FranÃ§ois Xavier Coudert

List of Publications by Year
in descending order

157 papers	14,315 citations	20817 60 h-index	20358 116 g-index
235 all docs	235 docs citations	235 times ranked	12184 citing authors

#	Article	IF	Citations
1	Identification of a Grotthuss proton hopping mechanism at protonated polyhedral oligomeric silsesquioxane (POSS) â€“ water interface. Journal of Colloid and Interface Science, 2022, 605, 701-709.	9.4	9
2	Prediction of Thermal Properties of Zeolites through Machine Learning. Journal of Physical Chemistry C, 2022, 126, 1651-1660.	3.1	20
3	Atomistic Models of Amorphous Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2022, 126, 6905-6914.	3.1	14
4	Tunable acetylene sorption by flexible catenated metalâ€“organic frameworks. Nature Chemistry, 2022, 14, 816-822.	13.6	62
5	Chiral Lanthanum Metalâ€“Organic Framework with Gated CO₂ Sorption and Concerted Framework Flexibility. Journal of the American Chemical Society, 2022, 144, 8725-8733.	13.7	18
6	High-throughput computational screening of nanoporous materials in targeted applications. , 2022, 1, 355-374.		19
7	Defective Nature of CdSe Quantum Dots Embedded in Inorganic Matrices. Journal of the American Chemical Society, 2022, 144, 11296-11305.	13.7	5
8	CrystalNets.jl: Identification of Crystal Topologies. SciPost Chemistry, 2022, 1, .	4.0	5
9	The role of temperature and adsorbate on negative gas adsorption transitions of the mesoporous metalâ€“organic framework DUT-49. Faraday Discussions, 2021, 225, 168-183.	3.2	19
10	Carbon species solvated in molten carbonate electrolyser cell from first-principles simulations. International Journal of Hydrogen Energy, 2021, 46, 15008-15023.	7.1	6
11	Transient Catenation in a Zirconium-Based Metalâ€“Organic Framework and Its Effect on Mechanical Stability and Sorption Properties. Journal of the American Chemical Society, 2021, 143, 1503-1512.	13.7	28
12	The changing state of porous materials. Nature Materials, 2021, 20, 1179-1187.	27.5	147
13	Melting of hybrid organicâ€“inorganic perovskites. Nature Chemistry, 2021, 13, 778-785.	13.6	65
14	Best practices in machine learning for chemistry. Nature Chemistry, 2021, 13, 505-508.	13.6	240
15	Emergence of Coupled Rotor Dynamics in Metalâ€“Organic Frameworks via Tuned Steric Interactions. Journal of the American Chemical Society, 2021, 143, 12053-12062.	13.7	18
16	Open questions on water confined in nanoporous materials. Communications Chemistry, 2021, 4, .	4.5	15
17	Systematic Study of the Thermal Properties of Zeolitic Frameworks. Journal of Physical Chemistry C, 2021, 125, 15647-15658.	3.1	7
18	Influence of Glass Composition on the Luminescence Mechanisms of CdSe Quantum-Dot-Doped Glasses. Journal of Physical Chemistry C, 2021, 125, 18916-18926.	3.1	3

