

Francois Xavier Coudert

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/152199/francois-xavier-coudert-publications-by-year.pdf>

Version: 2024-04-27

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Prediction of Thermal Properties of Zeolites through Machine Learning. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 1651-1660	3.8	2
146	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	9.3	1
145	The changing state of porous materials. <i>Nature Materials</i> , 2021 , 20, 1179-1187	27	18
144	Melting of hybrid organic-inorganic perovskites. <i>Nature Chemistry</i> , 2021 , 13, 778-785	17.6	19
143	Best practices in machine learning for chemistry. <i>Nature Chemistry</i> , 2021 , 13, 505-508	17.6	61
142	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	16.4	2
141	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	3.6	13
140	Carbon species solvated in molten carbonate electrolyser cell from first-principles simulations. <i>International Journal of Hydrogen Energy</i> , 2021 , 46, 15008-15023	6.7	2
139	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	16.4	9
138	Systematic Study of the Thermal Properties of Zeolitic Frameworks. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 15647-15658	3.8	1
137	Influence of Glass Composition on the Luminescence Mechanisms of CdSe Quantum-Dot-Doped Glasses. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 18916-18926	3.8	0
136	MechElastic: A Python library for analysis of mechanical and elastic properties of bulk and 2D materials. <i>Computer Physics Communications</i> , 2021 , 267, 108068	4.2	6
135	Thermodynamic exploration of xenon/krypton separation based on a high-throughput screening. <i>Faraday Discussions</i> , 2021 , 231, 201-223	3.6	0
134	The rise of preprints in chemistry. <i>Nature Chemistry</i> , 2020 , 12, 499-502	17.6	4
133	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	9.6	12
132	Structure and chemistry of graphene oxide in liquid water from first principles. <i>Nature Communications</i> , 2020 , 11, 1566	17.4	68
131	Water Adsorption in Soft and Heterogeneous Nanopores. <i>Accounts of Chemical Research</i> , 2020 , 53, 1342-1350	13.5	8

130	Speeding Up Discovery of Auxetic Zeolite Frameworks by Machine Learning. <i>Chemistry of Materials</i> , 2020 , 32, 2653-2663	9.6	15
129	Ab Initio Molecular Dynamics of CdSe Quantum-Dot-Doped Glasses. <i>Journal of the American Chemical Society</i> , 2020 , 142, 3905-3912	16.4	8
128	Machine learning approaches for the prediction of materials properties. <i>APL Materials</i> , 2020 , 8, 080701	5.7	46
127	Structure of Metal-Organic Framework Glasses by Ab Initio Molecular Dynamics. <i>Chemistry of Materials</i> , 2020 , 32, 8004-8011	9.6	9
126	Engineering micromechanics of soft porous crystals for negative gas adsorption. <i>Chemical Science</i> , 2020 , 11, 9468-9479	9.4	16
125	Rich Polymorphism of a Metal-Organic Framework in Pressure-Temperature Space. <i>Journal of the American Chemical Society</i> , 2019 , 141, 9330-9337	16.4	35
124	Structure, Dynamics, and Thermodynamics of Intruded Electrolytes in ZIF-8. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 15589-15598	3.8	9
123	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		9
122	Metal-organic framework crystal-glass composites. <i>Nature Communications</i> , 2019 , 10, 2580	17.4	49
121	Mixed-metal metal-organic frameworks. <i>Chemical Society Reviews</i> , 2019 , 48, 2535-2565	58.5	292
120	Pressure promoted low-temperature melting of metal-organic frameworks. <i>Nature Materials</i> , 2019 , 18, 370-376	27	74
119	Nanoscale metamaterials: Meta-MOFs and framework materials with anomalous behavior. <i>Coordination Chemistry Reviews</i> , 2019 , 388, 48-62	23.2	31
118	Rotational Dynamics of Linkers in Metal-Organic Frameworks. <i>Nanomaterials</i> , 2019 , 9,	5.4	52
117	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	6.4	24
116	MOF Decomposition and Introduction of Repairable Defects Using a Photodegradable Strut. <i>Chemistry - A European Journal</i> , 2019 , 25, 8393-8400	4.8	5
115	Towards general network architecture design criteria for negative gas adsorption transitions in ultraporous frameworks. <i>Nature Communications</i> , 2019 , 10, 3632	17.4	46
114	Systematic exploration of the mechanical properties of 13 621 inorganic compounds. <i>Chemical Science</i> , 2019 , 10, 8589-8599	9.4	15
113	Materials Databases: The Need for Open, Interoperable Databases with Standardized Data and Rich Metadata. <i>Advanced Theory and Simulations</i> , 2019 , 2, 1900131	3.5	11

