Sotiris S Xantheas

List of Publications by Year
in descending order

189	13,062	19608 61	24179 110
papers	citations	h-index	g-index

193	193	193	7135
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Gas phase protonated nicotine is a mixture of pyridine- and pyrrolidine-protonated conformers: implications for its native structure in the nicotinic acetylcholine receptor. Physical Chemistry Chemical Physics, 2022, 24, 5786-5793.	1.3	8
2	The Effect of Geometry, Spin, and Orbital Optimization in Achieving Accurate, Correlated Results for Ironâ€“Sulfur Cubanes. Journal of Chemical Theory and Computation, 2022, 18, 687-702.	2.3	10
3	Breaking covalent bonds in the context of the many-body expansion (MBE). I. The purported â€œfirst row anomalyâ€•in XHn (X = C, Si, Ge, Sn; n = 1â€“4). Journal of Chemical Physics, 2022, 156, .	1.2	4
4	The many-body expansion for aqueous systems revisited: III. Hofmeister ionâ€“water interactions. Physical Chemistry Chemical Physics, 2021, 23, 11196-11210.	1.3	16
5	The Many-Body Expansion for Aqueous Systems Revisited: II. Alkali Metal and Halide Ionâ€“Water Interactions. Journal of Chemical Theory and Computation, 2021, 17, 2200-2216.	2.3	22
6	Cryogenic Vibrationally Resolved Photoelectron Spectroscopy of OH^{â€“}(H₂O): Confirmation of Multidimensional Franckâ€“Condon Simulation Results for the Transition State of the OH + H₂O Reaction. Journal of Physical Chemistry A, 2021, 125, 2154-2162.	1.1	3
7	Guestâ€“Host Interactions in Clathrate Hydrates: Benchmark MP2 and CCSD(T)/CBS Binding Energies of CH₄, CO₂, and H₂S in (H₂O)₂₀Cages. Journal of Physical Chemistry Letters, 2021, 12, 7574-7582.	2.1	16
8	Quantitative Account of the Bonding Properties of a Rubredoxin Model Complex [Fe(SCH₃)₄]^q, q = â^’2, â^’1, +2, +3. Journal of Chemical Theory and Computation, 2021, 17, 6080-6091.	2.3	5
9	Co-design Center for Exascale Machine Learning Technologies (ExaLearn). International Journal of High Performance Computing Applications, 2021, 35, 598-616.	2.4	6
10	Massively parallel quantum chemical density matrix renormalization group method. Journal of Computational Chemistry, 2021, 42, 534-544.	1.5	34
11	Towards complete assignment of the infrared spectrum of the protonated water cluster H+(H2O)21. Nature Communications, 2021, 12, 6141.	5.8	35
12	Molecular Dynamics Driven by the Many-Body Expansion (MBE-MD). Journal of Chemical Theory and Computation, 2021, 17, 7341-7352.	2.3	10
13	Mapping the temperature-dependent and network site-specific onset of spectral diffusion at the surface of a water cluster cage. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26047-26052.	3.3	15
14	The Many-Body Expansion for Aqueous Systems Revisited: I. Waterâ€“Water Interactions. Journal of Chemical Theory and Computation, 2020, 16, 6843-6855.	2.3	31
15	A look inside the black box: Using graph-theoretical descriptors to interpret a Continuous-Filter Convolutional Neural Network (CF-CNN) trained on the global and local minimum energy structures of neutral water clusters. Journal of Chemical Physics, 2020, 153, 024302.	1.2	14
16	Isolating the Contributions of Specific Network Sites to the Diffuse Vibrational Spectrum of Interfacial Water with Isotopomer-Selective Spectroscopy of Cold Clusters. Journal of Physical Chemistry A, 2020, 124, 10393-10406.	1.1	16
17	Characterization of the alkali metal oxalates (MC₂O₄^{â^’}) and their formation by CO₂ reduction via the alkali metal carbonites (MCO₂^{â^’}). Physical Chemistry Chemical Physics, 2020, 22, 7460-7473.	1.3	11
18	Going large(r): general discussion. Faraday Discussions, 2019, 217, 476-513.	1.6	1

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19	Controlling internal degrees: general discussion. Faraday Discussions, 2019, 217, 138-171.	1.6	1
20	Pushing resolution in frequency and time: general discussion. Faraday Discussions, 2019, 217, 290-321.	1.6	1
21	Properties of perhalogenated {closo-B₁₀} and {closo-B₁₁} multiply charged anions and a critical comparison with {closo-B₁₂} in the gas and the condensed phase. Physical Chemistry Chemical Physics, 2019, 21, 5903-5915.	1.3	24
