Francesco Paesani

List of Publications by Year
in descending order

129	7,644	46918 47	58464 82
papers	citations	h-index	g-index

192	192	192	5837
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Static and Dynamic Correlations in Water: Comparison of Classical Ab Initio Molecular Dynamics at Elevated Temperature with Path Integral Simulations at Ambient Temperature. Journal of Chemical Theory and Computation, 2022, 18, 2124-2131.	2.3	16
2	Combined Theoretical, Bioinformatic, and Biochemical Analyses of RNA Editing by Adenine Base Editors. CRISPR Journal, 2022, 5, 294-310.	1.4	4
3	Transferability of data-driven, many-body models for CO2 simulations in the vapor and liquid phases. Journal of Chemical Physics, 2022, 156, 104503.	1.2	12
4	Density functional theory of water with the machine-learned DM21 functional. Journal of Chemical Physics, 2022, 156, 161103.	1.2	8
5	Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model. Journal of Physical Chemistry Letters, 2022, 13, 3652-3658.	2.1	25
6	Assessing the Interplay between Functional-Driven and Density-Driven Errors in DFT Models of Water. Journal of Chemical Theory and Computation, 2022, 18, 3410-3426.	2.3	14
7	The behavior of methaneâ€“water mixtures under elevated pressures from simulations using many-body potentials. Journal of Chemical Physics, 2022, 156, .	1.2	7
8	Phase diagram of the TIP4P/Ice water model by enhanced sampling simulations. Journal of Chemical Physics, 2022, 157, .	1.2	8
9	How Good Is the Density-Corrected SCAN Functional for Neutral and Ionic Aqueous Systems, and What Is So Right about the Hartreeâ€“Fock Density?. Journal of Chemical Theory and Computation, 2022, 18, 4745-4761.	2.3	20
10	Relationship between Hydrogen-Bonding Motifs and the 1b₁ Splitting in the X-ray Emission Spectrum of Liquid Water. Journal of Physical Chemistry Letters, 2021, 12, 3996-4002.	2.1	21
11	Highly Accurate Many-Body Potentials for Simulations of N₂O₅ in Water: Benchmarks, Development, and Validation. Journal of Chemical Theory and Computation, 2021, 17, 3931-3945.	2.3	13
12	Simulation Meets Experiment: Unraveling the Properties of Water in Metalâ€“Organic Frameworks through Vibrational Spectroscopy. Journal of Physical Chemistry C, 2021, 125, 12451-12460.	1.5	16
13	Assessing the Accuracy of the SCAN Functional for Water through a Many-Body Analysis of the Adiabatic Connection Formula. Journal of Chemical Theory and Computation, 2021, 17, 3739-3749.	2.3	13
14	Vaporâ€“liquid equilibrium of water with the MB-pol many-body potential. Journal of Chemical Physics, 2021, 154, 211103.	1.2	32
15	Data-driven many-body models enable a quantitative description of chloride hydration from clusters to bulk. Journal of Chemical Physics, 2021, 155, 064502.	1.2	21
16	General Many-Body Framework for Data-Driven Potentials with Arbitrary Quantum Mechanical Accuracy: Water as a Case Study. Journal of Chemical Theory and Computation, 2021, 17, 5635-5650.	2.3	28
17	MB-Fit: Software infrastructure for data-driven many-body potential energy functions. Journal of Chemical Physics, 2021, 155, 124801.	1.2	18
18	Topology-Mediated Enhanced Polaron Coherence in Covalent Organic Frameworks. Journal of Physical Chemistry Letters, 2021, 12, 9442-9448.	2.1	7

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19	Unraveling the effect of defects, domain size, and chemical doping on photophysics and charge transport in covalent organic frameworks. Chemical Science, 2021, 12, 8373-8384.	3.7	23
20	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. Nature Communications, 2021, 12, 6359.	5.8	45