112	Soft Porous Crystals: Extraordinary Responses to Stimulation. <i>Bulletin of Japan Society of Coordination Chemistry</i> , 2019 , 73, 15-23	0.3	3
111	van der Waals forces stabilize low-energy polymorphism in B ₂ O ₃ : Implications for the crystallization anomaly. <i>Physical Review Materials</i> , 2019 , 3,	3.2	8
110	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	2.6	20
109	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	3.4	6
108	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	3.5	33
107	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	3.8	33
106	Adsorption Contraction Mechanics: Understanding Breathing Energetics in Isoreticular Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 19171-19179	3.8	39
105	Air separation with graphene mediated by nanowindow-rim concerted motion. <i>Nature Communications</i> , 2018 , 9, 1812	17.4	42
104	Emissive Azobenzenes Delivered on a Silver Coordination Polymer. <i>Inorganic Chemistry</i> , 2018 , 57, 15009-15022	4.5	10
103	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	3.8	28
102	Structure and Dynamics of Water Confined in Imogolite Nanotubes. <i>Langmuir</i> , 2018 , 34, 6748-6756	4	16
101	Conformational chiral polymorphism in cis-bis-triphenylphosphine complexes of transition metals. <i>CrystEngComm</i> , 2018 , 20, 5137-5142	3.3	2
100	Negative Hydration Expansion in ZrW ₂ O ₈ : Microscopic Mechanism, Spaghetti Dynamics, and Negative Thermal Expansion. <i>Physical Review Letters</i> , 2018 , 120, 265501	7.4	16
99	Molecular Insight into CO ₂ "rapdoor" Adsorption in Zeolite Na-RHO. <i>Chemistry of Materials</i> , 2017 , 29, 2724-2730	9.6	43
98	Kinetic Accessibility of Porous Material Adsorption Sites Studied through the Lattice Boltzmann Method. <i>Langmuir</i> , 2017 , 33, 1405-1411	4	12
97	Recent advances in the computational chemistry of soft porous crystals. <i>Chemical Communications</i> , 2017 , 53, 7211-7221	5.8	30
96	Macroscopic Simulation of Deformation in Soft Microporous Composites. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 1578-1584	6.4	11
95	Transport and adsorption under liquid flow: the role of pore geometry. <i>Soft Matter</i> , 2017 , 13, 875-885	3.6	25

94	Liquid metal-organic frameworks. <i>Nature Materials</i> , 2017 , 16, 1149-1154	27	207
93	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	58.5	50
92	Predicting the Mechanical Properties of Zeolite Frameworks by Machine Learning. <i>Chemistry of Materials</i> , 2017 , 29, 7833-7839	9.6	95
91	Molecular Mechanism of Swing Effect in Zeolitic Imidazolate Framework ZIF-8: Continuous Deformation upon Adsorption. <i>ChemPhysChem</i> , 2017 , 18, 2732-2738	3.2	53
90	Computational Chemistry Methods for Nanoporous Materials. <i>Chemistry of Materials</i> , 2017 , 29, 199-212	9.6	54
89	Computational characterization and prediction of metal-organic framework properties. <i>Coordination Chemistry Reviews</i> , 2016 , 307, 211-236	23.2	162
88	Interplay between defects, disorder and flexibility in metal-organic frameworks. <i>Nature Chemistry</i> , 2016 , 9, 11-16	17.6	256
87	Modelling photophysical properties of metal-organic frameworks: a density functional theory based approach. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 25176-25182	3.6	20
86	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	3.8	28
85	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	307
84	A Computational and Experimental Approach Linking Disorder, High-Pressure Behavior, and Mechanical Properties in UiO Frameworks. <i>Angewandte Chemie</i> , 2016 , 128, 2447-2451	3.6	20
83	A Computational and Experimental Approach Linking Disorder, High-Pressure Behavior, and Mechanical Properties in UiO Frameworks. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 2401-5	16.4	80
82	Controlled partial interpenetration in metal-organic frameworks. <i>Nature Chemistry</i> , 2016 , 8, 250-7	17.6	87
81	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	5.3	12
80	Encoding complexity within supramolecular analogues of frustrated magnets. <i>Nature Chemistry</i> , 2016 , 8, 442-7	17.6	22
79	Carbon dioxide transport in molten calcium carbonate occurs through an oxo-Grothuss mechanism via a pyrocarbonate anion. <i>Nature Chemistry</i> , 2016 , 8, 454-60	17.6	44
78	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, 3371-81	16.4	91
77	Adsorption deformation of microporous composites. <i>Dalton Transactions</i> , 2016 , 45, 4136-40	4.3	11

