

François Xavier Coudert

List of Publications by Year in descending order

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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	Necessary and sufficient elastic stability conditions in various crystal systems. <i>Physical Review B</i> , 2014, 90, .	3.2	2,555
2	ELATE: an open-source online application for analysis and visualization of elastic tensors. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 275201.	1.8	605
3	Correlated defect nanoregions in a metal-organic framework. <i>Nature Communications</i> , 2014, 5, 4176.	12.8	550
4	A pressure-amplifying framework material with negative gas adsorption transitions. <i>Nature</i> , 2016, 532, 348-352.	27.8	490
5	Mixed-metal metal-organic frameworks. <i>Chemical Society Reviews</i> , 2019, 48, 2535-2565.	38.1	474
6	Responsive Metal-Organic Frameworks and Framework Materials: Under Pressure, Taking the Heat, in the Spotlight, with Friends. <i>Chemistry of Materials</i> , 2015, 27, 1905-1916.	6.7	432
7	Interplay between defects, disorder and flexibility in metal-organic frameworks. <i>Nature Chemistry</i> , 2017, 9, 11-16.	13.6	342
8	Liquid metal-organic frameworks. <i>Nature Materials</i> , 2017, 16, 1149-1154.	27.5	326
9	Thermodynamics of Guest-Induced Structural Transitions in Hybrid Organic-Inorganic Frameworks. <i>Journal of the American Chemical Society</i> , 2008, 130, 14294-14302.	13.7	299
10	Anisotropic Elastic Properties of Flexible Metal-Organic Frameworks: How Soft are Soft Porous Crystals?. <i>Physical Review Letters</i> , 2012, 109, 195502.	7.8	265
11	Best practices in machine learning for chemistry. <i>Nature Chemistry</i> , 2021, 13, 505-508.	13.6	240
12	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. <i>CrystEngComm</i> , 2009, 11, 2272.	2.6	217
13	Stress-Based Model for the Breathing of Metal-Organic Frameworks. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 445-449.	4.6	209
14	Computational characterization and prediction of metal-organic framework properties. <i>Coordination Chemistry Reviews</i> , 2016, 307, 211-236.	18.8	206
15	The Behavior of Flexible MIL-53(Al) upon CH ₄ and CO ₂ Adsorption. <i>Journal of Physical Chemistry C</i> , 2010, 114, 22237-22244.	3.1	197
16	Breathing Transitions in MIL-53(Al) Metal-Organic Framework Upon Xenon Adsorption. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 8314-8317.	13.8	176
17	Structure and chemistry of graphene oxide in liquid water from first principles. <i>Nature Communications</i> , 2020, 11, 1566.	12.8	169
18	Defects and disorder in metal organic frameworks. <i>Dalton Transactions</i> , 2016, 45, 4113-4126.	3.3	159