21	Water Capture Mechanisms at Zeolitic Imidazolate Framework Interfaces. Journal of the American Chemical Society, 2021, 143, 21189-21194.	6.6	28
22	Near- and long-term quantum algorithmic approaches for vibrational spectroscopy. Physical Review A, 2021, 104, .	1.0	17
23	Modeling Spontaneous Charge Transfer at Metal/Organic Hybrid Heterostructures. Journal of Physical Chemistry C, 2020, 124, 4802-4809.	1.5	8
24	A Many-Body, Fully Polarizable Approach to QM/MM Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7462-7472.	2.3	11
25	Infrared signatures of isomer selectivity and symmetry breaking in the Cs+(H2O)3 complex using many-body potential energy functions. Journal of Chemical Physics, 2020, 153, 044306.	1.2	15
26	How good are polarizable and flexible models for water: Insights from a many-body perspective. Journal of Chemical Physics, 2020, 153, 060901.	1.2	39
27	Data-Driven Many-Body Models for Molecular Fluids: CO₂/H₂O Mixtures as a Case Study. Journal of Chemical Theory and Computation, 2020, 16, 2246-2257.	2.3	44
28	Computer simulations explain mutation-induced effects on the DNA editing by adenine base editors. Science Advances, 2020, 6, eaaz2309.	4.7	18
29	Nature of Alkali Ionâ€“Water Interactions: Insights from Many-Body Representations and Density Functional Theory. II. Journal of Chemical Theory and Computation, 2020, 16, 3055-3072.	2.3	16
30	Active learning of many-body configuration space: Application to the Cs+â€“water MB-nrg potential energy function as a case study. Journal of Chemical Physics, 2020, 152, 144103.	1.2	18
31	Water: Many-Body Potential from First Principles (From the Gas to the Liquid Phase). , 2020, , 635-660.		10
32	Data-Driven Many-Body Models with Chemical Accuracy for CH₄/H₂O Mixtures. Journal of Physical Chemistry B, 2020, 124, 11207-11221.	1.2	28
33	A Ligand Field Molecular Mechanics Study of CO 2 â€Induced Breathing in the Metalâ€“Organic Framework DUTâ€8(Ni). Advanced Theory and Simulations, 2019, 2, 1900098.	1.3	9
34	Assessing Many-Body Effects of Water Self-Ions. II: H₃O⁺(H₂O)_n Clusters. Journal of Chemical Theory and Computation, 2019, 15, 4816-4833.	2.3	20
35	Low-order many-body interactions determine the local structure of liquid water. Chemical Science, 2019, 10, 8211-8218.	3.7	35
36	Chemical accuracy in modeling halide ion hydration from many-body representations. Advances in Physics: X, 2019, 4, 1631212.	1.5	32

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37	Water is not a dynamic polydisperse branched polymer. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 13169-13170.	3.3	10
38	Hydrogen bonding structure of confined water templated by a metal-organic framework with open metal sites. Nature Communications, 2019, 10, 4771.	5.8	86
39	The end of ice I. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 24413-24419.	3.3	50
40	Sun etÂal. Reply:. Physical Review Letters, 2019, 123, 099602.	2.9	1
41	Water structure at the interface of alcohol monolayers as determined by molecular dynamics simulations and computational vibrational sum-frequency generation spectroscopy. Journal of Chemical Physics, 2019, 150, 034701.	1.2	8
42	Specific Ion Effects on Hydrogen-Bond Rearrangements in the Halideâ€“Dihydrate Complexes. Journal of Physical Chemistry Letters, 2019, 10, 2823-2828.	2.1	26
43	Ion-mediated hydrogen-bond rearrangement through tunnelling in the iodideâ€“dihydrate complex. Nature Chemistry, 2019, 11, 367-374.	6.6	55
44	Nature of Halideâ€“Water Interactions: Insights from Many-Body Representations and Density Functional Theory. Journal of Chemical Theory and Computation, 2019, 15, 2983-2995.	2.3	26