22	Probing the selectivity of Li⁺and Na⁺cations on noradrenaline at the molecular level. Faraday Discussions, 2019, 217, 396-413.	1.6	3
23	A benchmark photoelectron spectroscopic and theoretical study of the electronic stability of [B12H12]2â^'. Journal of Chemical Physics, 2019, 150, 164306.	1.2	29
24	Rational design of an argon-binding superelectrophilic anion. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 8167-8172.	3.3	69
25	Beyond Badgerâ€™s Rule: The Origins and Generality of the Structureâ€“Spectra Relationship of Aqueous Hydrogen Bonds. Journal of Physical Chemistry Letters, 2019, 10, 918-924.	2.1	52
26	Atlas of putative minima and low-lying energy networks of water clusters n = 3â€“25. Journal of Chemical Physics, 2019, 151, 214307.	1.2	41
27	Deviation from the trans-Effect in Ligand-Exchange Reactions of Zeiseâ€™s Ions PtCl₃(C₂H₄)^{â^'} with Heavier Halides (Br^{â€“},) Tj ETQq1 1 0.784314 rgB		
28	The water dimer II: Theoretical investigations. Chemical Physics Letters, 2018, 700, 163-175.	1.2	82
29	Communication: Water activation and splitting by single metal-atom anions. Journal of Chemical Physics, 2018, 149, 221101.	1.2	22
30	The activation of carbon dioxide by first row transition metals (Scâ€“Zn). Physical Chemistry Chemical Physics, 2018, 20, 25495-25505.	1.3	12
31	Benchmark Electronic Structure Calculations for H₃O⁺(H₂O)_n, n = 0â€“5, Clusters and Tests of an Existing 1,2,3-Body Potential Energy Surface with a New 4-Body Correction. Journal of Chemical Theory and Computation, 2018, 14, 4553-4566.	2.3	39
32	Structures, Energetics, and Spectroscopic Fingerprints of Water Clusters n = 2â€“24. , 2017, , 1139-1173.		6
33	Formation of Exotic Networks of Water Clusters in Helium Droplets Facilitated by the Presence of Neon Atoms. Journal of the American Chemical Society, 2017, 139, 4152-4156.	6.6	20
34	Molecular-Level Insight of the Effect of Hofmeister Anions on the Interfacial Surface Tension of a Model Protein. Journal of Physical Chemistry Letters, 2017, 8, 1574-1577.	2.1	11
35	Electronic Structure and Stability of [B₁₂X₁₂]^{2â€“} (X = Fâ€“At): A Combined Photoelectron Spectroscopic and Theoretical Study. Journal of the American Chemical Society, 2017, 139, 14749-14756.	6.6	60
36	Ortho-para interconversion in cation-water complexes: The case of V+(H2O) and Nb+(H2O) clusters. Journal of Chemical Physics, 2017, 146, 224305.	1.2	8

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37	A surprisingly simple correlation between the classical and quantum structural networks in liquid water. Journal of Chemical Physics, 2017, 147, 064506.	1.2	7
38	Spying on the neighbors' pool. Science, 2016, 354, 1101-1101.	6.0	7
39	Isotopomer-selective spectra of a single intact H2O molecule in the Cs+(D2O)5H2O isotopologue: Going beyond pattern recognition to harvest the structural information encoded in vibrational spectra. Journal of Chemical Physics, 2016, 144, 074305.	1.2	23
40	Modular polymer biosensors by solvent immersion imprint lithography. Journal of Polymer Science, Part B: Polymer Physics, 2016, 54, 98-103.	2.4	8
41	Mesoscale Polymer Dissolution Probed by Raman Spectroscopy and Molecular Simulations. Journal of Physical Chemistry B, 2016, 120, 10581-10587.	1.2	2
42	A New, Dispersion-Driven Intermolecular Arrangement for the Benzeneâ€“Water Octamer Complex: Isomers and Analysis of their Vibrational Spectra. Journal of Chemical Theory and Computation, 2016, 12, 4004-4014.	2.3	11
43	The Origin of the Reactivity of the Criegee Intermediate: Implications for Atmospheric Particle Growth. Angewandte Chemie, 2016, 128, 1027-1031.	1.6	14
44	Electronic origin of the dependence of hydrogen bond strengths on nearest-neighbor and next-nearest-neighbor hydrogen bonds in polyhedral water clusters (H₂O)_n, n = 8, 20 and 24. Physical Chemistry Chemical Physics, 2016, 18, 19746-19756.	1.3	8
45	The Origin of the Reactivity of the Criegee Intermediate: Implications for Atmospheric Particle Growth. Angewandte Chemie - International Edition, 2016, 55, 1015-1019.	7.2	36