#	ARTICLE	IF	CITATIONS
19	Adsorption Deformation and Structural Transitions in Metal-Organic Frameworks: From the Unit Cell to the Crystal. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3198-3205.	4.6	148
20	Investigating the Pressure-Induced Amorphization of Zeolitic Imidazolate Framework ZIF-8: Mechanical Instability Due to Shear Mode Softening. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1861-1865.	4.6	148
21	The changing state of porous materials. <i>Nature Materials</i> , 2021, 20, 1179-1187.	27.5	147
22	Prediction of Breathing and Gate-Opening Transitions Upon Binary Mixture Adsorption in Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2009, 131, 11329-11331.	13.7	144
23	Predicting the Mechanical Properties of Zeolite Frameworks by Machine Learning. <i>Chemistry of Materials</i> , 2017, 29, 7833-7839.	6.7	144
24	Structural Transitions in MIL-53 (Cr): View from Outside and Inside. <i>Langmuir</i> , 2011, 27, 4734-4741.	3.5	143
25	What makes zeolitic imidazolate frameworks hydrophobic or hydrophilic? The impact of geometry and functionalization on water adsorption. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9940-9949.	2.8	142
26	Defects in metal-organic frameworks: a compromise between adsorption and stability?. <i>Dalton Transactions</i> , 2016, 45, 4352-4359.	3.3	140
27	Metal-organic frameworks with wine-rack motif: What determines their flexibility and elastic properties?. <i>Journal of Chemical Physics</i> , 2013, 138, 174703.	3.0	139
28	Pressure promoted low-temperature melting of metal-organic frameworks. <i>Nature Materials</i> , 2019, 18, 370-376.	27.5	134
29	Defect-dependent colossal negative thermal expansion in UiO-66(Hf) metal-organic framework. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11586-11592.	2.8	127
30	Experimental evidence of negative linear compressibility in the MIL-53 metal-organic framework family. <i>CrystEngComm</i> , 2015, 17, 276-280.	2.6	119
31	How Can a Hydrophobic MOF be Water-Unstable? Insight into the Hydration Mechanism of IRMOFs. <i>ChemPhysChem</i> , 2012, 13, 3497-3503.	2.1	116
32	Controlled partial interpenetration in metal-organic frameworks. <i>Nature Chemistry</i> , 2016, 8, 250-257.	13.6	113
33	Machine learning approaches for the prediction of materials properties. <i>APL Materials</i> , 2020, 8, 080701.	5.1	113
34	Thermodynamic Methods and Models to Study Flexible Metal-Organic Frameworks. <i>ChemPhysChem</i> , 2011, 12, 247-258.	2.1	105
35	Non-Interpenetrated Metal-Organic Frameworks Based on Copper(II) Paddlewheel and Oligoparaxylene-Isophthalate Linkers: Synthesis, Structure, and Gas Adsorption. <i>Journal of the American Chemical Society</i> , 2016, 138, 3371-3381.	13.7	104
36	A Computational and Experimental Approach Linking Disorder, High-Pressure Behavior, and Mechanical Properties in UiO Frameworks. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2401-2405.	13.8	103

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37	Thermal and mechanical stability of zeolitic imidazolate frameworks polymorphs. <i>APL Materials</i> , 2014, 2, .	5.1	99
38	Metal-organic framework crystal-glass composites. <i>Nature Communications</i> , 2019, 10, 2580.	12.8	97
39	Dipole Moment, Hydrogen Bonding and IR Spectrum of Confined Water. <i>ChemPhysChem</i> , 2006, 7, 2464-2467.	2.1	91
40	Origins of Negative Gas Adsorption. <i>Chem</i> , 2016, 1, 873-886.	11.7	89
41	Insulator-to-Proton-Conductor Transition in a Dense Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2015, 137, 6428-6431.	13.7	83
42	Rotational Dynamics of Linkers in Metal-Organic Frameworks. <i>Nanomaterials</i> , 2019, 9, 330.	4.1	83
43	Remarkable Pressure Responses of Metal-Organic Frameworks: Proton Transfer and Linker Coiling in Zinc Alkyl Gates. <i>Journal of the American Chemical Society</i> , 2014, 136, 11540-11545.	13.7	82
44	Distribution of Sodium Cations in Faujasite-Type Zeolite: A Canonical Parallel Tempering Simulation Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 399-404.	2.6	79
45	Thermodynamic analysis of the breathing of amino-functionalized MIL-53(Al) upon CO ₂ adsorption. <i>Microporous and Mesoporous Materials</i> , 2011, 140, 108-113.	4.4	78
46	Forced intrusion of water and aqueous solutions in microporous materials: from fundamental thermodynamics to energy storage devices. <i>Chemical Society Reviews</i> , 2017, 46, 7421-7437.	38.1	78
47	The osmotic framework adsorbed solution theory: predicting mixture coadsorption in flexible nanoporous materials. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10904.	2.8	76
48	Molecular Mechanism of Swing Effect in Zeolitic Imidazolate Framework ZIF-8: Continuous Deformation upon Adsorption. <i>ChemPhysChem</i> , 2017, 18, 2732-2738.	2.1	75
49	Mechanism of Breathing Transitions in Metal-Organic Frameworks. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2033-2037.	4.6	74
50	Adsorption induced transitions in soft porous crystals: An osmotic potential approach to multistability and intermediate structures. <i>Journal of Chemical Physics</i> , 2013, 138, 174706.	3.0	74
51	Towards general network architecture design criteria for negative gas adsorption transitions in ultraporous frameworks. <i>Nature Communications</i> , 2019, 10, 3632.	12.8	73
52	Double Structural Transition in Hybrid Material MIL-53 upon Hydrocarbon Adsorption: The Thermodynamics Behind the Scenes. <i>Journal of the American Chemical Society</i> , 2009, 131, 3442-3443.	13.7	72
53	Water adsorption in hydrophobic MOF channels. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8123.	2.8	72
54	Water nanodroplets confined in zeolite pores. <i>Faraday Discussions</i> , 2009, 141, 377-398.	3.2	71