45	Assessment of Density Functional Theory in Predicting Interaction Energies between Water and Polycyclic Aromatic Hydrocarbons: from Water on Benzene to Water on Graphene. Journal of Chemical Theory and Computation, 2019, 15, 2359-2374.	2.3	18
46	Halide Ion Microhydration: Structure, Energetics, and Spectroscopy of Small Halideâ€“Water Clusters. Journal of Physical Chemistry A, 2019, 123, 2843-2852.	1.1	35
47	Halogen bonding in UiO-66 frameworks promotes superior chemical warfare agent simulant degradation. Chemical Communications, 2019, 55, 3481-3484.	2.2	68
48	Many-Body Effects Determine the Local Hydration Structure of Cs⁺ in Solution. Journal of Physical Chemistry Letters, 2019, 10, 406-412.	2.1	45
49	Vibrational spectra of halide-water dimers: Insights on ion hydration from full-dimensional quantum calculations on many-body potential energy surfaces. Journal of Chemical Physics, 2018, 148, 102321.	1.2	40
50	Second-Order Vibrational Lineshapes from the Air/Water Interface. Journal of Physical Chemistry A, 2018, 122, 4457-4464.	1.1	63
51	Temperature Dependence of the Air/Water Interface Revealed by Polarization Sensitive Sum-Frequency Generation Spectroscopy. Journal of Physical Chemistry B, 2018, 122, 4356-4365.	1.2	59
52	Comparison of permutationally invariant polynomials, neural networks, and Gaussian approximation potentials in representing water interactions through many-body expansions. Journal of Chemical Physics, 2018, 148, 241725.	1.2	142
53	Electron affinity of liquid water. Nature Communications, 2018, 9, 247.	5.8	114
54	Transmission Electron Microscopy Reveals Deposition of Metal Oxide Coatings onto Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2018, 140, 1348-1357.	6.6	51

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55	Engineering the entropy-driven free-energy landscape of a dynamic nanoporous protein assembly. Nature Chemistry, 2018, 10, 732-739.	6.6	51
56	Assessing Many-Body Effects of Water Self-Ions. I: OH^{â€“}(H₂O)_n Clusters. Journal of Chemical Theory and Computation, 2018, 14, 1982-1997.	2.3	38
57	Ice-Nucleating and Antifreeze Proteins Recognize Ice through a Diversity of Anchored Clathrate and Ice-like Motifs. Journal of the American Chemical Society, 2018, 140, 4905-4912.	6.6	117
58	Neat Waterâ€“Vapor Interface: Proton Continuum and the Nonresonant Background. Journal of Physical Chemistry Letters, 2018, 9, 6744-6749.	2.1	25
59	Disentangling Coupling Effects in the Infrared Spectra of Liquid Water. Journal of Physical Chemistry B, 2018, 122, 10754-10761.	1.2	48
60	Orientational Distribution of Free O-H Groups of Interfacial Water is Exponential. Physical Review Letters, 2018, 121, 246101.	2.9	49
61	Electron-Hole Theory of the Effect of Quantum Nuclei on the X-Ray Absorption Spectra of Liquid Water. Physical Review Letters, 2018, 121, 137401.	2.9	35
62	Molecular-Level Interpretation of Vibrational Spectra of Ordered Ice Phases. Journal of Physical Chemistry B, 2018, 122, 10572-10581.	1.2	36
63	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
64	Water: Many-Body Potential from First Principles (From the Gas to the Liquid Phase). , 2018, , 1-25.		2
65	Isomeric Equilibria, Nuclear Quantum Effects, and Vibrational Spectra of M⁺(H₂O)_{n=1â€“3} Clusters, with M = Li, Na, K, Rb, and Cs, through Many-Body Representations. Journal of Physical Chemistry A, 2018, 122, 5811-5821.	1.1	27
66	Guest-Dependent Stabilization of the Low-Spin State in Spin-Crossover Metal-Organic Frameworks. Inorganic Chemistry, 2018, 57, 9839-9843.	1.9	23