46	Why Is MP2-Water â€œCoolerâ€•and â€œDenserâ€•than DFT-Water?. Journal of Physical Chemistry Letters, 2016, 7, 680-684.	2.1	47
47	On the validity of the basis set superposition error and complete basis set limit extrapolations for the binding energy of the formic acid dimer. Journal of Chemical Physics, 2015, 142, 094311.	1.2	40
48	Laser spectroscopic and theoretical studies of the structures and encapsulation motifs of functional molecules. , 2015, , .		0
49	Ultrafast Dynamics of Liquid Water: Energy Relaxation and Transfer Processes of the OH Stretch and the HOH Bend. Journal of Physical Chemistry B, 2015, 119, 11068-11078.	1.2	35
50	Snapshots of Proton Accommodation at a Microscopic Water Surface: Understanding the Vibrational Spectral Signatures of the Charge Defect in Cryogenically Cooled H⁺(H₂O)_{n=2â€“28} Clusters. Journal of Physical Chemistry A, 2015, 119, 9425-9440.	1.1	111
51	An accurate and efficient computational protocol for obtaining the complete basis set limits of the binding energies of water clusters at the MP2 and CCSD(T) levels of theory: Application to (H2O)m, m = 2-6, 8, 11, 16, and 17. Journal of Chemical Physics, 2015, 142, 234303.	1.2	54
52	Ground and Excited States of the [Fe(H₂O)₆]²⁺ and [Fe(H₂O)₆]³⁺ Clusters: Insight into the Electronic Structure of the [Fe(H₂O)₆]²⁺â€“[Fe(H₂O)₆]³⁺ Complex. Journal of Chemical Theory and Computation, 2015, 11, 1549-1563.	2.3	22
53	The Melting Temperature of Liquid Water with the Effective Fragment Potential. Journal of Physical Chemistry Letters, 2015, 6, 3555-3559.	2.1	10
54	A new variation of the Buckingham exponential-6 potential with a tunable, singularity-free short-range repulsion and an adjustable long-range attraction. Chemical Physics Letters, 2015, 619, 133-138.	1.2	9

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55	Structures, Energetics, and Spectroscopic Fingerprints of Water Clusters n = 2â€“24. , 2015, , 1-35.		0
56	Infrared detection of (H₂O)₂₀ isomers of exceptional stability: a drop-like and a face-sharing pentagonal prism cluster. Physical Chemistry Chemical Physics, 2014, 16, 26691-26696.	1.3	28
57	Low energy isomers of (H2O)25 from a hierarchical method based on Monte Carlo temperature basin paving and molecular tailoring approaches benchmarked by MP2 calculations. Journal of Chemical Physics, 2014, 141, 164304.	1.2	23
58	Universal scaling of potential energy functions describing intermolecular interactions. II. The halide-water and alkali metal-water interactions. Journal of Chemical Physics, 2014, 141, 064118.	1.2	19
59	Unimolecular and hydrolysis channels for the detachment of water from microsolvated alkaline earth dication (Mg2+, Ca2+, Sr2+, Ba2+) clusters. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	11
60	Elucidating the mechanism behind the stabilization of multi-charged metal cations in water: a case study of the electronic states of microhydrated Mg2+, Ca2+ and Al3+. Physical Chemistry Chemical Physics, 2014, 16, 6886.	1.3	16
61	Solvent immersion imprint lithography. Lab on A Chip, 2014, 14, 2072.	3.1	21
62	Universal scaling of potential energy functions describing intermolecular interactions. I. Foundations and scalable forms of new generalized Mie, Lennard-Jones, Morse, and Buckingham exponential-6 potentials. Journal of Chemical Physics, 2014, 141, 064117.	1.2	19
63	On the Bonding Nature of Ozone (O₃) and Its Sulfur-Substituted Analogues SO₂, OS₂, and S₃: Correlation between Their Biradical Character and Molecular Properties. Journal of the American Chemical Society, 2014, 136, 2808-2817.	6.6	66
64	Isomers and Conformational Barriers of Gas-Phase Nicotine, Nornicotine, and Their Protonated Forms. Journal of Physical Chemistry B, 2014, 118, 8273-8285.	1.2	12
65	Benchmark Theoretical Study of the Ï€â€“Ï€ Binding Energy in the Benzene Dimer. Journal of Physical Chemistry A, 2014, 118, 7568-7578.	1.1	77
66	Ultrafast dynamics of liquid water: Frequency fluctuations of the OH stretch and the HOH bend. Journal of Chemical Physics, 2013, 139, 044503.	1.2	30
