

Francesco Paesani

List of Publications by Year in descending order

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129
papers

7,644
citations

46918

47
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82
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192
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192
docs citations

192
times ranked

5837
citing authors

#	ARTICLE	IF	CITATIONS
1	Development of a "First Principles" Water Potential with Flexible Monomers: Dimer Potential Energy Surface, VRT Spectrum, and Second Virial Coefficient. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5395-5403.	2.3	398
2	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. <i>Chemical Reviews</i> , 2016, 116, 7501-7528.	23.0	314
3	Development of a "First Principles" Water Potential with Flexible Monomers. II: Trimer Potential Energy Surface, Third Virial Coefficient, and Small Clusters. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1599-1607.	2.3	313
4	Development of a "First-Principles" Water Potential with Flexible Monomers. III. Liquid Phase Properties. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2906-2910.	2.3	292
5	On the accuracy of the MB-pol many-body potential for water: Interaction energies, vibrational frequencies, and classical thermodynamic and dynamical properties from clusters to liquid water and ice. <i>Journal of Chemical Physics</i> , 2016, 145, 194504.	1.2	214
6	The Properties of Water: Insights from Quantum Simulations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5702-5719.	1.2	199
7	An accurate and simple quantum model for liquid water. <i>Journal of Chemical Physics</i> , 2006, 125, 184507.	1.2	187
8	Infrared and Raman Spectroscopy of Liquid Water through "First-Principles" Many-Body Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1145-1154.	2.3	182
9	MIL-101(Fe) as a lithium-ion battery electrode material: a relaxation and intercalation mechanism during lithium insertion. <i>Journal of Materials Chemistry A</i> , 2015, 3, 4738-4744.	5.2	168
10	Dissecting the Molecular Structure of the Air/Water Interface from Quantum Simulations of the Sum-Frequency Generation Spectrum. <i>Journal of the American Chemical Society</i> , 2016, 138, 3912-3919.	6.6	153
11	Proton Transport in a Highly Conductive Porous Zirconium-Based Metal-Organic Framework: Molecular Insight. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 3919-3924.	7.2	152
12	Quantum effects in liquid water from an <i>ab initio</i> -based polarizable force field. <i>Journal of Chemical Physics</i> , 2007, 127, 074506.	1.2	151
13	Comparison of permutationally invariant polynomials, neural networks, and Gaussian approximation potentials in representing water interactions through many-body expansions. <i>Journal of Chemical Physics</i> , 2018, 148, 241725.	1.2	142
14	Toward a Universal Water Model: First Principles Simulations from the Dimer to the Liquid Phase. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3765-3769.	2.1	137
15	The Water Hexamer: Cage, Prism, or Both. Full Dimensional Quantum Simulations Say Both. <i>Journal of the American Chemical Society</i> , 2012, 134, 11116-11119.	6.6	132
16	Ice Nucleation Efficiency of Hydroxylated Organic Surfaces Is Controlled by Their Structural Fluctuations and Mismatch to Ice. <i>Journal of the American Chemical Society</i> , 2017, 139, 3052-3064.	6.6	132
17	A Critical Assessment of Two-Body and Three-Body Interactions in Water. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1103-1114.	2.3	126
18	Infrared Spectroscopy and Hydrogen-Bond Dynamics of Liquid Water from Centroid Molecular Dynamics with an Ab Initio-Based Force Field. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13118-13130.	1.2	123