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55	Computational Chemistry Methods for Nanoporous Materials. <i>Chemistry of Materials</i> , 2017, 29, 199-212.	6.7	69
56	Rich Polymorphism of a Metal-Organic Framework in Pressure-Temperature Space. <i>Journal of the American Chemical Society</i> , 2019, 141, 9330-9337.	13.7	68
57	Air separation with graphene mediated by nanowindow-rim concerted motion. <i>Nature Communications</i> , 2018, 9, 1812.	12.8	67
58	Melting of hybrid organic-inorganic perovskites. <i>Nature Chemistry</i> , 2021, 13, 778-785.	13.6	65
59	Molecular Insight into CO ₂ Trapdoor Adsorption in Zeolite Na-RHO. <i>Chemistry of Materials</i> , 2017, 29, 2724-2730.	6.7	64
60	Systematic investigation of the mechanical properties of pure silica zeolites: stiffness, anisotropy, and negative linear compressibility. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16012.	2.8	62
61	Melting of Zeolitic Imidazolate Frameworks with Different Topologies: Insight from First-Principles Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6730-6736.	3.1	62
62	Tunable acetylene sorption by flexible catenated metal-organic frameworks. <i>Nature Chemistry</i> , 2022, 14, 816-822.	13.6	62
63	Carbon dioxide transport in molten calcium carbonate occurs through an oxo-Grothuss mechanism via a pyrocarbonate anion. <i>Nature Chemistry</i> , 2016, 8, 454-460.	13.6	60
64	Temperature-Induced Structural Transitions in the Gallium-Based MIL-53 Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8180-8188.	3.1	59
65	Free energy landscapes for the thermodynamic understanding of adsorption-induced deformations and structural transitions in porous materials. <i>Journal of Chemical Physics</i> , 2012, 137, 044118.	3.0	57
66	Water Adsorption in Flexible Gallium-Based MIL-53 Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5397-5405.	3.1	55
67	MechElastic: A Python library for analysis of mechanical and elastic properties of bulk and 2D materials. <i>Computer Physics Communications</i> , 2021, 267, 108068.	7.5	54
68	Adsorption Contraction Mechanics: Understanding Breathing Energetics in Isoreticular Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19171-19179.	3.1	52
69	Nanoscale metamaterials: Meta-MOFs and framework materials with anomalous behavior. <i>Coordination Chemistry Reviews</i> , 2019, 388, 48-62.	18.8	52
70	Multicomponent Metal-Organic Frameworks as Defect-Tolerant Materials. <i>Chemistry of Materials</i> , 2016, 28, 368-375.	6.7	51
71	Investigation of structure and dynamics of the hydrated metal-organic framework MIL-53(Cr) using first-principles molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 19049.	2.8	50
72	Polycatenated 2D Hydrogen-Bonded Binary Supramolecular Organic Frameworks (SOFs) with Enhanced Gas Adsorption and Selectivity. <i>Crystal Growth and Design</i> , 2018, 18, 2555-2562.	3.0	49