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19	MechElastic: A Python library for analysis of mechanical and elastic properties of bulk and 2D materials. Computer Physics Communications, 2021, 267, 108068.	7.5	54
20	Thermodynamic exploration of xenon/krypton separation based on a high-throughput screening. Faraday Discussions, 2021, 231, 201-223.	3.2	8
21	Novel computational tools: general discussion. Faraday Discussions, 2021, 225, 341-357.	3.2	1
22	Flexibility of a Metalâ€“Organic Framework Enhances Gas Separation and Enables Quantum Sieving. Chemistry of Materials, 2021, 33, 8886-8894.	6.7	23
23	Ab Initio Molecular Dynamics of CdSe Quantum-Dot-Doped Glasses. Journal of the American Chemical Society, 2020, 142, 3905-3912.	13.7	17
24	Machine learning approaches for the prediction of materials properties. APL Materials, 2020, 8, 080701.	5.1	113
25	Structure of Metalâ€“Organic Framework Glasses by Ab Initio Molecular Dynamics. Chemistry of Materials, 2020, 32, 8004-8011.	6.7	24
26	Engineering micromechanics of soft porous crystals for negative gas adsorption. Chemical Science, 2020, 11, 9468-9479.	7.4	30
27	The rise of preprints in chemistry. Nature Chemistry, 2020, 12, 499-502.	13.6	9
28	Isolating the Role of the Node-Linker Bond in the Compression of UiO-66 Metalâ€“Organic Frameworks. Chemistry of Materials, 2020, 32, 5864-5871.	6.7	24
29	Structure and chemistry of graphene oxide in liquid water from first principles. Nature Communications, 2020, 11, 1566.	12.8	169
30	Water Adsorption in Soft and Heterogeneous Nanopores. Accounts of Chemical Research, 2020, 53, 1342-1350.	15.6	15
31	Speeding Up Discovery of Auxetic Zeolite Frameworks by Machine Learning. Chemistry of Materials, 2020, 32, 2653-2663.	6.7	32
32	Towards general network architecture design criteria for negative gas adsorption transitions in ultraporous frameworks. Nature Communications, 2019, 10, 3632.	12.8	73
33	Systematic exploration of the mechanical properties of 13â€‰621 inorganic compounds. Chemical Science, 2019, 10, 8589-8599.	7.4	24
34	Materials Databases: The Need for Open, Interoperable Databases with Standardized Data and Rich Metadata. Advanced Theory and Simulations, 2019, 2, 1900131.	2.8	18
35	Soft Porous Crystals: Extraordinary Responses to Stimulation. Bulletin of Japan Society of Coordination Chemistry, 2019, 73, 15-23.	0.2	5
36	Rich Polymorphism of a Metalâ€“Organic Framework in Pressureâ€“Temperature Space. Journal of the American Chemical Society, 2019, 141, 9330-9337.	13.7	68

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37	Correcting the Scientific Record: Retraction Practices in Chemistry and Materials Science. Chemistry of Materials, 2019, 31, 3593-3598.	6.7	17
38	Structure, Dynamics, and Thermodynamics of Intruded Electrolytes in ZIF-8. Journal of Physical Chemistry C, 2019, 123, 15589-15598.	3.1	22
39	Modelling of framework materials at multiple scales: current practices and open questions. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180220.	3.4	15
40	Metal-organic framework crystal-glass composites. Nature Communications, 2019, 10, 2580.	12.8	97
41	Mixed-metal metalâ€“organic frameworks. Chemical Society Reviews, 2019, 48, 2535-2565.	38.1	474
42	Pressure promoted low-temperature melting of metalâ€“organic frameworks. Nature Materials, 2019, 18, 370-376.	27.5	134
43	Nanoscale metamaterials: Meta-MOFs and framework materials with anomalous behavior. Coordination Chemistry Reviews, 2019, 388, 48-62.	18.8	52
44	Rotational Dynamics of Linkers in Metalâ€“Organic Frameworks. Nanomaterials, 2019, 9, 330.	4.1	83
45	Charting a course for chemistry. Nature Chemistry, 2019, 11, 286-294.	13.6	18
46	Ab Initio Derived Force Fields for Zeolitic Imidazolate Frameworks: MOF-FF for ZIFs. Journal of Chemical Theory and Computation, 2019, 15, 2420-2432.	5.3	45
47	MOF Decomposition and Introduction of Repairable Defects Using a Photodegradable Strut. Chemistry - A European Journal, 2019, 25, 8393-8400.	3.3	7
48	van der Waals forces stabilize low-energy polymorphism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> : Implications for the crystallization anomaly. Physical Review Materials, 2019, 3, .	2.4	9
49	On the use of the IAST method for gas separation studies in porous materials with gate-opening behavior. Adsorption, 2018, 24, 233-241.	3.0	30
50	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.	2.6	9
51	Polycatenated 2D Hydrogen-Bonded Binary Supramolecular Organic Frameworks (SOFs) with Enhanced Gas Adsorption and Selectivity. Crystal Growth and Design, 2018, 18, 2555-2562.	3.0	49
52	Melting of Zeolitic Imidazolate Frameworks with Different Topologies: Insight from First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2018, 122, 6730-6736.	3.1	62
53	Emissive Azobenzenes Delivered on a Silver Coordination Polymer. Inorganic Chemistry, 2018, 57, 15009-15022.	4.0	14
54	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.	3.1	40