67	Optimal geometries and harmonic vibrational frequencies of the global minima of water clusters (H2O)n, n = 2â€“6, and several hexamer local minima at the CCSD(T) level of theory. Journal of Chemical Physics, 2013, 139, 114302.	1.2	105
68	Molecular origin of the difference in the HOH bend of the IR spectra between liquid water and ice. Journal of Chemical Physics, 2013, 138, 054506.	1.2	43
69	Cooperative Roles of Charge Transfer and Dispersion Terms in Hydrogen-Bonded Networks of (H₂O)_n, n = 6, 11, and 16. Journal of Physical Chemistry A, 2013, 117, 6641-6651.	1.1	24
70	Unusual Inorganic Biradicals: A Theoretical Analysis. Angewandte Chemie - International Edition, 2013, 52, 5736-5739.	7.2	75
71	Microhydration Effects on the Intermediates of the S_N2 Reaction of Iodide Anion with Methyl Iodide. Angewandte Chemie - International Edition, 2013, 52, 4380-4383.	7.2	32
72	Efficient Procedure for the Numerical Calculation of Harmonic Vibrational Frequencies Based on Internal Coordinates. Journal of Physical Chemistry A, 2013, 117, 7019-7029.	1.1	9

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73	The Performance of Density Functionals for Sulfateâ€“Water Clusters. Journal of Chemical Theory and Computation, 2013, 9, 1368-1380.	2.3	69
74	Second-order many-body perturbation study of ice Ih. Journal of Chemical Physics, 2012, 137, 204505.	1.2	69
75	Vapor Phase Infrared Spectroscopy and Ab Initio Fundamental Anharmonic Frequencies of Ammonia Borane. Journal of Physical Chemistry A, 2012, 116, 3124-3136.	1.1	22
76	Refined energetic ordering for sulphateâ€“water (nâ€‰=â€‰3â€“6) clusters using high-level electronic structure calculations. Molecular Physics, 2012, 110, 2513-2521.	0.8	22
77	Titelbild: A Combined Gas-Phase Photoelectron Spectroscopic and Theoretical Study of Zeiseâ€™s Anion and Its Bromine and Iodine Analogues (Angew. Chem. 26/2012). Angewandte Chemie, 2012, 124, 6385-6385.	1.6	0
78	A Combined Gasâ€Phase Photoelectron Spectroscopic and Theoretical Study of Zeiseâ€™s Anion and Its Bromine and Iodine Analogues. Angewandte Chemie - International Edition, 2012, 51, 6356-6360.	7.2	11
79	Lowâ€lying energy isomers and global minima of aqueous nanoclusters: Structures and spectroscopic features of the pentagonal dodecahedron (H₂O)₂₀ and (H₃O)⁺(H₂O)₂₀. Canadian Journal of Chemical Engineering, 2012, 90, 843-851.	0.9	36
80	Structures, Energetics, and Spectroscopic Fingerprints of Water Clusters n = 2â€“24. , 2012, , 761-792.		14
81	Enhancement of hydrogen storage capacity in hydrate lattices. Chemical Physics Letters, 2012, 525-526, 13-18.	1.2	46
82	Laser Spectroscopic and Theoretical Studies of Encapsulation Complexes of Calix[4]arene. Journal of Physical Chemistry A, 2011, 115, 10846-10853.	1.1	20
83	Photodetachment of Isolated Bicarbonate Anion: Electron Binding Energy of HCO₃^{â€“}. Journal of Physical Chemistry Letters, 2011, 2, 1204-1210.	2.1	16
84	The Role of Hydrophobic Surfaces in Altering Water-Mediated Peptideâ^'Peptide Interactions in an Aqueous Environment. Journal of Physical Chemistry A, 2011, 115, 6088-6092.	1.1	0
85	Dynamics of Weak, Bifurcated, and Strong Hydrogen Bonds in Lithium Nitrate Trihydrate. Journal of Physical Chemistry Letters, 2011, 2, 1633-1638.	2.1	13
86	Is Electronegativity a Useful Descriptor for the Pseudoâ€Alkali Metal NH₄?. Chemistry - A European Journal, 2011, 17, 13197-13205.	1.7	16
87	Insights in quantum dynamical effects in the infrared spectroscopy of liquid water from a semiclassical study with an ab initio-based flexible and polarizable force field. Journal of Chemical Physics, 2011, 135, 244503.	1.2	63
88	Communication: The effect of dispersion corrections on the melting temperature of liquid water. Journal of Chemical Physics, 2011, 134, 121105.	1.2	149
89	Structures and Encapsulation Motifs of Functional Molecules Probed by Laser Spectroscopic and Theoretical Methods. Sensors, 2010, 10, 3519-3548.	2.1	16