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19	Getting the Right Answers for the Right Reasons: Toward Predictive Molecular Simulations of Water with Many-Body Potential Energy Functions. <i>Accounts of Chemical Research</i> , 2016, 49, 1844-1851.	7.6	121
20	Ice-Nucleating and Antifreeze Proteins Recognize Ice through a Diversity of Anchored Clathrate and Ice-like Motifs. <i>Journal of the American Chemical Society</i> , 2018, 140, 4905-4912.	6.6	117
21	Electron affinity of liquid water. <i>Nature Communications</i> , 2018, 9, 247.	5.8	114
22	Preordering of water is not needed for ice recognition by hyperactive antifreeze proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 8266-8271.	3.3	89
23	Molecular-Level Characterization of the Breathing Behavior of the Jungle-Gym-type DMOF-1 Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2012, 134, 4207-4215.	6.6	87
24	Temperature-dependent vibrational spectra and structure of liquid water from classical and quantum simulations with the MB-pol potential energy function. <i>Journal of Chemical Physics</i> , 2017, 147, 244504.	1.2	87
25	Hydrogen bonding structure of confined water templated by a metal-organic framework with open metal sites. <i>Nature Communications</i> , 2019, 10, 4771.	5.8	86
26	Toward Chemical Accuracy in the Description of Ion-Water Interactions through Many-Body Representations. I. Halide-Water Dimer Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2698-2705.	2.3	81
27	On the representation of many-body interactions in water. <i>Journal of Chemical Physics</i> , 2015, 143, 104102.	1.2	80
28	A Refined MS-EVB Model for Proton Transport in Aqueous Environments. <i>Journal of Physical Chemistry B</i> , 2012, 116, 343-352.	1.2	79
29	Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase. <i>Journal of Chemical Physics</i> , 2014, 141, 181101.	1.2	74
30	Monitoring Water Clusters Through Vibrational Spectroscopy. <i>Journal of the American Chemical Society</i> , 2017, 139, 7082-7088.	6.6	69
31	Bulk Contributions Modulate the Sum-Frequency Generation Spectra of Water on Model Sea-Spray Aerosols. <i>CheM</i> , 2018, 4, 1629-1644.	5.8	69
32	Halogen bonding in UiO-66 frameworks promotes superior chemical warfare agent simulant degradation. <i>Chemical Communications</i> , 2019, 55, 3481-3484.	2.2	68
33	Molecular Origin of the Vibrational Structure of Ice I _h . <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2579-2583.	2.1	66
34	A quantitative assessment of the accuracy of centroid molecular dynamics for the calculation of the infrared spectrum of liquid water. <i>Journal of Chemical Physics</i> , 2010, 132, 014105.	1.2	63
35	Second-Order Vibrational Lineshapes from the Air/Water Interface. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4457-4464.	1.1	63
36	Nuclear Quantum Effects in the Reorientation of Water. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2316-2321.	2.1	62

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37	i-TTM Model for Ab Initio-Based Ion-Water Interaction Potentials. 1. Halide-Water Potential Energy Functions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1822-1832.	1.2	61
38	Many-Body Interactions in Ice. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1778-1784.	2.3	60
39	Temperature Dependence of the Air/Water Interface Revealed by Polarization Sensitive Sum-Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4356-4365.	1.2	59
40	Toward chemical accuracy in the description of ion-water interactions through many-body representations. Alkali-water dimer potential energy surfaces. <i>Journal of Chemical Physics</i> , 2017, 147, 161715.	1.2	57
41	Pore Breathing of Metal-Organic Frameworks by Environmental Transmission Electron Microscopy. <i>Journal of the American Chemical Society</i> , 2017, 139, 13973-13976.	6.6	56
42	Ion-mediated hydrogen-bond rearrangement through tunnelling in the iodide-dihydrate complex. <i>Nature Chemistry</i> , 2019, 11, 367-374.	6.6	55
43	Application of Adaptive QM/MM Methods to Molecular Dynamics Simulations of Aqueous Systems. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2868-2877.	2.3	54
44	Negative Ion Photoelectron Spectroscopy Reveals Thermodynamic Advantage of Organic Acids in Facilitating Formation of Bisulfate Ion Clusters: Atmospheric Implications. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 779-785.	2.1	53
45	Transmission Electron Microscopy Reveals Deposition of Metal Oxide Coatings onto Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2018, 140, 1348-1357.	6.6	51
46	Engineering the entropy-driven free-energy landscape of a dynamic nanoporous protein assembly. <i>Nature Chemistry</i> , 2018, 10, 732-739.	6.6	51
47	Local superfluidity in inhomogeneous quantum fluids. <i>Physical Review B</i> , 2006, 74, .	1.1	50
48	The end of ice I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 24413-24419.	3.3	50
49	Orientational Distribution of Free O-H Groups of Interfacial Water is Exponential. <i>Physical Review Letters</i> , 2018, 121, 246101.	2.9	49
50	Disentangling Coupling Effects in the Infrared Spectra of Liquid Water. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10754-10761.	1.2	48
51	The effects of electronic polarization on water adsorption in metal-organic frameworks: H ₂ O in MIL-53(Cr). <i>Journal of Chemical Physics</i> , 2012, 137, 054704.	1.2	45
52	Many-Body Effects Determine the Local Hydration Structure of Cs ⁺ in Solution. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 406-412.	2.1	45
53	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. <i>Nature Communications</i> , 2021, 12, 6359.	5.8	45
54	Ultrafast direct electron transfer at organic semiconductor and metal interfaces. <i>Science Advances</i> , 2017, 3, e1701508.	4.7	44

