Sotiris S Xantheas

List of Publications by Year
in descending order

189	13,062	19657 61	24258 110
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	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.	3.0	765
2	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.	3.0	653
3	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.	3.0	642
4	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€‰ Issues and Scientific Advances. Chemical Reviews, 2005, 105, 355-390.	47.7	560
5	Cooperativity and hydrogen bonding network in water clusters. Chemical Physics, 2000, 258, 225-231.	1.9	402
6	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.	3.0	382
7	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.	3.0	363
8	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.	3.0	332
9	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.	3.0	236
10	The structure of the water trimer from ab initio calculations. Journal of Chemical Physics, 1993, 98, 8037-8040.	3.0	235
11	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.	3.0	232
12	Quantitative Description of Hydrogen Bonding in Chlorideâ^'Water Clusters. The Journal of Physical Chemistry, 1996, 100, 9703-9713.	2.9	218
13	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.	3.0	203
14	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.	2.5	192
15	Microscopic hydration of the fluoride anion. Journal of Chemical Physics, 1999, 110, 5-8.	3.0	192
16	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.	3.0	190
17	Theoretical Study of Hydroxide Ion-Water Clusters. Journal of the American Chemical Society, 1995, 117, 10373-10380.	13.7	183
18	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.	3.0	173

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19	Molecular multipole moments of water molecules in ice Ih. Journal of Chemical Physics, 1998, 109, 4546-4551.	3.0	167
20	The Flexible, Polarizable, Thole-Type Interaction Potential for Water (TTM2-F) Revisited. Journal of Physical Chemistry A, 2006, 110, 4100-4106.	2.5	166
21	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.	4.6	152
22	Communication: The effect of dispersion corrections on the melting temperature of liquid water. Journal of Chemical Physics, 2011, 134, 121105.	3.0	149
23	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.	3.0	137
24	Fast electron correlation methods for molecular clusters in the ground and excited states. Molecular Physics, 2005, 103, 2255-2265.	1.7	137
25	The formation of cyclic water complexes by sequential ring insertion: Experiment and theory. Journal of Chemical Physics, 2002, 117, 1109-1122.	3.0	134
26	Potential energy surfaces of ozone. I. Journal of Chemical Physics, 1991, 94, 8054-8069.	3.0	129
27	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.	2.5	128
28	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.	3.0	127
29	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
30	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.	2.6	123
31	Predicting the Proton Affinities of H2O and NH3. Journal of Physical Chemistry A, 1998, 102, 2449-2454.	2.5	116
32	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
33	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.	2.5	113
34	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.	2.5	111
35	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.	3.0	105
36	Critical Study of Fluorideâ^'Water Interactions. The Journal of Physical Chemistry, 1996, 100, 3989-3995.	2.9	101

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37	Multipole moments of water molecules in clusters and ice Ih from first principles calculations. Journal of Chemical Physics, 1999, 111, 6011-6015.	3.0	98
38	Nitric Acidâ^'Water Complexes:â€‰ Theoretical Calculations and Comparison to Experiment. Journal of Physical Chemistry A, 2002, 106, 7628-7635.	2.5	90
39	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.	3.0	84
40	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.	3.0	83
41	The water dimer II: Theoretical investigations. Chemical Physics Letters, 2018, 700, 163-175.	2.6	82
42	Lowest-Energy Structures of Water Clusters (H2O)11 and (H2O)13. Journal of Physical Chemistry A, 2006, 110, 11781-11784.	2.5	81
43	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.	3.0	79
44	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.	2.6	79
45	A quantitative account of quantum effects in liquid water. Journal of Chemical Physics, 2006, 125, 141102.	3.0	77
46	Benchmark Theoretical Study of the Ï€â€“Ï€ Binding Energy in the Benzene Dimer. Journal of Physical Chemistry A, 2014, 118, 7568-7578.	2.5	77
47	Interaction potential of Al3+ in water from first principles calculations. Journal of Chemical Physics, 1997, 106, 9769-9780.	3.0	75
48	Unusual Inorganic Biradicals: A Theoretical Analysis. Angewandte Chemie - International Edition, 2013, 52, 5736-5739.	13.8	75
49	Identifying the most stable networks in polyhedral water clusters. Chemical Physics Letters, 2008, 461, 180-188.	2.6	74
50	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
51	A New Determination of the Fluoride Ionâ^'Water Bond Energy. Journal of the American Chemical Society, 1999, 121, 3531-3532.	13.7	69
52	Second-order many-body perturbation study of ice Ih. Journal of Chemical Physics, 2012, 137, 204505.	3.0	69
53	The Performance of Density Functionals for Sulfateâ€“Water Clusters. Journal of Chemical Theory and Computation, 2013, 9, 1368-1380.	5.3	69
54	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.	7.1	69