67	Preordering of water is not needed for ice recognition by hyperactive antifreeze proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 8266-8271.	3.3	89
68	Solvation-Guided Design of Fluorescent Probes for Discrimination of Amyloids. Scientific Reports, 2018, 8, 6950.	1.6	21
69	Analytical STEM Investigation of the Post-Synthetic Modification (PMS) of Metal-Organic Frameworks (MOFs): Metal- and Ligand-Exchange in UiO-66. Microscopy and Microanalysis, 2018, 24, 1970-1971.	0.2	3
70	Bulk Contributions Modulate the Sum-Frequency Generation Spectra of Water on Model Sea-Spray Aerosols. CheM, 2018, 4, 1629-1644.	5.8	69
71	Ice Nucleation Efficiency of Hydroxylated Organic Surfaces Is Controlled by Their Structural Fluctuations and Mismatch to Ice. Journal of the American Chemical Society, 2017, 139, 3052-3064.	6.6	132
72	Computational Exploration of the Water Concentration Dependence of the Proton Transport in the Porous UiOâ€“66(Zr)â€“(CO₂H)₂ Metalâ€“Organic Framework. Chemistry of Materials, 2017, 29, 1569-1576.	3.2	40

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73	Many-Body Interactions in Ice. Journal of Chemical Theory and Computation, 2017, 13, 1778-1784.	2.3	60
74	Sodiumâ€“carboxylate contact ion pair formation induces stabilization of palmitic acid monolayers at high pH. Physical Chemistry Chemical Physics, 2017, 19, 10481-10490.	1.3	42
75	Monitoring Water Clusters â€œMeltâ€•Through Vibrational Spectroscopy. Journal of the American Chemical Society, 2017, 139, 7082-7088.	6.6	69
76	Molecular Origin of the Vibrational Structure of Ice I_h. Journal of Physical Chemistry Letters, 2017, 8, 2579-2583.	2.1	66
77	Pore Breathing of Metalâ€“Organic Frameworks by Environmental Transmission Electron Microscopy. Journal of the American Chemical Society, 2017, 139, 13973-13976.	6.6	56
78	Toward chemical accuracy in the description of ionâ€“water interactions through many-body representations. Alkali-water dimer potential energy surfaces. Journal of Chemical Physics, 2017, 147, 161715.	1.2	57
79	Ultrafast direct electron transfer at organic semiconductor and metal interfaces. Science Advances, 2017, 3, e1701508.	4.7	44
80	Temperature-dependent vibrational spectra and structure of liquid water from classical and quantum simulations with the MB-pol potential energy function. Journal of Chemical Physics, 2017, 147, 244504.	1.2	87
81	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. Journal of Chemical Physics, 2016, 145, 194504.	1.2	214
82	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. Chemical Reviews, 2016, 116, 7501-7528.	23.0	314
83	Exploring Electrostatic Effects on the Hydrogen Bond Network of Liquid Water through Many-Body Molecular Dynamics. Journal of Physical Chemistry B, 2016, 120, 8539-8546.	1.2	35
84	Toward Chemical Accuracy in the Description of Ionâ€“Water Interactions through Many-Body Representations. I. Halideâ€“Water Dimer Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2016, 12, 2698-2705.	2.3	81
85	Molecular Mechanisms of Spin Crossover in the {Fe(pz)[Pt(CN)₄]} Metalâ€“Organic Framework upon Water Adsorption. Journal of the American Chemical Society, 2016, 138, 6123-6126.	6.6	41
86	Spin Crossover in the {Fe(pz)[Pt(CN)₄]} Metalâ€“Organic Framework upon Pyrazine Adsorption. Journal of Physical Chemistry Letters, 2016, 7, 4022-4026.	2.1	26
87	Getting the Right Answers for the Right Reasons: Toward Predictive Molecular Simulations of Water with Many-Body Potential Energy Functions. Accounts of Chemical Research, 2016, 49, 1844-1851.	7.6	121