90	High-Level Ab Initio Electronic Structure Calculations of Water Clusters (H₂O)₁₆ and (H₂O)₁₇: A New Global Minimum for (H₂O)₁₆. Journal of Physical Chemistry Letters, 2010, 1, 3122-3127.	2.1	152

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91	Dimerization of Indanedioneketene to Spiro-oxetanone: A Theoretical Study. Journal of Organic Chemistry, 2010, 75, 5499-5504.	1.7	5
92	Analysis of Bonding Patterns in the Valence Isoelectronic Series O₃, S₃, SO₂, and OS₂in Terms of Oriented Quasi-Atomic Molecular Orbitals^{â€}. Journal of Physical Chemistry A, 2010, 114, 8923-8931.	1.1	31
93	Structure of the Calix[4]areneâ^'(H₂O) Cluster: The Worldâ€™s Smallest Cup of Water. Journal of Physical Chemistry A, 2010, 114, 2967-2972.	1.1	38
94	An Empirical Correlation between the Enthalpy of Solution of Aqueous Salts and Their Ability to Form Hydrates. Journal of Physical Chemistry A, 2010, 114, 10454-10457.	1.1	11
95	Nuclear Quantum Effects in the Reorientation of Water. Journal of Physical Chemistry Letters, 2010, 1, 2316-2321.	2.1	62
96	Stepwise hydration of the cyanide anion: A temperature-controlled photoelectron spectroscopy and ab initio computational study of CNâ^'(H2O)n, n=2â€“5. Journal of Chemical Physics, 2010, 132, 124306.	1.2	24
97	Encapsulation of Arn complexes by calix[4]arene: endo- vs. exo-complexes. Physical Chemistry Chemical Physics, 2010, 12, 4569.	1.3	12
98	Hydrogen Bonds in Aqueous Hydrates: Experiment and Theory. , 2010, , .		0
99	On the phase diagram of water with density functional theory potentials: The melting temperature of ice Ih with the Perdewâ€“Burkeâ€“Ernzerhof and Beckeâ€“Leeâ€“Yangâ€“Parr functionals. Journal of Chemical Physics, 2009, 130, 221102.	1.2	203
100	Liquid water. , 2009, , .		44
101	Dances with hydrogen cations. Nature, 2009, 457, 673-674.	13.7	21
102	The reorientation mechanism of hydroxide ions in water: A molecular dynamics study. Chemical Physics Letters, 2009, 481, 9-16.	1.2	27
103	The melting temperature of bulk silicon from ab initio molecular dynamics simulations. Chemical Physics Letters, 2009, 481, 88-90.	1.2	22
104	Accurate dipole polarizabilities for water clusters n=2â€“12 at the coupled-cluster level of theory and benchmarking of various density functionals. Journal of Chemical Physics, 2009, 131, 214103.	1.2	83
105	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
106	Low-Energy Networks of the T-Cage (H₂O)₂₄ Cluster and Their Use in Constructing Periodic Unit Cells of the Structure I (sI) Hydrate Lattice. Journal of the American Chemical Society, 2009, 131, 7564-7566.	6.6	60
107	Aqueous Solutions and Their Interfaces. Journal of Physical Chemistry B, 2009, 113, 3997-3999.	1.2	6
108	Observation of a Remarkable Temperature Effect in the Hydrogen Bonding Structure and Dynamics of the CN^{â^'}(H₂O) Cluster. Journal of Physical Chemistry A, 2009, 113, 9579-9584.	1.1	10

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109	Computational Investigation of the First Solvation Shell Structure of Interfacial and Bulk Aqueous Chloride and Iodide Ions. Journal of Physical Chemistry B, 2009, 113, 4141-4146.	1.2	79
110	Clusterâ€Controlled Photofragmentation: The Case of the Xeâ€“Pyrrole Cluster. ChemPhysChem, 2008, 9, 1838-1841.	1.0	15
111	Identifying the most stable networks in polyhedral water clusters. Chemical Physics Letters, 2008, 461, 180-188.	1.2	74
112	Development of transferable interaction potentials for water. V. Extension of the flexible, polarizable, Thole-type model potential (<scp>TTM3-F</scp>, v. 3.0) to describe the vibrational spectra of water clusters and liquid water. Journal of Chemical Physics, 2008, 128, 074506.	1.2	332
113	On the Determination of Monomer Dissociation Energies of Small Water Clusters from Photoionization Experiments. Journal of Physical Chemistry A, 2008, 112, 1851-1853.	1.1	5
114	Infrared spectrum of NH4+(H2O): Evidence for mode specific fragmentation. Journal of Chemical Physics, 2007, 126, 074307.	1.2	63
115	Photofragment slice imaging studies of pyrrole and the Xeâ‹¯pyrrole cluster. Journal of Chemical Physics, 2007, 127, 064306.	1.2	43