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55	Structure and Dynamics of Water Confined in Imogolite Nanotubes. Langmuir, 2018, 34, 6748-6756.	3.5	22
56	Conformational chiral polymorphism in cis-bis-triphenylphosphine complexes of transition metals. CrystEngComm, 2018, 20, 5137-5142.	2.6	2
57	Negative Hydration Expansion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>ZrW</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>8</mml:mn></mml:mrow></mml:mrow></mml:math> : Microscopic Mechanism, Spaghetti Dynamics, and Negative Thermal Expansion. Physical Review Letters, 2018, 120, 265501.	7.8	21
58	Adsorption Contraction Mechanics: Understanding Breathing Energetics in Isoreticular Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2018, 122, 19171-19179.	3.1	52
59	Air separation with graphene mediated by nanowindow-rim concerted motion. Nature Communications, 2018, 9, 1812.	12.8	67
60	Molecular Insight into CO₂ â€œTrapdoorâ€•Adsorption in Zeolite Na-RHO. Chemistry of Materials, 2017, 29, 2724-2730.	6.7	64
61	Kinetic Accessibility of Porous Material Adsorption Sites Studied through the Lattice Boltzmann Method. Langmuir, 2017, 33, 1405-1411.	3.5	14
62	Reproducible Research in Computational Chemistry of Materials. Chemistry of Materials, 2017, 29, 2615-2617.	6.7	28
63	Recent advances in the computational chemistry of soft porous crystals. Chemical Communications, 2017, 53, 7211-7221.	4.1	37
64	Macroscopic Simulation of Deformation in Soft Microporous Composites. Journal of Physical Chemistry Letters, 2017, 8, 1578-1584.	4.6	13
65	Transport and adsorption under liquid flow: the role of pore geometry. Soft Matter, 2017, 13, 875-885.	2.7	31
66	Interplay between defects, disorder and flexibility in metal-organic frameworks. Nature Chemistry, 2017, 9, 11-16.	13.6	342
67	Liquid metalâ€“organic frameworks. Nature Materials, 2017, 16, 1149-1154.	27.5	326
68	Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices. Chemical Society Reviews, 2017, 46, 7421-7437.	38.1	78
69	Predicting the Mechanical Properties of Zeolite Frameworks by Machine Learning. Chemistry of Materials, 2017, 29, 7833-7839.	6.7	144
70	Molecular Mechanism of Swing Effect in Zeolitic Imidazolate Framework ZIFâ€8: Continuous Deformation upon Adsorption. ChemPhysChem, 2017, 18, 2732-2738.	2.1	75
71	Computational Chemistry Methods for Nanoporous Materials. Chemistry of Materials, 2017, 29, 199-212.	6.7	69
72	Complexity in supramolecular analogues of frustrated magnets at high pressure. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1420-C1420.	0.1	0