88	The i-TTM model for ab initio-based ionâ€“water interaction potentials. II. Alkali metal ionâ€“water potential energy functions. Physical Chemistry Chemical Physics, 2016, 18, 30334-30343.	1.3	43
89	Proton Transport in a Highly Conductive Porous Zirconiumâ€Based Metalâ€“Organic Framework: Molecular Insight. Angewandte Chemie, 2016, 128, 3987-3992.	1.6	37
90	Proton Transport in a Highly Conductive Porous Zirconiumâ€Based Metalâ€“Organic Framework: Molecular Insight. Angewandte Chemie - International Edition, 2016, 55, 3919-3924.	7.2	152

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91	i-TTM Model for Ab Initio-Based Ionâ€“Water Interaction Potentials. 1. Halideâ€“Water Potential Energy Functions. Journal of Physical Chemistry B, 2016, 120, 1822-1832.	1.2	61
92	The effects of framework dynamics on the behavior of water adsorbed in the [Zn(l-L)(Cl)] and Co-MOF-74 metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2016, 18, 8196-8204.	1.3	12
93	Dissecting the Molecular Structure of the Air/Water Interface from Quantum Simulations of the Sum-Frequency Generation Spectrum. Journal of the American Chemical Society, 2016, 138, 3912-3919.	6.6	153
94	Infrared and Raman Spectroscopy of Liquid Water through â€œFirst-Principlesâ€•Many-Body Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 1145-1154.	2.3	182
95	Thermodynamics of Water Dimer Dissociation in the Primary Hydration Shell of the Iodide Ion with Temperature-Dependent Vibrational Predissociation Spectroscopy. Journal of Physical Chemistry A, 2015, 119, 1859-1866.	1.1	37
96	Effects of Surface Pressure on the Properties of Langmuir Monolayers and Interfacial Water at the Airâ€“Water Interface. Langmuir, 2015, 31, 2147-2156.	1.6	27
97	MIL-101(Fe) as a lithium-ion battery electrode material: a relaxation and intercalation mechanism during lithium insertion. Journal of Materials Chemistry A, 2015, 3, 4738-4744.	5.2	168
98	Water Structure and Dynamics in Homochiral [Zn(l-L)(X)] Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 18239-18247.	1.5	11
99	On the interplay of the potential energy and dipole moment surfaces in controlling the infrared activity of liquid water. Journal of Chemical Physics, 2015, 142, 212411.	1.2	33
100	On the representation of many-body interactions in water. Journal of Chemical Physics, 2015, 143, 104102.	1.2	80
101	Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase. Journal of Chemical Physics, 2014, 141, 181101.	1.2	74
102	Water Dynamics in Metalâ€“Organic Frameworks: Effects of Heterogeneous Confinement Predicted by Computational Spectroscopy. Journal of Physical Chemistry Letters, 2014, 5, 2897-2902.	2.1	43
103	Theoretical Modeling of Spin Crossover in Metalâ€“Organic Frameworks: [Fe(pz)₂Pt(CN)₄] as a Case Study. Inorganic Chemistry, 2014, 53, 11020-11028.	1.9	38
104	Development of a â€œFirst Principlesâ€•Water Potential with Flexible Monomers. II: Trimer Potential Energy Surface, Third Virial Coefficient, and Small Clusters. Journal of Chemical Theory and Computation, 2014, 10, 1599-1607.	2.3	313
105	Development of a â€œFirst-Principlesâ€•Water Potential with Flexible Monomers. III. Liquid Phase Properties. Journal of Chemical Theory and Computation, 2014, 10, 2906-2910.	2.3	292
106	Molecular Mechanisms of Water-Mediated Proton Transport in MIL-53 Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 19508-19516.	1.5	42
107	The curious case of the water hexamer: Cage vs. Prism. Chemical Physics Letters, 2013, 580, 1-8.	1.2	41