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73	Prediction of flexibility of metal-organic frameworks CAU-13 and NOTT-300 by first principles molecular simulations. <i>Chemical Communications</i> , 2014, 50, 5867.	4.1	46
74	Predicting Mixture Coadsorption in Soft Porous Crystals: Experimental and Theoretical Study of CO ₂ /CH ₄ in MIL-53(Al). <i>Langmuir</i> , 2012, 28, 494-498.	3.5	45
75	Ab Initio Derived Force Fields for Zeolitic Imidazolate Frameworks: MOF-FF for ZIFs. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2420-2432.	5.3	45
76	Heterometallic Metal-Organic Frameworks of MOF-5 and UiO-66 Families: Insight from Computational Chemistry. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24885-24894.	3.1	43
77	Reorientational Dynamics of Water Confined in Zeolites. <i>ChemPhysChem</i> , 2014, 15, 521-529.	2.1	42
78	Microscopic Mechanism of Chiral Induction in a Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2016, 138, 6131-6134.	13.7	41
79	Impacts of the Imidazolate Linker Substitution (CH ₃ , Cl, or Br) on the Structural and Adsorptive Properties of ZIF-8. <i>Journal of Physical Chemistry C</i> , 2018, 122, 26945-26955.	3.1	40
80	Recent advances in the computational chemistry of soft porous crystals. <i>Chemical Communications</i> , 2017, 53, 7211-7221.	4.1	37
81	Understanding adsorption-induced structural transitions in metal-organic frameworks: From the unit cell to the crystal. <i>Journal of Chemical Physics</i> , 2012, 137, 184702.	3.0	35
82	Speeding Up Discovery of Auxetic Zeolite Frameworks by Machine Learning. <i>Chemistry of Materials</i> , 2020, 32, 2653-2663.	6.7	32
83	Insight into the Li ₂ CO ₃ -K ₂ CO ₃ eutectic mixture from classical molecular dynamics: Thermodynamics, structure, and dynamics. <i>Journal of Chemical Physics</i> , 2016, 144, 104507.	3.0	31
84	Transport and adsorption under liquid flow: the role of pore geometry. <i>Soft Matter</i> , 2017, 13, 875-885.	2.7	31
85	On the use of the IAST method for gas separation studies in porous materials with gate-opening behavior. <i>Adsorption</i> , 2018, 24, 233-241.	3.0	30
86	Engineering micromechanics of soft porous crystals for negative gas adsorption. <i>Chemical Science</i> , 2020, 11, 9468-9479.	7.4	30
87	Reproducible Research in Computational Chemistry of Materials. <i>Chemistry of Materials</i> , 2017, 29, 2615-2617.	6.7	28
88	Transient Catenation in a Zirconium-Based Metal-Organic Framework and Its Effect on Mechanical Stability and Sorption Properties. <i>Journal of the American Chemical Society</i> , 2021, 143, 1503-1512.	13.7	28
89	Understanding the Effect of Confinement on the Liquid-Gas Transition: A Study of Adsorption Isotherms in a Family of Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21631-21637.	3.1	27
90	A systematic typology for negative Poisson's ratio materials and the prediction of complete auxeticity in pure silica zeolite JST. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17927-17933.	2.8	27

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91	Unexpected coupling between flow and adsorption in porous media. <i>Soft Matter</i> , 2015, 11, 6125-6133.	2.7	27
92	Modelling photophysical properties of metal-organic frameworks: a density functional theory based approach. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25176-25182.	2.8	27
93	Encoding complexity within supramolecular analogues of frustrated magnets. <i>Nature Chemistry</i> , 2016, 8, 442-447.	13.6	26
94	Flexibility and disorder in metal-organic frameworks. <i>Dalton Transactions</i> , 2016, 45, 4058-4059.	3.3	26
95	Challenges in first-principles NPT molecular dynamics of soft porous crystals: A case study on MIL-53(Ga). <i>Journal of Chemical Physics</i> , 2014, 141, 064703.	3.0	25
96	A Computational and Experimental Approach Linking Disorder, High-Pressure Behavior, and Mechanical Properties in UiO Frameworks. <i>Angewandte Chemie</i> , 2016, 128, 2447-2451.	2.0	24
97	Systematic exploration of the mechanical properties of 13621 inorganic compounds. <i>Chemical Science</i> , 2019, 10, 8589-8599.	7.4	24
98	Structure of Metal-Organic Framework Glasses by <i>Ab Initio</i> Molecular Dynamics. <i>Chemistry of Materials</i> , 2020, 32, 8004-8011.	6.7	24
99	Isolating the Role of the Node-Linker Bond in the Compression of UiO-66 Metal-Organic Frameworks. <i>Chemistry of Materials</i> , 2020, 32, 5864-5871.	6.7	24
100	Hydrothermal Breakdown of Flexible Metal-Organic Frameworks: A Study by First-Principles Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4365-4370.	4.6	23
101	Flexibility of a Metal-Organic Framework Enhances Gas Separation and Enables Quantum Sieving. <i>Chemistry of Materials</i> , 2021, 33, 8886-8894.	6.7	23
102	Structure and Dynamics of Water Confined in Imogolite Nanotubes. <i>Langmuir</i> , 2018, 34, 6748-6756.	3.5	22
103	Structure, Dynamics, and Thermodynamics of Intruded Electrolytes in ZIF-8. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15589-15598.	3.1	22
104	Negative Hydration Expansion in ZrW_2O_8 : Microscopic Mechanism, Spaghetti Dynamics, and Negative Thermal Expansion. <i>Physical Review Letters</i> , 2018, 120, 265501.	7.8	21
105	Softening upon Adsorption in Microporous Materials: A Counterintuitive Mechanical Response. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4265-4269.	4.6	20
106	Prediction of Thermal Properties of Zeolites through Machine Learning. <i>Journal of Physical Chemistry C</i> , 2022, 126, 1651-1660.	3.1	20
107	The role of temperature and adsorbate on negative gas adsorption transitions of the mesoporous metal-organic framework DUT-49. <i>Faraday Discussions</i> , 2021, 225, 168-183.	3.2	19
108	High-throughput computational screening of nanoporous materials in targeted applications. , 2022, 1, 355-374.		19

