanopores. *Accounts of Chemical Research*, **2020**, 53, 1342-1350	21.3	8
30	Comment on "Volume shrinkage of a metal-organic framework host induced by the dispersive attraction of guest gas molecules". *Physical Chemistry Chemical Physics*, **2014**, 16, 4394-5	3.6	8
29	van der Waals forces stabilize low-energy polymorphism in B2O3: Implications for the crystallization anomaly. *Physical Review Materials*, **2019**, 3,	3.2	8
28	Ab Initio Molecular Dynamics of CdSe Quantum-Dot-Doped Glasses. *Journal of the American Chemical Society*, **2020**, 142, 3905-3912	16.4	8
27	Strontium's scarlet sparkles. *Nature Chemistry*, **2015**, 7, 940	17.6	7
26	Metal-organic frameworks: the pressure is on. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2015**, 71, 585-6	1.8	7
25	Structure and Dynamics of Solvated Polymers near a Silica Surface: On the Different Roles Played by Solvent. *Journal of Physical Chemistry B*, **2018**, 122, 4573-4582	3.4	6
24	Confinement effect on the hydrated electron behaviour. *Chemical Physics Letters*, **2006**, 428, 68-72	2.5	6
23	MechElastic: A Python library for analysis of mechanical and elastic properties of bulk and 2D materials. *Computer Physics Communications*, **2021**, 267, 108068	4.2	6

22	MOF Decomposition and Introduction of Repairable Defects Using a Photodegradable Strut. *Chemistry - A European Journal*, **2019**, 25, 8393-8400	4.8	5
21	Molecular Simulation of a Zn Triazamacrocyle Metal Organic Frameworks Family with Extraframework Anions. *Journal of Physical Chemistry C*, **2012**, 116, 2952-2959	3.8	5
20	Flexibility of a Metal Organic Framework Enhances Gas Separation and Enables Quantum Sieving. *Chemistry of Materials*,	9.6	5
19	How Reproducible Are Surface Areas Calculated from the BET Equation?		5
18	The rise of preprints in chemistry. *Nature Chemistry*, **2020**, 12, 499-502	17.6	4
17	Soft Porous Crystals: Extraordinary Responses to Stimulation. *Bulletin of Japan Society of Coordination Chemistry*, **2019**, 73, 15-23	0.3	3
16	THEORETICAL STUDY OF NEUTRAL DIPOLAR ATOM IN WATER: STRUCTURE, SPECTROSCOPY AND FORMATION OF AN EXCITONIC STATE. *Modern Physics Letters B*, **2004**, 18, 1327-1345	1.6	3
15	Reactivity of an Excess Electron with Monovalent Cations in Bulk Water by Mixed Quantum Classical Molecular Dynamics Simulations. *Molecular Simulation*, **2004**, 30, 749-754	2	3
14	Atomistic Models of Amorphous Metal Organic Frameworks. *Journal of Physical Chemistry C*,	3.8	3
13	Adsorption in complex porous networks with geometrical and chemical heterogeneity. *Molecular Simulation*, **2014**, 40, 16-24	2	2
12	Thermodynamic Methods for Prediction of Gas Separation in Flexible Frameworks **2011**, 49-68		2
11	Prediction of Thermal Properties of Zeolites through Machine Learning. *Journal of Physical Chemistry C*, **2022**, 126, 1651-1660	3.8	2
10	Control of hysteretic sorption of flexible MOF for practical acetylene safe storage		2
9	Hybrid Inorganic-Organic Perovskite Glasses		2
8	Hybrid Inorganic-Organic Perovskite Glasses		2
7	Emergence of Coupled Rotor Dynamics in Metal-Organic Frameworks via Tuned Steric Interactions. *Journal of the American Chemical Society*, **2021**, 143, 12053-12062	16.4	2
6	Carbon species solvated in molten carbonate electrolyser cell from first-principles simulations. *International Journal of Hydrogen Energy*, **2021**, 46, 15008-15023	6.7	2
5	Conformational chiral polymorphism in cis-bis-triphenylphosphine complexes of transition metals. *CrystEngComm*, **2018**, 20, 5137-5142	3.3	2

4	Systematic Study of the Thermal Properties of Zeolitic Frameworks. *Journal of Physical Chemistry C*, **2021**, 125, 15647-15658	3.8	1
3	Identification of a Grotthuss proton hopping mechanism at protonated polyhedral oligomeric silsesquioxane (POSS) - water interface. *Journal of Colloid and Interface Science*, **2022**, 605, 701-709	9.3	1
2	Influence of Glass Composition on the Luminescence Mechanisms of CdSe Quantum-Dot-Doped Glasses. *Journal of Physical Chemistry C*, **2021**, 125, 18916-18926	3.8	0
1	Thermodynamic exploration of xenon/krypton separation based on a high-throughput screening. *Faraday Discussions*, **2021**, 231, 201-223	3.6	0