Lars G M Pettersson

List of Publications by Year
in descending order

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		8208	13274
327	22,588	78	135
papers	citations	h-index	g-index

334	334	334	17577
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Simulations of x-ray absorption spectra for CO desorbing from Ru(0001) with transition-potential and time-dependent density functional theory approaches. Structural Dynamics, 2022, 9, 014101.	0.9	1
2	Hydrogen Evolution Linked to Selective Oxidation of Glycerol over CoMoO₄â€"A Theoretically Predicted Catalyst. Advanced Energy Materials, 2022, 12, .	10.2	37
3	The local structure of water from combining diffraction and X-ray spectroscopy. Journal of Non-Crystalline Solids: X, 2022, 14, 100087.	0.5	3
4	In Situ Surface-Sensitive Investigation of Multiple Carbon Phases on Fe(110) in the Fischerâ€"Tropsch Synthesis. ACS Catalysis, 2022, 12, 7609-7621.	5.5	13
5	Selectivity of the First Two Glycerol Dehydrogenation Steps Determined Using Scaling Relationships. ACS Catalysis, 2021, 11, 3487-3497.	5.5	19
6	Properties of interfaces between copper and copper sulphide/oxide films. Corrosion Science, 2021, 183, 109313.	3.0	9
7	Electrocatalytic Glycerol Oxidation with Concurrent Hydrogen Evolution Utilizing an Efficient MoO_x/Pt Catalyst. Small, 2021, 17, e2104288.	5.2	63
8	X-ray emission spectroscopy: a genetic algorithm to disentangle coreâ€"hole-induced dynamics. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	6
9	Time-resolved observation of transient precursor state of CO on Ru(0001) using carbon K-edge spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 2677-2684.	1.3	15
10	Electrochemical Interface during Corrosion of Copper in Anoxic Sulfide-Containing Groundwaterâ€"A Computational Study. Journal of Physical Chemistry C, 2020, 124, 469-481.	1.5	8
11	Photodriven CO dimerization on Cu₂O from an electronic-structure perspective. Sustainable Energy and Fuels, 2020, 4, 670-677.	2.5	0
12	Uncovering the electrochemical interface of low-index copper surfaces in deep groundwater environments. Electrochimica Acta, 2020, 362, 137111.	2.6	5
13	Elucidating the role of Ni to enhance the methanol oxidation reaction on Pd electrocatalysts. Electrochimica Acta, 2020, 360, 136954.	2.6	34
14	Partial Electrooxidation of Glycerol on Close-Packed Transition Metal Surfaces: Insights from First-Principles Calculations. Journal of Physical Chemistry C, 2020, 124, 17907-17915.	1.5	13
15	Some useful correlations for H-bonded systems. Molecular Crystals and Liquid Crystals, 2020, 696, 15-28.	0.4	6
16	Nanoscale Spatial Distribution of Supported Nanoparticles Controls Activity and Stability in Powder Catalysts for CO Oxidation and Photocatalytic H₂ Evolution. Journal of the American Chemical Society, 2020, 142, 14481-14494.	6.6	25
17	Accurate SCC-DFTB Parametrization for Bulk Water. Journal of Chemical Theory and Computation, 2020, 16, 1768-1778.	2.3	17
18	Accuracy of XAS theory for unraveling structural changes of adsorbates: CO on Ni(100). AIP Advances, 2020, 10, 115014.	0.6	6