116	Study of NH Stretching Vibrations in Small Ammonia Clusters by Infrared Spectroscopy in He Droplets and ab Initio Calculationsâ€. Journal of Physical Chemistry A, 2007, 111, 7460-7471.	1.1	59
117	High-Resolution Infrared Spectroscopy in the 1200â‹'1300 cm⁻¹ Region and Accurate Theoretical Estimates for the Structure and Ring-Puckering Barrier of Perfluorocyclobutane. Journal of Physical Chemistry A, 2007, 111, 11328-11341.	1.1	6
118	The Flexible, Polarizable, Thole-Type Interaction Potential for Water (TTM2-F) Revisited. Journal of Physical Chemistry A, 2006, 110, 4100-4106.	1.1	166
119	Anharmonic vibrational spectra of hydrogen bonded clusters: comparison between higher energy derivative and mean-field grid based methods. International Reviews in Physical Chemistry, 2006, 25, 719-733.	0.9	21
120	The bend angle of water in ice Ih and liquid water: The significance of implementing the nonlinear monomer dipole moment surface in classical interaction potentials. Journal of Chemical Physics, 2006, 124, 174504.	1.2	65
121	Lowest-Energy Structures of Water Clusters (H2O)11 and (H2O)13. Journal of Physical Chemistry A, 2006, 110, 11781-11784.	1.1	81
122	Structure, Vibrational Spectrum, and Ring Puckering Barrier of Cyclobutane. Journal of Physical Chemistry A, 2006, 110, 10487-10494.	1.1	17
123	New Experimental and Theoretical Approach to the Heterogeneous Hydrolysis of NO2:Â Key Role of Molecular Nitric Acid and Its Complexesâ€. Journal of Physical Chemistry A, 2006, 110, 6886-6897.	1.1	113
124	An efficient parallelization scheme for molecular dynamics simulations with many-body, flexible, polarizable empirical potentials: application to water. Theoretical Chemistry Accounts, 2006, 117, 73-84.	0.5	8
125	A quantitative account of quantum effects in liquid water. Journal of Chemical Physics, 2006, 125, 141102.	1.2	77
126	High-level ab initio calculations for the four low-lying families of minima of(H2O)20. II. Spectroscopic signatures of the dodecahedron, fused cubes, face-sharing pentagonal prisms, and edge-sharing pentagonal prisms hydrogen bonding networks. Journal of Chemical Physics, 2005, 122, 134304.	1.2	84

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127	The spectroscopic signature of the â€œall-surfaceâ€•to â€œinternally solvatedâ€•structural transition in water clusters in the n=17â€“21 size regime. Journal of Chemical Physics, 2005, 122, 194310.	1.2	79
128	Competition between van der Waals and Hydrogen Bonding Interactions:Â Structure of thetrans-1-Naphthol/N2Cluster. Journal of Physical Chemistry A, 2005, 109, 9584-9589.	1.1	1
129	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	23.0	560
130	Fast electron correlation methods for molecular clusters in the ground and excited states. Molecular Physics, 2005, 103, 2255-2265.	0.8	137
131	On the importance of zero-point effects in molecular level classical simulations of water. Journal of Molecular Liquids, 2004, 110, 177-192.	2.3	9
132	"Morphing" of ab initio-based interaction potentials to spectroscopic accuracy: Application to Cl-(H2O). Pure and Applied Chemistry, 2004, 76, 29-35.	0.9	22
133	The binding energies of the D2d and S4 water octamer isomers: High-level electronic structure and empirical potential results. Journal of Chemical Physics, 2004, 120, 823-828.	1.2	137
134	High-level ab initio calculations for the four low-lying families of minima of (H[sub 2]O)[sub 20]. I. Estimates of MP2/CBS binding energies and comparison with empirical potentials. Journal of Chemical Physics, 2004, 121, 2655.	1.2	190
135	Intermolecular Interactions and Cooperative Effects from Electronic Structure Calculations: An Effective Means for Developing Interaction Potentials for Condensed Phase Simulations. , 2004, , 1-15.		0
136	Anharmonic Vibrational Spectroscopy of the F-(H2O)nComplexes,n= 1, 2. Journal of Physical Chemistry A, 2003, 107, 4952-4956.	1.1	65
137	The formation of cyclic water complexes by sequential ring insertion: Experiment and theory. Journal of Chemical Physics, 2002, 117, 1109-1122.	1.2	134