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55	Probing Temperature Effects on the Hydrogen Bonding Network of the Cl-(H2O)2 Cluster. Journal of Physical Chemistry A, 1999, 103, 3351-3355.	2.5	66
56	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.	13.7	66
57	Anharmonic Vibrational Spectroscopy of the F-(H2O)nComplexes,n= 1, 2. Journal of Physical Chemistry A, 2003, 107, 4952-4956.	2.5	65
58	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.	3.0	65
59	Infrared spectrum of NH4+(H2O): Evidence for mode specific fragmentation. Journal of Chemical Physics, 2007, 126, 074307.	3.0	63
60	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.	3.0	63
61	Ab-Initio Total Energy Studies of the Static and Dynamical Properties of Ice Ih. Journal of Physical Chemistry B, 1997, 101, 6146-6150.	2.6	62
62	Nuclear Quantum Effects in the Reorientation of Water. Journal of Physical Chemistry Letters, 2010, 1, 2316-2321.	4.6	62
63	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.	13.7	60
64	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.	13.7	60
65	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.	2.5	59
66	The ring opening of cyclopropylidene to allene: global features of the reaction surface. Theoretica Chimica Acta, 1991, 78, 287-326.	0.8	56
67	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.	3.0	54
68	A systematic ab initio investigation of the open and ring structures of ozone. Chemical Physics Letters, 1998, 293, 72-80.	2.6	53
69	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
70	Electric fields in ice and near water clusters. Journal of Chemical Physics, 2000, 112, 3285-3292.	3.0	52
71	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.	4.6	52
72	First Principles Examination of the Acetyleneâ‹¯Water Clusters, HCCHâ‹¯(H2O)x,x= 2, 3, and 4. Journal of Physical Chemistry A, 2002, 106, 11327-11337.	2.5	49

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73	Structures of anion-water clusters: H-(H2O)n, n = 1-3. The Journal of Physical Chemistry, 1992, 96, 7505-7506.	2.9	47
74	Why Is MP2-Water â€œCoolerâ€•and â€œDenserâ€•than DFT-Water?. Journal of Physical Chemistry Letters, 2016, 7, 680-684.	4.6	47
75	Enhancement of hydrogen storage capacity in hydrate lattices. Chemical Physics Letters, 2012, 525-526, 13-18.	2.6	46
76	Liquid water. , 2009, , .		44
77	The ring opening of cyclopropylidene to allene: key features of the accurate reaction surface. Theoretica Chimica Acta, 1991, 78, 365-395.	0.8	43
78	Photofragment slice imaging studies of pyrrole and the Xeâ¯pyrrole cluster. Journal of Chemical Physics, 2007, 127, 064306.	3.0	43
79	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.	3.0	43
80	Atlas of putative minima and low-lying energy networks of water clusters n = 3â€“25. Journal of Chemical Physics, 2019, 151, 214307.	3.0	41
81	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.	3.0	40
82	Exploiting regularity in systematic sequences of wavefunctions which approach the full CI limit. Theoretica Chimica Acta, 1992, 83, 31-55.	0.8	39
83	Photofragmentation spectra and structures of Sr+Arn,â€‰n=2â€“8 clusters: Experiment and theory. Journal of Chemical Physics, 1998, 109, 108-120.	3.0	39
84	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.	5.3	39
85	Structure of the Calix[4]areneâ¯(H₂O) Cluster: The Worldâ€™s Smallest Cup of Water. Journal of Physical Chemistry A, 2010, 114, 2967-2972.	2.5	38
86	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.	1.7	36
87	The Origin of the Reactivity of the Criegee Intermediate: Implications for Atmospheric Particle Growth. Angewandte Chemie - International Edition, 2016, 55, 1015-1019.	13.8	36
88	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.	2.6	35
89	Towards complete assignment of the infrared spectrum of the protonated water cluster H+(H2O)21. Nature Communications, 2021, 12, 6141.	12.8	35
90	A first principles study of the acetyleneâ€“water interaction. Journal of Chemical Physics, 2000, 112, 6178-6189.	3.0	34

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91	Massively parallel quantum chemical density matrix renormalization group method. Journal of Computational Chemistry, 2021, 42, 534-544.	3.3	34
92	Microhydration Effects on the Intermediates of the S_N2 Reaction of Iodide Anion with Methyl Iodide. Angewandte Chemie - International Edition, 2013, 52, 4380-4383.	13.8	32
93	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.	2.5	31
94	The Many-Body Expansion for Aqueous Systems Revisited: I. Waterâ€“Water Interactions. Journal of Chemical Theory and Computation, 2020, 16, 6843-6855.	5.3	31
95	Ultrafast dynamics of liquid water: Frequency fluctuations of the OH stretch and the HOH bend. Journal of Chemical Physics, 2013, 139, 044503.	3.0	30
96	A benchmark photoelectron spectroscopic and theoretical study of the electronic stability of [B12H12]2â^'. Journal of Chemical Physics, 2019, 150, 164306.	3.0	29
97	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.	2.8	28
98	Interaction Potentials for Water from Accurate Cluster Calculations. , 0, , 119-148.		27
99	The reorientation mechanism of hydroxide ions in water: A molecular dynamics study. Chemical Physics Letters, 2009, 481, 9-16.	2.6	27
100	Potential energy surfaces of carbon dioxide. International Journal of Quantum Chemistry, 1994, 49, 409-427.	2.0	24
101	The Hamiltonian for a weakly interacting trimer of polyatomic monomers. Journal of Chemical Physics, 1995, 103, 8022-8030.	3.0	24
102	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.	3.0	24
103	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.	2.5	24
104	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.	2.8	24
105	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.	0.8	23
106	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.	3.0	23
107	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.	3.0	23
108	"Morphing" of ab initio-based interaction potentials to spectroscopic accuracy: Application to Cl-(H2O). Pure and Applied Chemistry, 2004, 76, 29-35.	1.9	22