108	Many-Body Convergence of the Electrostatic Properties of Water. Journal of Chemical Theory and Computation, 2013, 9, 4844-4852.	2.3	29

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109	A Critical Assessment of Two-Body and Three-Body Interactions in Water. Journal of Chemical Theory and Computation, 2013, 9, 1103-1114.	2.3	126
110	Development of a â€œFirst Principlesâ€•Water Potential with Flexible Monomers: Dimer Potential Energy Surface, VRT Spectrum, and Second Virial Coefficient. Journal of Chemical Theory and Computation, 2013, 9, 5395-5403.	2.3	398
111	Negative Ion Photoelectron Spectroscopy Reveals Thermodynamic Advantage of Organic Acids in Facilitating Formation of Bisulfate Ion Clusters: Atmospheric Implications. Journal of Physical Chemistry Letters, 2013, 4, 779-785.	2.1	53
112	Toward a Universal Water Model: First Principles Simulations from the Dimer to the Liquid Phase. Journal of Physical Chemistry Letters, 2012, 3, 3765-3769.	2.1	137
113	A Refined MS-EVB Model for Proton Transport in Aqueous Environments. Journal of Physical Chemistry B, 2012, 116, 343-352.	1.2	79
114	Application of Adaptive QM/MM Methods to Molecular Dynamics Simulations of Aqueous Systems. Journal of Chemical Theory and Computation, 2012, 8, 2868-2877.	2.3	54
115	Water in metal-organic frameworks: structure and diffusion of H₂O in MIL-53(Cr) from quantum simulations. Molecular Simulation, 2012, 38, 631-641.	0.9	28
116	The effects of electronic polarization on water adsorption in metal-organic frameworks: H2O in MIL-53(Cr). Journal of Chemical Physics, 2012, 137, 054704.	1.2	45
117	The Water Hexamer: Cage, Prism, or Both. Full Dimensional Quantum Simulations Say Both. Journal of the American Chemical Society, 2012, 134, 11116-11119.	6.6	132
118	Molecular-Level Characterization of the Breathing Behavior of the Jungle-Gym-type DMOF-1 Metalâ€“Organic Framework. Journal of the American Chemical Society, 2012, 134, 4207-4215.	6.6	87
119	Hydrogen bond dynamics in heavy water studied with quantum dynamical simulations. Physical Chemistry Chemical Physics, 2011, 13, 19865.	1.3	16
120	Temperature-Dependent Infrared Spectroscopy of Water from a First-Principles Approach. Journal of Physical Chemistry A, 2011, 115, 6861-6871.	1.1	25
121	A quantitative assessment of the accuracy of centroid molecular dynamics for the calculation of the infrared spectrum of liquid water. Journal of Chemical Physics, 2010, 132, 014105.	1.2	63
122	Nuclear Quantum Effects in the Reorientation of Water. Journal of Physical Chemistry Letters, 2010, 1, 2316-2321.	2.1	62
123	Infrared Spectroscopy and Hydrogen-Bond Dynamics of Liquid Water from Centroid Molecular Dynamics with an Ab Initio-Based Force Field. Journal of Physical Chemistry B, 2009, 113, 13118-13130.	1.2	123
124	The Properties of Water: Insights from Quantum Simulations. Journal of Physical Chemistry B, 2009, 113, 5702-5719.	1.2	199
125	Nonlinear quantum time correlation functions from centroid molecular dynamics and the maximum entropy method. Journal of Chemical Physics, 2008, 129, 194113.	1.2	15
126	Quantum effects in liquid water from an ab initio-based polarizable force field. Journal of Chemical Physics, 2007, 127, 074506.	1.2	151

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127	Rovibrational Spectra for the HCCCNÂ·HCN and HCNÂ·HCCCN Binary Complexes in4He Dropletsâ€. Journal of Physical Chemistry A, 2007, 111, 7516-7528.	1.1	8
128	Local superfluidity in inhomogeneous quantum fluids. Physical Review B, 2006, 74, .	1.1	50
129	An accurate and simple quantum model for liquid water. Journal of Chemical Physics, 2006, 125, 184507.	1.2	187