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109	A thermodynamic description of the adsorption-induced structural transitions in flexible MIL-53 metal-organic framework. <i>Molecular Physics</i> , 2014, 112, 1257-1261.	1.7	18
110	Materials Databases: The Need for Open, Interoperable Databases with Standardized Data and Rich Metadata. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900131.	2.8	18
111	Charting a course for chemistry. <i>Nature Chemistry</i> , 2019, 11, 286-294.	13.6	18
112	Emergence of Coupled Rotor Dynamics in Metal-Organic Frameworks via Tuned Steric Interactions. <i>Journal of the American Chemical Society</i> , 2021, 143, 12053-12062.	13.7	18
113	Chiral Lanthanum Metal-Organic Framework with Gated CO ₂ Sorption and Concerted Framework Flexibility. <i>Journal of the American Chemical Society</i> , 2022, 144, 8725-8733.	13.7	18
114	Correcting the Scientific Record: Retraction Practices in Chemistry and Materials Science. <i>Chemistry of Materials</i> , 2019, 31, 3593-3598.	6.7	17
115	Ab Initio Molecular Dynamics of CdSe Quantum-Dot-Doped Glasses. <i>Journal of the American Chemical Society</i> , 2020, 142, 3905-3912.	13.7	17
116	Molecular Dynamics Simulations of Electron-Alkali Cation Pairs in Bulk Water. <i>Journal of Physical Chemistry B</i> , 2006, 110, 607-615.	2.6	15
117	Modelling of framework materials at multiple scales: current practices and open questions. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2019, 377, 20180220.	3.4	15
118	Water Adsorption in Soft and Heterogeneous Nanopores. <i>Accounts of Chemical Research</i> , 2020, 53, 1342-1350.	15.6	15
119	Open questions on water confined in nanoporous materials. <i>Communications Chemistry</i> , 2021, 4, .	4.5	15
120	Molecular dynamics simulations of the temperature and density dependence of the absorption spectra of hydrated electron and solvated silver atom in water. <i>Chemical Physics Letters</i> , 2005, 409, 219-223.	2.6	14
121	Strontium's scarlet sparkles. <i>Nature Chemistry</i> , 2015, 7, 940-940.	13.6	14
122	Novel Porous Polymorphs of Zinc Cyanide with Rich Thermal and Mechanical Behavior. <i>Chemistry of Materials</i> , 2015, 27, 4422-4430.	6.7	14
123	Mechanism of water adsorption in the large pore form of the gallium-based MIL-53 metal-organic framework. <i>Microporous and Mesoporous Materials</i> , 2016, 222, 145-152.	4.4	14
124	Adsorption deformation of microporous composites. <i>Dalton Transactions</i> , 2016, 45, 4136-4140.	3.3	14
125	Kinetic Accessibility of Porous Material Adsorption Sites Studied through the Lattice Boltzmann Method. <i>Langmuir</i> , 2017, 33, 1405-1411.	3.5	14
126	Emissive Azobenzenes Delivered on a Silver Coordination Polymer. <i>Inorganic Chemistry</i> , 2018, 57, 15009-15022.	4.0	14