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73	Origins of Negative Gas Adsorption. CheM, 2016, 1, 873-886.	11.7	89
74	Insight into the Li2CO3â€“K2CO3 eutectic mixture from classical molecular dynamics: Thermodynamics, structure, and dynamics. Journal of Chemical Physics, 2016, 144, 104507.	3.0	31
75	A pressure-amplifying framework material with negative gas adsorption transitions. Nature, 2016, 532, 348-352.	27.8	490
76	Microscopic Mechanism of Chiral Induction in a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2016, 138, 6131-6134.	13.7	41
77	Modelling photophysical properties of metalâ€“organic frameworks: a density functional theory based approach. Physical Chemistry Chemical Physics, 2016, 18, 25176-25182.	2.8	27
78	Heterometallic Metalâ€“Organic Frameworks of MOF-5 and UiO-66 Families: Insight from Computational Chemistry. Journal of Physical Chemistry C, 2016, 120, 24885-24894.	3.1	43
79	ELATE: an open-source online application for analysis and visualization of elastic tensors. Journal of Physics Condensed Matter, 2016, 28, 275201.	1.8	605
80	A Computational and Experimental Approach Linking Disorder, Highâ€Pressure Behavior, and Mechanical Properties in UiO Frameworks. Angewandte Chemie, 2016, 128, 2447-2451.	2.0	24
81	A Computational and Experimental Approach Linking Disorder, Highâ€Pressure Behavior, and Mechanical Properties in UiO Frameworks. Angewandte Chemie - International Edition, 2016, 55, 2401-2405.	13.8	103
82	Controlled partial interpenetration in metalâ€“organic frameworks. Nature Chemistry, 2016, 8, 250-257.	13.6	113
83	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.	4.4	14
84	Encoding complexity within supramolecular analogues of frustrated magnets. Nature Chemistry, 2016, 8, 442-447.	13.6	26
85	Flexibility and disorder in metalâ€“organic frameworks. Dalton Transactions, 2016, 45, 4058-4059.	3.3	26
86	Carbon dioxide transport in molten calcium carbonate occurs through an oxo-Grotthuss mechanism via a pyrocarbonate anion. Nature Chemistry, 2016, 8, 454-460.	13.6	60
87	Non-Interpenetrated Metalâ€“Organic Frameworks Based on Copper(II) Paddlewheel and Oligoparaxylene-Isophthalate Linkers: Synthesis, Structure, and Gas Adsorption. Journal of the American Chemical Society, 2016, 138, 3371-3381.	13.7	104
88	Adsorption deformation of microporous composites. Dalton Transactions, 2016, 45, 4136-4140.	3.3	14
89	Defects in metalâ€“organic frameworks: a compromise between adsorption and stability?. Dalton Transactions, 2016, 45, 4352-4359.	3.3	140
90	Multicomponent Metalâ€“Organic Frameworks as Defect-Tolerant Materials. Chemistry of Materials, 2016, 28, 368-375.	6.7	51

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91	Defects and disorder in metal organic frameworks. Dalton Transactions, 2016, 45, 4113-4126.	3.3	159
92	Computational characterization and prediction of metalâ€“organic framework properties. Coordination Chemistry Reviews, 2016, 307, 211-236.	18.8	206
93	Strontium's scarlet sparkles. Nature Chemistry, 2015, 7, 940-940.	13.6	14
94	Novel Porous Polymorphs of Zinc Cyanide with Rich Thermal and Mechanical Behavior. Chemistry of Materials, 2015, 27, 4422-4430.	6.7	14
95	Metalâ€“organic frameworks: the pressure is on. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 585-586.	1.1	8
96	Responsive Metalâ€“Organic Frameworks and Framework Materials: Under Pressure, Taking the Heat, in the Spotlight, with Friends. Chemistry of Materials, 2015, 27, 1905-1916.	6.7	432
97	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, 17927-17933.	2.8	27
98	Unexpected coupling between flow and adsorption in porous media. Soft Matter, 2015, 11, 6125-6133.	2.7	27
99	Defect-dependent colossal negative thermal expansion in UiO-66(Hf) metalâ€“organic framework. Physical Chemistry Chemical Physics, 2015, 17, 11586-11592.	2.8	127
100	Insulator-to-Proton-Conductor Transition in a Dense Metalâ€“Organic Framework. Journal of the American Chemical Society, 2015, 137, 6428-6431.	13.7	83
101	Hydrothermal Breakdown of Flexible Metalâ€“Organic Frameworks: A Study by First-Principles Molecular Dynamics. Journal of Physical Chemistry Letters, 2015, 6, 4365-4370.	4.6	23
102	Softening upon Adsorption in Microporous Materials: A Counterintuitive Mechanical Response. Journal of Physical Chemistry Letters, 2015, 6, 4265-4269.	4.6	20
103	Molecular simulation of framework materials. Molecular Simulation, 2015, 41, 1309-1310.	2.0	0
104	Experimental evidence of negative linear compressibility in the MIL-53 metalâ€“organic framework family. CrystEngComm, 2015, 17, 276-280.	2.6	119
105	Adsorption in complex porous networks with geometrical and chemical heterogeneity. Molecular Simulation, 2014, 40, 16-24.	2.0	3
106	Thermal and mechanical stability of zeolitic imidazolate frameworks polymorphs. APL Materials, 2014, 2, .	5.1	99
107	A thermodynamic description of the adsorption-induced structural transitions in flexible MIL-53 metal-organic framework. Molecular Physics, 2014, 112, 1257-1261.	1.7	18
108	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.	3.0	25