76	Defects in metal-organic frameworks: a compromise between adsorption and stability?. <i>Dalton Transactions</i> , 2016 , 45, 4352-9	4.3	114
75	Multicomponent Metal-Organic Frameworks as Defect-Tolerant Materials. <i>Chemistry of Materials</i> , 2016 , 28, 368-375	9.6	43
74	Defects and disorder in metal organic frameworks. <i>Dalton Transactions</i> , 2016 , 45, 4113-26	4.3	125
73	Origins of Negative Gas Adsorption. <i>Chem</i> , 2016 , 1, 873-886	16.2	68
72	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	3.9	23
71	A pressure-amplifying framework material with negative gas adsorption transitions. <i>Nature</i> , 2016 , 532, 348-52	50.4	380
70	Microscopic Mechanism of Chiral Induction in a Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2016 , 138, 6131-4	16.4	31
69	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, 17927-33	3.6	19
68	Unexpected coupling between flow and adsorption in porous media. <i>Soft Matter</i> , 2015 , 11, 6125-33	3.6	23
67	Defect-dependent colossal negative thermal expansion in UiO-66(Hf) metal-organic framework. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 11586-92	3.6	99
66	Insulator-to-Proton-Conductor Transition in a Dense Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2015 , 137, 6428-31	16.4	61
65	Hydrothermal Breakdown of Flexible Metal-Organic Frameworks: A Study by First-Principles Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4365-70	6.4	18
64	Softening upon Adsorption in Microporous Materials: A Counterintuitive Mechanical Response. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4265-9	6.4	12
63	Experimental Evidence of Negative Linear Compressibility in the MIL-53 Metal-Organic Framework Family. <i>CrystEngComm</i> , 2015 , 17, 276-280	3.3	99
62	Strontium's scarlet sparkles. <i>Nature Chemistry</i> , 2015 , 7, 940	17.6	7
61	Novel Porous Polymorphs of Zinc Cyanide with Rich Thermal and Mechanical Behavior. <i>Chemistry of Materials</i> , 2015 , 27, 4422-4430	9.6	10
60	Metal-organic frameworks: the pressure is on. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2015 , 71, 585-6	1.8	7
59	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	9.6	370

58	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, 4394-5	3.6	8
57	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, 11540-5	16.4	66
56	Prediction of flexibility of metal-organic frameworks CAU-13 and NOTT-300 by first principles molecular simulations. <i>Chemical Communications</i> , 2014 , 50, 5867-70	5.8	35
55	Correlated defect nanoregions in a metal-organic framework. <i>Nature Communications</i> , 2014 , 5, 4176	17.4	420
54	Water Adsorption in Flexible Gallium-Based MIL-53 Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 5397-5405	3.8	44
53	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, 9940-9	3.6	106
52	Reorientational dynamics of water confined in zeolites. <i>ChemPhysChem</i> , 2014 , 15, 521-9	3.2	37
51	Adsorption in complex porous networks with geometrical and chemical heterogeneity. <i>Molecular Simulation</i> , 2014 , 40, 16-24	2	2
50	Thermal and mechanical stability of zeolitic imidazolate frameworks polymorphs. <i>APL Materials</i> , 2014 , 2, 124110	5.7	83
49	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	15
48	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	3.9	23
47	Necessary and sufficient elastic stability conditions in various crystal systems. <i>Physical Review B</i> , 2014 , 90,	3.3	1370
46	Water evaporation in silica colloidal deposits. <i>Journal of Colloid and Interface Science</i> , 2013 , 408, 206-11	9.3	9
45	Metal-organic frameworks with wine-rack motif: what determines their flexibility and elastic properties?. <i>Journal of Chemical Physics</i> , 2013 , 138, 174703	3.9	124
44	Systematic investigation of the mechanical properties of pure silica zeolites: stiffness, anisotropy, and negative linear compressibility. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 16012-8	3.6	52
43	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	3.9	67
42	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	6.4	121
41	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, 19049-56	3.6	45