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109	The melting temperature of bulk silicon from ab initio molecular dynamics simulations. Chemical Physics Letters, 2009, 481, 88-90.	2.6	22
110	Vapor Phase Infrared Spectroscopy and Ab Initio Fundamental Anharmonic Frequencies of Ammonia Borane. Journal of Physical Chemistry A, 2012, 116, 3124-3136.	2.5	22
111	Refined energetic ordering for sulphateâ€“water (nâ€‰=â€‰3â€“6) clusters using high-level electronic structure calculations. Molecular Physics, 2012, 110, 2513-2521.	1.7	22
112	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.	5.3	22
113	Communication: Water activation and splitting by single metal-atom anions. Journal of Chemical Physics, 2018, 149, 221101.	3.0	22
114	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.	5.3	22
115	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.	2.3	21
116	Dances with hydrogen cations. Nature, 2009, 457, 673-674.	27.8	21
117	Solvent immersion imprint lithography. Lab on A Chip, 2014, 14, 2072.	6.0	21
118	Laser Spectroscopic and Theoretical Studies of Encapsulation Complexes of Calix[4]arene. Journal of Physical Chemistry A, 2011, 115, 10846-10853.	2.5	20
119	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.	13.7	20
120	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.	3.0	19
121	Rotationally resolved spectroscopy of a librational fundamental band of hydrogen fluoride tetramer. Journal of Chemical Physics, 2000, 113, 707-718.	3.0	19
122	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.	3.0	19
123	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.	3.0	19
124	A molecular level study of the aqueous microsolvation of acetylene. Chemical Physics Letters, 2001, 340, 538-546.	2.6	18
125	Structure, Vibrational Spectrum, and Ring Puckering Barrier of Cyclobutane. Journal of Physical Chemistry A, 2006, 110, 10487-10494.	2.5	17
126	Structures and Encapsulation Motifs of Functional Molecules Probed by Laser Spectroscopic and Theoretical Methods. Sensors, 2010, 10, 3519-3548.	3.8	16

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127	Photodetachment of Isolated Bicarbonate Anion: Electron Binding Energy of HCO₃^{â€“}. Journal of Physical Chemistry Letters, 2011, 2, 1204-1210.	4.6	16
128	Is Electronegativity a Useful Descriptor for the Pseudoâ€Alkali Metal NH₄?. Chemistry - A European Journal, 2011, 17, 13197-13205.	3.3	16
129	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.	2.8	16
130	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.	2.5	16
131	The many-body expansion for aqueous systems revisited: III. Hofmeister ionâ€“water interactions. Physical Chemistry Chemical Physics, 2021, 23, 11196-11210.	2.8	16
132	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.	4.6	16
133	Clusterâ€Controlled Photofragmentation: The Case of the Xeâ€“Pyrrole Cluster. ChemPhysChem, 2008, 9, 1838-1841.	2.1	15
134	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.	7.1	15
135	Structures, Energetics, and Spectroscopic Fingerprints of Water Clusters n = 2â€“24. , 2012, , 761-792.		14
136	The Origin of the Reactivity of the Criegee Intermediate: Implications for Atmospheric Particle Growth. Angewandte Chemie, 2016, 128, 1027-1031.	2.0	14
137	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.	3.0	14
138	The potential energy surface of the ground state of carbon dioxide. Chemical Physics Letters, 1990, 166, 39-42.	2.6	13
139	Dynamics of Weak, Bifurcated, and Strong Hydrogen Bonds in Lithium Nitrate Trihydrate. Journal of Physical Chemistry Letters, 2011, 2, 1633-1638.	4.6	13
140	Encapsulation of Arn complexes by calix[4]arene: endo- vs. exo-complexes. Physical Chemistry Chemical Physics, 2010, 12, 4569.	2.8	12
141	Isomers and Conformational Barriers of Gas-Phase Nicotine, Nornicotine, and Their Protonated Forms. Journal of Physical Chemistry B, 2014, 118, 8273-8285.	2.6	12
142	The activation of carbon dioxide by first row transition metals (Scâ€“Zn). Physical Chemistry Chemical Physics, 2018, 20, 25495-25505.	2.8	12
143	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.	2.5	11
144	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.	13.8	11

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145	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.	1.4	11
146	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.	5.3	11
147	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.	4.6	11
148	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.	2.8	11
149	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.	2.5	10
150	The Melting Temperature of Liquid Water with the Effective Fragment Potential. Journal of Physical Chemistry Letters, 2015, 6, 3555-3559.	4.6	10
151	AB initio characterization of water and anion-water clusters. Advances in Molecular Vibrations and Collision Dynamics, 1998, , 281-309.	0.8	10
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