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109	Necessary and sufficient elastic stability conditions in various crystal systems. Physical Review B, 2014, 90, .	3.2	2,555
110	Comment on â€œVolume shrinkage of a metalâ€“organic framework host induced by the dispersive attraction of guest gas moleculesâ€• Physical Chemistry Chemical Physics, 2014, 16, 4394.	2.8	8
111	Remarkable Pressure Responses of Metalâ€“Organic Frameworks: Proton Transfer and Linker Coiling in Zinc Alkyl Gates. Journal of the American Chemical Society, 2014, 136, 11540-11545.	13.7	82
112	Prediction of flexibility of metalâ€“organic frameworks CAU-13 and NOTT-300 by first principles molecular simulations. Chemical Communications, 2014, 50, 5867.	4.1	46
113	Correlated defect nanoregions in a metalâ€“organic framework. Nature Communications, 2014, 5, 4176.	12.8	550
114	Water Adsorption in Flexible Gallium-Based MIL-53 Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2014, 118, 5397-5405.	3.1	55
115	What makes zeolitic imidazolate frameworks hydrophobic or hydrophilic? The impact of geometry and functionalization on water adsorption. Physical Chemistry Chemical Physics, 2014, 16, 9940-9949.	2.8	142
116	Reorientational Dynamics of Water Confined in Zeolites. ChemPhysChem, 2014, 15, 521-529.	2.1	42
117	Water evaporation in silica colloidal deposits. Journal of Colloid and Interface Science, 2013, 408, 206-211.	9.4	11
118	Metalâ€“organic frameworks with wine-rack motif: What determines their flexibility and elastic properties?. Journal of Chemical Physics, 2013, 138, 174703.	3.0	139
119	Systematic investigation of the mechanical properties of pure silica zeolites: stiffness, anisotropy, and negative linear compressibility. Physical Chemistry Chemical Physics, 2013, 15, 16012.	2.8	62
120	Adsorption induced transitions in soft porous crystals: An osmotic potential approach to multistability and intermediate structures. Journal of Chemical Physics, 2013, 138, 174706.	3.0	74
121	Hydrothermal and Mechanical Stability of Metal-Organic Frameworks. , 2013, , .		0
122	Adsorption Deformation and Structural Transitions in Metalâ€“Organic Frameworks: From the Unit Cell to the Crystal. Journal of Physical Chemistry Letters, 2013, 4, 3198-3205.	4.6	148
123	Investigation of structure and dynamics of the hydrated metalâ€“organic framework MIL-53(Cr) using first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 19049.	2.8	50
124	Temperature-Induced Structural Transitions in the Gallium-Based MIL-53 Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2013, 117, 8180-8188.	3.1	59
125	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, 1861-1865.	4.6	148
126	Adsorption-Induced Breathing Transitions in Metal-Organic Frameworks. , 2013, , .		0