40	Temperature-Induced Structural Transitions in the Gallium-Based MIL-53 Metal-Organic Framework. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 8180-8188	3.8	52
39	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, 1861-1864	6.4	110
38	Anisotropic elastic properties of flexible metal-organic frameworks: how soft are soft porous crystals?. <i>Physical Review Letters</i> , 2012 , 109, 195502	7.4	222
37	Molecular Simulation of a Zn-Triazamacrocyclic Metal-Organic Frameworks Family with Extraframework Anions. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 2952-2959	3.8	5
36	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, 494-8	4	43
35	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	3.9	50
34	How can a hydrophobic MOF be water-unstable? Insight into the hydration mechanism of IRMOFs. <i>ChemPhysChem</i> , 2012 , 13, 3497-503	3.2	99
33	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	3.9	27
32	Thermodynamic Methods for Prediction of Gas Separation in Flexible Frameworks 2011 , 49-68		2
31	Structural transitions in MIL-53 (Cr): view from outside and inside. <i>Langmuir</i> , 2011 , 27, 4734-41	4	125
30	Mechanism of Breathing Transitions in Metal-Organic Frameworks. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 2033-2037	6.4	63
29	Thermodynamic methods and models to study flexible metal-organic frameworks. <i>ChemPhysChem</i> , 2011 , 12, 247-58	3.2	100
28	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	5.3	72
27	The osmotic framework adsorbed solution theory: predicting mixture coadsorption in flexible nanoporous materials. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 10904-13	3.6	66
26	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	3.8	171
25	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	3.8	22
24	Water adsorption in hydrophobic MOF channels. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 8123-9	3.6	66
23	Stress-Based Model for the Breathing of Metal-Organic Frameworks. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 445-9	6.4	187

22	Breathing Transitions in MIL-53(Al) Metal-Organic Framework Upon Xenon Adsorption. <i>Angewandte Chemie</i> , 2009 , 121, 8464-8467	3.6	23
21	Breathing transitions in MIL-53(Al) metal-organic framework upon xenon adsorption. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 8314-7	16.4	161
20	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, 3442-3	16.4	69
19	Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues. <i>CrystEngComm</i> , 2009 , 11, 2272	3.3	181
18	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, 11329-31	16.4	133
17	Water nanodroplets confined in zeolite pores. <i>Faraday Discussions</i> , 2009 , 141, 377-98; discussion 443-65	3.6	61
16	Thermodynamics of guest-induced structural transitions in hybrid organic-inorganic frameworks. <i>Journal of the American Chemical Society</i> , 2008 , 130, 14294-302	16.4	259
15	Mechanism and kinetics of hydrated electron diffusion. <i>Journal of Chemical Physics</i> , 2008 , 129, 054505	3.9	9
14	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, 3548-53	2.8	11
13	Dipole moment, hydrogen bonding and IR spectrum of confined water. <i>ChemPhysChem</i> , 2006 , 7, 2464-7	3.2	82
12	Molecular dynamics simulations of electron-alkali cation pairs in bulk water. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 607-15	3.4	14
11	Confinement effect on the hydrated electron behaviour. <i>Chemical Physics Letters</i> , 2006 , 428, 68-72	2.5	6
10	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	2.5	14
9	THEORETICAL STUDY OF NEUTRAL DIPOLAR ATOM IN WATER: STRUCTURE, SPECTROSCOPY AND FORMATION OF AN EXCITONIC STATE. <i>Modern Physics Letters B</i> , 2004 , 18, 1327-1345	1.6	3
8	Reactivity of an Excess Electron with Monovalent Cations in Bulk Water by Mixed Quantum Classical Molecular Dynamics Simulations. <i>Molecular Simulation</i> , 2004 , 30, 749-754	2	3
7	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	3.4	66
6	Flexibility of a Metal-Organic Framework Enhances Gas Separation and Enables Quantum Sieving. <i>Chemistry of Materials</i> ,	9.6	5
5	Control of hysteretic sorption of flexible MOF for practical acetylene safe storage		2

4	Hybrid Inorganic-Organic Perovskite Glasses	2
3	Hybrid Inorganic-Organic Perovskite Glasses	2
2	How Reproducible Are Surface Areas Calculated from the BET Equation?	5
1	Atomistic Models of Amorphous Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> ,	3.8 3