138	Nitric Acidâˆ’Water Complexes:â€‰ Theoretical Calculations and Comparison to Experiment. Journal of Physical Chemistry A, 2002, 106, 7628-7635.	1.1	90
139	First Principles Examination of the Acetyleneâˆ’Water Clusters, HCCHâˆ’(H2O)x,x= 2, 3, and 4. Journal of Physical Chemistry A, 2002, 106, 11327-11337.	1.1	49
140	Development of transferable interaction models for water. I. Prominent features of the water dimer potential energy surface. Journal of Chemical Physics, 2002, 116, 1479-1492.	1.2	127
141	Development of transferable interaction models for water. II. Accurate energetics of the first few water clusters from first principles. Journal of Chemical Physics, 2002, 116, 1493-1499.	1.2	363
142	Development of transferable interaction models for water. III. Reparametrization of an all-atom polarizable rigid model (TTM2â€“R) from first principles. Journal of Chemical Physics, 2002, 116, 1500-1510.	1.2	173
143	Development of transferable interaction models for water. IV. A flexible, all-atom polarizable potential (TTM2-F) based on geometry dependent charges derived from an ab initio monomer dipole moment surface. Journal of Chemical Physics, 2002, 116, 5115.	1.2	236
144	Promise and challenge of high-performance computing, with examples from molecular modelling. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2002, 360, 1079-1105.	1.6	10

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145	A molecular level study of the aqueous microsolvation of acetylene. Chemical Physics Letters, 2001, 340, 538-546.	1.2	18
146	Cooperativity and hydrogen bonding network in water clusters. Chemical Physics, 2000, 258, 225-231.	0.9	402
147	A first principles study of the acetyleneâ€“water interaction. Journal of Chemical Physics, 2000, 112, 6178-6189.	1.2	34
148	Electric fields in ice and near water clusters. Journal of Chemical Physics, 2000, 112, 3285-3292.	1.2	52
149	Rotationally resolved spectroscopy of a librational fundamental band of hydrogen fluoride tetramer. Journal of Chemical Physics, 2000, 113, 707-718.	1.2	19
150	Cooperative Effects in Water Clusters. , 2000, , 119-128.		1
151	Microscopic hydration of the fluoride anion. Journal of Chemical Physics, 1999, 110, 5-8.	1.2	192
152	Multipole moments of water molecules in clusters and ice Ih from first principles calculations. Journal of Chemical Physics, 1999, 111, 6011-6015.	1.2	98
153	Spectroscopic Observation of Ion-Induced Water Dimer Dissociation in the X-Â·(H2O)2(X = F, Cl, Br, I) Clusters. Journal of Physical Chemistry A, 1999, 103, 10665-10669.	1.1	128
154	Photofragmentation spectra and potential energy surfaces of Sr+Ar2. Physical Chemistry Chemical Physics, 1999, 1, 977-981.	1.3	8
155	A New Determination of the Fluoride Ionâ^'Water Bond Energy. Journal of the American Chemical Society, 1999, 121, 3531-3532.	6.6	69
156	The parametrization of a Thole-type all-atom polarizable water model from first principles and its application to the study of water clusters (n=2â€“21) and the phonon spectrum of ice Ih. Journal of Chemical Physics, 1999, 110, 4566-4581.	1.2	232
157	Probing Temperature Effects on the Hydrogen Bonding Network of the Cl-(H2O)2 Cluster. Journal of Physical Chemistry A, 1999, 103, 3351-3355.	1.1	66
158	A systematic ab initio investigation of the open and ring structures of ozone. Chemical Physics Letters, 1998, 293, 72-80.	1.2	53
159	Predicting the Proton Affinities of H2O and NH3. Journal of Physical Chemistry A, 1998, 102, 2449-2454.	1.1	116
160	Photofragmentation spectra and structures of Sr+Arn,â€‰n=2â€“8 clusters: Experiment and theory. Journal of Chemical Physics, 1998, 109, 108-120.	1.2	39
161	Spectroscopic constants of the Xâ€‰2Î£+ and Aâ€‰2Î states of Sr+Ar from first principles: Comparison with experiment. Journal of Chemical Physics, 1998, 108, 46-49.	1.2	19
162	Molecular multipole moments of water molecules in ice Ih. Journal of Chemical Physics, 1998, 109, 4546-4551.	1.2	167

#	Article	IF	Citations
163	AB initio characterization of water and anion-water clusters. Advances in Molecular Vibrations and Collision Dynamics, 1998, , 281-309.	0.8	10