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55	Data-Driven Many-Body Models for Molecular Fluids: CO ₂ /H ₂ O Mixtures as a Case Study. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2246-2257.	2.3	44
56	Water Dynamics in Metal-Organic Frameworks: Effects of Heterogeneous Confinement Predicted by Computational Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2897-2902.	2.1	43
57	The i-TTM model for ab initio-based ion-water interaction potentials. II. Alkali metal ion-water potential energy functions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30334-30343.	1.3	43
58	Molecular Mechanisms of Water-Mediated Proton Transport in MIL-53 Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2013, 117, 19508-19516.	1.5	42
59	Sodium-carboxylate contact ion pair formation induces stabilization of palmitic acid monolayers at high pH. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10481-10490.	1.3	42
60	The curious case of the water hexamer: Cage vs. Prism. <i>Chemical Physics Letters</i> , 2013, 580, 1-8.	1.2	41
61	Molecular Mechanisms of Spin Crossover in the {Fe(pz)[Pt(CN) ₄]} Metal-Organic Framework upon Water Adsorption. <i>Journal of the American Chemical Society</i> , 2016, 138, 6123-6126.	6.6	41
62	Computational Exploration of the Water Concentration Dependence of the Proton Transport in the Porous UiO-66(Zr)(CO ₂ /H ₂) Metal-Organic Framework. <i>Chemistry of Materials</i> , 2017, 29, 1569-1576.	3.2	40
63	Vibrational spectra of halide-water dimers: Insights on ion hydration from full-dimensional quantum calculations on many-body potential energy surfaces. <i>Journal of Chemical Physics</i> , 2018, 148, 102321.	1.2	40
64	How good are polarizable and flexible models for water: Insights from a many-body perspective. <i>Journal of Chemical Physics</i> , 2020, 153, 060901.	1.2	39
65	Theoretical Modeling of Spin Crossover in Metal-Organic Frameworks: [Fe(pz) ₂ Pt(CN) ₄] as a Case Study. <i>Inorganic Chemistry</i> , 2014, 53, 11020-11028.	1.9	38
66	Assessing Many-Body Effects of Water Self-Ions. I: OH ⁺ (H ₂ O) _n Clusters. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1982-1997.	2.3	38
67	Thermodynamics of Water Dimer Dissociation in the Primary Hydration Shell of the Iodide Ion with Temperature-Dependent Vibrational Predissociation Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1859-1866.	1.1	37
68	Proton Transport in a Highly Conductive Porous Zirconium-Based Metal-Organic Framework: Molecular Insight. <i>Angewandte Chemie</i> , 2016, 128, 3987-3992.	1.6	37
69	Molecular-Level Interpretation of Vibrational Spectra of Ordered Ice Phases. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10572-10581.	1.2	36
70	Exploring Electrostatic Effects on the Hydrogen Bond Network of Liquid Water through Many-Body Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8539-8546.	1.2	35
71	Electron-Hole Theory of the Effect of Quantum Nuclei on the X-Ray Absorption Spectra of Liquid Water. <i>Physical Review Letters</i> , 2018, 121, 137401.	2.9	35
72	Low-order many-body interactions determine the local structure of liquid water. <i>Chemical Science</i> , 2019, 10, 8211-8218.	3.7	35