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127	Understanding adsorption-induced structural transitions in metal-organic frameworks: From the unit cell to the crystal. Journal of Chemical Physics, 2012, 137, 184702.	3.0	35
128	Anisotropic Elastic Properties of Flexible Metal-Organic Frameworks: How Soft are Soft Porous Crystals?. Physical Review Letters, 2012, 109, 195502.	7.8	265
129	Molecular Simulation of a Znâ€“Triazamacrocyle Metalâ€“Organic Frameworks Family with Extraframework Anions. Journal of Physical Chemistry C, 2012, 116, 2952-2959.	3.1	5
130	Predicting Mixture Coadsorption in Soft Porous Crystals: Experimental and Theoretical Study of CO₂/CH₄ in MIL-53(Al). Langmuir, 2012, 28, 494-498.	3.5	45
131	Free energy landscapes for the thermodynamic understanding of adsorption-induced deformations and structural transitions in porous materials. Journal of Chemical Physics, 2012, 137, 044118.	3.0	57
132	How Can a Hydrophobic MOF be Waterâ€Unstable? Insight into the Hydration Mechanism of IRMOFs. ChemPhysChem, 2012, 13, 3497-3503.	2.1	116
133	Thermodynamic Methods for Prediction of Gas Separation in Flexible Frameworks. , 2011, , 49-68.		2
134	Structural Transitions in MIL-53 (Cr): View from Outside and Inside. Langmuir, 2011, 27, 4734-4741.	3.5	143
135	Mechanism of Breathing Transitions in Metalâ€“Organic Frameworks. Journal of Physical Chemistry Letters, 2011, 2, 2033-2037.	4.6	74
136	Thermodynamic Methods and Models to Study Flexible Metalâ€“Organic Frameworks. ChemPhysChem, 2011, 12, 247-258.	2.1	105
137	Thermodynamic analysis of the breathing of amino-functionalized MIL-53(Al) upon CO2 adsorption. Microporous and Mesoporous Materials, 2011, 140, 108-113.	4.4	78
138	Stress-Based Model for the Breathing of Metalâ^'Organic Frameworks. Journal of Physical Chemistry Letters, 2010, 1, 445-449.	4.6	209
139	The osmotic framework adsorbed solution theory: predicting mixture coadsorption in flexible nanoporous materials. Physical Chemistry Chemical Physics, 2010, 12, 10904.	2.8	76
140	The Behavior of Flexible MIL-53(Al) upon CH₄and CO₂Adsorption. Journal of Physical Chemistry C, 2010, 114, 22237-22244.	3.1	197
141	Understanding the Effect of Confinement on the Liquidâ^'Gas Transition: A Study of Adsorption Isotherms in a Family of Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2010, 114, 21631-21637.	3.1	27
142	Water adsorption in hydrophobic MOF channels. Physical Chemistry Chemical Physics, 2010, 12, 8123.	2.8	72
143	Breathing Transitions in MILâ€53(Al) Metalâ€“Organic Framework Upon Xenon Adsorption. Angewandte Chemie - International Edition, 2009, 48, 8314-8317.	13.8	176
144	Double Structural Transition in Hybrid Material MIL-53 upon Hydrocarbon Adsorption: The Thermodynamics Behind the Scenes. Journal of the American Chemical Society, 2009, 131, 3442-3443.	13.7	72

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145	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. CrystEngComm, 2009, 11, 2272.	2.6	217
146	Prediction of Breathing and Gate-Opening Transitions Upon Binary Mixture Adsorption in Metalâ^'Organic Frameworks. Journal of the American Chemical Society, 2009, 131, 11329-11331.	13.7	144
147	Water nanodroplets confined in zeolite pores. Faraday Discussions, 2009, 141, 377-398.	3.2	71
148	Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organicâ^'Inorganic Frameworks. Journal of the American Chemical Society, 2008, 130, 14294-14302.	13.7	299
149	Mechanism and kinetics of hydrated electron diffusion. Journal of Chemical Physics, 2008, 129, 054505.	3.0	10
150	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, 3548-3553.	2.5	11
151	Molecular Dynamics Simulations of Electronâ^'Alkali Cation Pairs in Bulk Water. Journal of Physical Chemistry B, 2006, 110, 607-615.	2.6	15
152	Confinement effect on the hydrated electron behaviour. Chemical Physics Letters, 2006, 428, 68-72.	2.6	7
153	Dipole Moment, Hydrogen Bonding and IR Spectrum of Confined Water. ChemPhysChem, 2006, 7, 2464-2467.	2.1	91
154	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.	2.6	14
155	THEORETICAL STUDY OF NEUTRAL DIPOLAR ATOM IN WATER: STRUCTURE, SPECTROSCOPY AND FORMATION OF AN EXCITONIC STATE. Modern Physics Letters B, 2004, 18, 1327-1345.	1.9	3
156	Reactivity of an Excess Electron with Monovalent Cations in Bulk Water by Mixed Quantum Classical Molecular Dynamics Simulations. Molecular Simulation, 2004, 30, 749-754.	2.0	3
157	Distribution of Sodium Cations in Faujasite-Type Zeolite:Â A Canonical Parallel Tempering Simulation Study. Journal of Physical Chemistry B, 2004, 108, 399-404.	2.6	79