164	Contribution of Many-Body Terms to the Energy for Small Water Clusters:â€‰ A Comparison of ab Initio Calculations and Accurate Model Potentials. Journal of Physical Chemistry A, 1997, 101, 9163-9168.	1.1	192
165	Interaction potential of Al3+ in water from first principles calculations. Journal of Chemical Physics, 1997, 106, 9769-9780.	1.2	75
166	Ab-Initio Total Energy Studies of the Static and Dynamical Properties of Ice Ih. Journal of Physical Chemistry B, 1997, 101, 6146-6150.	1.2	62
167	On the importance of the fragment relaxation energy terms in the estimation of the basis set superposition error correction to the intermolecular interaction energy. Journal of Chemical Physics, 1996, 104, 8821-8824.	1.2	642
168	Quantitative Description of Hydrogen Bonding in Chlorideâ^'Water Clusters. The Journal of Physical Chemistry, 1996, 100, 9703-9713.	2.9	218
169	Significance of higher-order many-body interaction energy terms in water clusters and bulk water. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1996, 73, 107-115.	0.6	52
170	Critical Study of Fluorideâ^'Water Interactions. The Journal of Physical Chemistry, 1996, 100, 3989-3995.	2.9	101
171	Theoretical Study of Hydroxide Ion-Water Clusters. Journal of the American Chemical Society, 1995, 117, 10373-10380.	6.6	183
172	The Hamiltonian for a weakly interacting trimer of polyatomic monomers. Journal of Chemical Physics, 1995, 103, 8022-8030.	1.2	24
173	Ab initio studies of cyclic water clusters (H2O)n, n=1â€“6. III. Comparison of density functional with MP2 results. Journal of Chemical Physics, 1995, 102, 4505-4517.	1.2	382
174	Structures and Energetics of F-(H2O)n, n = 1-3 Clusters from ab Initio Calculations. The Journal of Physical Chemistry, 1994, 98, 13489-13497.	2.9	114
175	Potential energy surfaces of carbon dioxide. International Journal of Quantum Chemistry, 1994, 49, 409-427.	1.0	24
176	Ab initio studies of cyclic water clusters (H2O)n, n=1â€“6. II. Analysis of manyâ€body interactions. Journal of Chemical Physics, 1994, 100, 7523-7534.	1.2	653
177	The structure of the water trimer from ab initio calculations. Journal of Chemical Physics, 1993, 98, 8037-8040.	1.2	235
178	Theoretical estimate of the enthalpy of formation of sulfhydryl radical (HSO) and HSO-SOH isomerization energy. The Journal of Physical Chemistry, 1993, 97, 18-19.	2.9	124
179	Ab initio studies of cyclic water clusters (H2O)n, n=1â€“6. I. Optimal structures and vibrational spectra. Journal of Chemical Physics, 1993, 99, 8774-8792.	1.2	765
180	Theoretical studies of sulfurous species of importance in atmospheric chemistry. 1. Characterization of the mercaptooxy (HSO) and hydroxythio (SOH) isomers. The Journal of Physical Chemistry, 1993, 97, 6616-6627.	2.9	69

#	Article	IF	Citations
181	Structures of anion-water clusters: H-(H2O)n, n = 1-3. The Journal of Physical Chemistry, 1992, 96, 7505-7506.	2.9	47
182	Exploiting regularity in systematic sequences of wavefunctions which approach the full CI limit. Theoretica Chimica Acta, 1992, 83, 31-55.	0.9	39
183	Potential energy surfaces of ozone. I. Journal of Chemical Physics, 1991, 94, 8054-8069.	1.2	129
184	The ring opening of cyclopropylidene to allene: global features of the reaction surface. Theoretica Chimica Acta, 1991, 78, 287-326.	0.9	56
185	The ring opening of cyclopropylidene to allene and the isomerization of allene:ab initio interpretation of the electronic rearrangements in terms of quasi-atomic orbitals. Theoretica Chimica Acta, 1991, 78, 327-363.	0.9	23
186	The ring opening of cyclopropylidene to allene: key features of the accurate reaction surface. Theoretica Chimica Acta, 1991, 78, 365-395.	0.9	43
187	The potential energy surface of the ground state of carbon dioxide. Chemical Physics Letters, 1990, 166, 39-42.	1.2	13
188	Interaction Potentials for Water from Accurate Cluster Calculations. , 0, , 119-148.		27
189	A Classical Model for 3-body Interactions in Aqueous Ionic Systems. Journal of Chemical Physics, 0, , .	1.2	3