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73	Halide Ion Microhydration: Structure, Energetics, and Spectroscopy of Small Halide–Water Clusters. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2843-2852.	1.1	35
74	On the interplay of the potential energy and dipole moment surfaces in controlling the infrared activity of liquid water. <i>Journal of Chemical Physics</i> , 2015, 142, 212411.	1.2	33
75	Chemical accuracy in modeling halide ion hydration from many-body representations. <i>Advances in Physics: X</i> , 2019, 4, 1631212.	1.5	32
76	Vapor–liquid equilibrium of water with the MB-pol many-body potential. <i>Journal of Chemical Physics</i> , 2021, 154, 211103.	1.2	32
77	Many-Body Convergence of the Electrostatic Properties of Water. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4844-4852.	2.3	29
78	Water in metal-organic frameworks: structure and diffusion of H ₂ O in MIL-53(Cr) from quantum simulations. <i>Molecular Simulation</i> , 2012, 38, 631-641.	0.9	28
79	General Many-Body Framework for Data-Driven Potentials with Arbitrary Quantum Mechanical Accuracy: Water as a Case Study. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5635-5650.	2.3	28
80	Data-Driven Many-Body Models with Chemical Accuracy for CH ₄ /H ₂ O Mixtures. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11207-11221.	1.2	28
81	Water Capture Mechanisms at Zeolitic Imidazolate Framework Interfaces. <i>Journal of the American Chemical Society</i> , 2021, 143, 21189-21194.	6.6	28
82	Effects of Surface Pressure on the Properties of Langmuir Monolayers and Interfacial Water at the Air–Water Interface. <i>Langmuir</i> , 2015, 31, 2147-2156.	1.6	27
83	Isomeric Equilibria, Nuclear Quantum Effects, and Vibrational Spectra of M ⁺ (H ₂ O) _n Clusters, with M = Li, Na, K, Rb, and Cs, through Many-Body Representations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5811-5821.	1.1	27
84	Spin Crossover in the {Fe(pz)[Pt(CN) ₄]} Metal–Organic Framework upon Pyrazine Adsorption. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4022-4026.	2.1	26
85	Specific Ion Effects on Hydrogen-Bond Rearrangements in the Halide–Dihydrate Complexes. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2823-2828.	2.1	26
86	Nature of Halide–Water Interactions: Insights from Many-Body Representations and Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2983-2995.	2.3	26
87	Temperature-Dependent Infrared Spectroscopy of Water from a First-Principles Approach. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6861-6871.	1.1	25
88	Neat Water–Vapor Interface: Proton Continuum and the Nonresonant Background. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6744-6749.	2.1	25
89	Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3652-3658.	2.1	25
90	Guest-Dependent Stabilization of the Low-Spin State in Spin-Crossover Metal-Organic Frameworks. <i>Inorganic Chemistry</i> , 2018, 57, 9839-9843.	1.9	23

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91	Unraveling the effect of defects, domain size, and chemical doping on photophysics and charge transport in covalent organic frameworks. <i>Chemical Science</i> , 2021, 12, 8373-8384.	3.7	23
92	Solvation-Guided Design of Fluorescent Probes for Discrimination of Amyloids. <i>Scientific Reports</i> , 2018, 8, 6950.	1.6	21
93	Relationship between Hydrogen-Bonding Motifs and the $1b_{1g}$ Splitting in the X-ray Emission Spectrum of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3996-4002.	2.1	21
94	Data-driven many-body models enable a quantitative description of chloride hydration from clusters to bulk. <i>Journal of Chemical Physics</i> , 2021, 155, 064502.	1.2	21
95	Assessing Many-Body Effects of Water Self-Ions. II: $H_3O^+(H_2O)_n$ Clusters. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4816-4833.	2.3	20
96	How Good Is the Density-Corrected SCAN Functional for Neutral and Ionic Aqueous Systems, and What Is So Right about the Hartree-Fock Density?. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4745-4761.	2.3	20
97	Assessment of Density Functional Theory in Predicting Interaction Energies between Water and Polycyclic Aromatic Hydrocarbons: from Water on Benzene to Water on Graphene. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2359-2374.	2.3	18
98	Computer simulations explain mutation-induced effects on the DNA editing by adenine base editors. <i>Science Advances</i> , 2020, 6, eaaz2309.	4.7	18
99	Active learning of many-body configuration space: Application to the Cs^+ -water MB-nrg potential energy function as a case study. <i>Journal of Chemical Physics</i> , 2020, 152, 144103.	1.2	18
100	MB-Fit: Software infrastructure for data-driven many-body potential energy functions. <i>Journal of Chemical Physics</i> , 2021, 155, 124801.	1.2	18
101	Near- and long-term quantum algorithmic approaches for vibrational spectroscopy. <i>Physical Review A</i> , 2021, 104, .	1.0	17
102	Hydrogen bond dynamics in heavy water studied with quantum dynamical simulations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19865.	1.3	16
103	Nature of Alkali Ion-Water Interactions: Insights from Many-Body Representations and Density Functional Theory. II. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3055-3072.	2.3	16
104	Simulation Meets Experiment: Unraveling the Properties of Water in Metal-Organic Frameworks through Vibrational Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12451-12460.	1.5	16
105	Static and Dynamic Correlations in Water: Comparison of Classical Ab Initio Molecular Dynamics at Elevated Temperature with Path Integral Simulations at Ambient Temperature. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2124-2131.	2.3	16
106	Nonlinear quantum time correlation functions from centroid molecular dynamics and the maximum entropy method. <i>Journal of Chemical Physics</i> , 2008, 129, 194113.	1.2	15
107	Infrared signatures of isomer selectivity and symmetry breaking in the $Cs+(H_2O)_3$ complex using many-body potential energy functions. <i>Journal of Chemical Physics</i> , 2020, 153, 044306.	1.2	15
108	Assessing the Interplay between Functional-Driven and Density-Driven Errors in DFT Models of Water. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3410-3426.	2.3	14