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127	Atomistic Models of Amorphous Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6905-6914.	3.1	14
128	Macroscopic Simulation of Deformation in Soft Microporous Composites. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1578-1584.	4.6	13
129	Temperature Effect on the Absorption Spectrum of the Hydrated Electron Paired with a Lithium Cation in Deuterated Water. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3548-3553.	2.5	11
130	Water evaporation in silica colloidal deposits. <i>Journal of Colloid and Interface Science</i> , 2013, 408, 206-211.	9.4	11
131	Mechanism and kinetics of hydrated electron diffusion. <i>Journal of Chemical Physics</i> , 2008, 129, 054505.	3.0	10
132	Structure and Dynamics of Solvated Polymers near a Silica Surface: On the Different Roles Played by Solvent. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4573-4582.	2.6	9
133	The rise of preprints in chemistry. <i>Nature Chemistry</i> , 2020, 12, 499-502.	13.6	9
134	Identification of a Grotthuss proton hopping mechanism at protonated polyhedral oligomeric silsesquioxane (POSS) water interface. <i>Journal of Colloid and Interface Science</i> , 2022, 605, 701-709.	9.4	9
135	van der Waals forces stabilize low-energy polymorphism in B_2O_3 : Implications for the crystallization anomaly. <i>Physical Review Materials</i> , 2019, 3, ...	2.4	9
136	Comment on "Volume shrinkage of a metal-organic framework host induced by the dispersive attraction of guest gas molecules". <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4394.	2.8	8
137	Metal-organic frameworks: the pressure is on. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2015, 71, 585-586.	1.1	8
138	Thermodynamic exploration of xenon/krypton separation based on a high-throughput screening. <i>Faraday Discussions</i> , 2021, 231, 201-223.	3.2	8
139	Confinement effect on the hydrated electron behaviour. <i>Chemical Physics Letters</i> , 2006, 428, 68-72.	2.6	7
140	MOF Decomposition and Introduction of Repairable Defects Using a Photodegradable Strut. <i>Chemistry - A European Journal</i> , 2019, 25, 8393-8400.	3.3	7
141	Systematic Study of the Thermal Properties of Zeolitic Frameworks. <i>Journal of Physical Chemistry C</i> , 2021, 125, 15647-15658.	3.1	7
142	Carbon species solvated in molten carbonate electrolyser cell from first-principles simulations. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 15008-15023.	7.1	6
143	Molecular Simulation of a Zn-Triazamacrocyle Metal-Organic Frameworks Family with Extraframework Anions. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2952-2959.	3.1	5
144	Soft Porous Crystals: Extraordinary Responses to Stimulation. <i>Bulletin of Japan Society of Coordination Chemistry</i> , 2019, 73, 15-23.	0.2	5

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145	Defective Nature of CdSe Quantum Dots Embedded in Inorganic Matrices. Journal of the American Chemical Society, 2022, 144, 11296-11305.	13.7	5
146	CrystalNets.jl: Identification of Crystal Topologies. SciPost Chemistry, 2022, 1, .	4.0	5
147	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
148	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
149	Adsorption in complex porous networks with geometrical and chemical heterogeneity. Molecular Simulation, 2014, 40, 16-24.	2.0	3
150	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
151	Thermodynamic Methods for Prediction of Gas Separation in Flexible Frameworks. , 2011, , 49-68.		2
152	Conformational chiral polymorphism in cis-bis-triphenylphosphine complexes of transition metals. CrystEngComm, 2018, 20, 5137-5142.	2.6	2
153	Novel computational tools: general discussion. Faraday Discussions, 2021, 225, 341-357.	3.2	1
154	Hydrothermal and Mechanical Stability of Metal-Organic Frameworks. , 2013, , .		0
155	Adsorption-Induced Breathing Transitions in Metal-Organic Frameworks. , 2013, , .		0
156	Molecular simulation of framework materials. Molecular Simulation, 2015, 41, 1309-1310.	2.0	0
157	Complexity in supramolecular analogues of frustrated magnets at high pressure. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1420-C1420.	0.1	0