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109	Highly Accurate Many-Body Potentials for Simulations of N_2O_5 in Water: Benchmarks, Development, and Validation. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3931-3945.	2.3	13
110	Assessing the Accuracy of the SCAN Functional for Water through a Many-Body Analysis of the Adiabatic Connection Formula. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3739-3749.	2.3	13
111	The effects of framework dynamics on the behavior of water adsorbed in the [Zn(I-L)(Cl)] and Co-MOF-74 metal-organic frameworks. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8196-8204.	1.3	12
112	Transferability of data-driven, many-body models for CO ₂ simulations in the vapor and liquid phases. <i>Journal of Chemical Physics</i> , 2022, 156, 104503.	1.2	12
113	Water Structure and Dynamics in Homochiral [Zn(I-L)(X)] Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18239-18247.	1.5	11
114	A Many-Body, Fully Polarizable Approach to QM/MM Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7462-7472.	2.3	11
115	Water is not a dynamic polydisperse branched polymer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 13169-13170.	3.3	10
116	Water: Many-Body Potential from First Principles (From the Gas to the Liquid Phase). , 2020, , 635-660.		10
117	A Ligand Field Molecular Mechanics Study of CO ₂ -Induced Breathing in the Metal-Organic Framework DUT-8(Ni). <i>Advanced Theory and Simulations</i> , 2019, 2, 1900098.	1.3	9
118	Rovibrational Spectra for the HCCCN-HCN and HCN-HCCCN Binary Complexes in 4He Droplets. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7516-7528.	1.1	8
119	Water structure at the interface of alcohol monolayers as determined by molecular dynamics simulations and computational vibrational sum-frequency generation spectroscopy. <i>Journal of Chemical Physics</i> , 2019, 150, 034701.	1.2	8
120	Modeling Spontaneous Charge Transfer at Metal/Organic Hybrid Heterostructures. <i>Journal of Physical Chemistry C</i> , 2020, 124, 4802-4809.	1.5	8
121	Density functional theory of water with the machine-learned DM21 functional. <i>Journal of Chemical Physics</i> , 2022, 156, 161103.	1.2	8
122	Phase diagram of the TIP4P/Ice water model by enhanced sampling simulations. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	8
123	Topology-Mediated Enhanced Polaron Coherence in Covalent Organic Frameworks. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9442-9448.	2.1	7
124	The behavior of methane-water mixtures under elevated pressures from simulations using many-body potentials. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	7
125	Combined Theoretical, Bioinformatic, and Biochemical Analyses of RNA Editing by Adenine Base Editors. <i>CRISPR Journal</i> , 2022, 5, 294-310.	1.4	4
126	Analytical STEM Investigation of the Post-Synthetic Modification (PMS) of Metal-Organic Frameworks (MOFs): Metal- and Ligand-Exchange in UiO-66. <i>Microscopy and Microanalysis</i> , 2018, 24, 1970-1971.	0.2	3

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127	Water: Many-Body Potential from First Principles (From the Gas to the Liquid Phase). , 2018, , 1-25.		2
128	Gas Absorption and Pore Breathing of Metal-Organic Frameworks Studied Using in situ Environmental Transmission Electron Microscopy (ETEM). Microscopy and Microanalysis, 2018, 24, 1880-1881.	0.2	1
129	Sun <i>etÂal.</i> Reply.. Physical Review Letters, 2019, 123, 099602.	2.9	1