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19	A proposal for the structure of high- and low-density fluctuations in liquid water. Journal of Chemical Physics, 2019, 151, 034508.	1.2	39
20	Radial distribution functions of water: Models vs experiments. Journal of Chemical Physics, 2019, 151, 044502.	1.2	25
21	Liquid water structure from X-ray absorption and emission, NMR shielding and X-ray diffraction. Science China: Physics, Mechanics and Astronomy, 2019, 62, 1.	2.0	5
22	Translational and rotational dynamics of high and low density TIP4P/2005 water. Journal of Chemical Physics, 2019, 150, 224507.	1.2	20
23	On the Nature of the Cathodic Reaction during Corrosion of Copper in Anoxic Sulfide Solutions. Journal of the Electrochemical Society, 2019, 166, C196-C208.	1.3	6
24	Do X-ray spectroscopies provide evidence for continuous distribution models of water at ambient conditions?. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 17156-17157.	3.3	16
25	X-ray absorption spectrum simulations of hexagonal ice. Journal of Chemical Physics, 2019, 150, 034501.	1.2	13
26	A Two-State Picture of Water and the Funnel of Life. Springer Proceedings in Physics, 2019, , 3-39.	0.1	8
27	Amorphous, Periodic Model of a Copper Electrocatalyst with Subsurface Oxygen for Enhanced CO Coverage and Dimerization. Journal of Physical Chemistry C, 2019, 123, 4961-4968.	1.5	13
28	Relationship between x-ray emission and absorption spectroscopy and the local H-bond environment in water. Journal of Chemical Physics, 2018, 148, 144507.	1.2	37
29	A Chemical View on Xâ€ray Photoelectron Spectroscopy: the ESCA Molecule and Surfaceâ€toâ€Bulk XPS Shifts. ChemPhysChem, 2018, 19, 169-174.	1.0	24
30	Atom-specific activation in CO oxidation. Journal of Chemical Physics, 2018, 149, 234707.	1.2	2
31	Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics. Nature Communications, 2018, 9, 1917.	5.8	59
32	Spin Uncoupling in Chemisorbed OCCO and CO₂: Two High-Energy Intermediates in Catalytic CO₂ Reduction. Journal of Physical Chemistry C, 2018, 122, 12251-12258.	1.5	22
33	X-ray Absorption Near-Edge Spectroscopy Calculations on Pristine and Modified Chalcopyrite Surfaces. Journal of Physical Chemistry C, 2018, 122, 20200-20209.	1.5	8
34	Temperature dependence of the intensity of the vibration-rotational absorption band Î½2 of H2O trapped in an argon matrix. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 172, 83-90.	2.0	13
35	MP4 Study of the Anharmonic Coupling of the Shared Proton Stretching Vibration of the Protonated Water Dimer in Equilibrium and Transition States. Journal of Physical Chemistry A, 2017, 121, 2151-2165.	1.1	8
36	Core-hole-induced dynamical effects in the x-ray emission spectrum of liquid methanol. Journal of Chemical Physics, 2017, 146, 134506.	1.2	18

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37	Calculation of the vibrationâ€“rotational transition intensities of water molecules trapped in an argon matrix: stretching Oâ€“H vibrations spectral region. Molecular Physics, 2017, 115, 2605-2613.	0.8	10
38	Stability, Structure, and Electronic Properties of the Pyrite/Arsenopyrite Solidâ€“Solid Interfaceâ€“A DFT Study. Journal of Physical Chemistry C, 2017, 121, 8042-8051.	1.5	34
39	Subsurface Oxygen in Oxide-Derived Copper Electrocatalysts for Carbon Dioxide Reduction. Journal of Physical Chemistry Letters, 2017, 8, 285-290.	2.1	332
40	Stability and Effects of Subsurface Oxygen in Oxide-Derived Cu Catalyst for CO₂ Reduction. Journal of Physical Chemistry C, 2017, 121, 25010-25017.	1.5	92
41	Nature and Distribution of Stable Subsurface Oxygen in Copper Electrodes During Electrochemical CO₂ Reduction. Journal of Physical Chemistry C, 2017, 121, 25003-25009.	1.5	98
42	How square ice helps lubrication. Physical Review B, 2017, 95, .	1.1	12
43	Real-Time Elucidation of Catalytic Pathways in CO Hydrogenation on Ru. Journal of Physical Chemistry Letters, 2017, 8, 3820-3825.	2.1	9
44	Temperature-Independent Nuclear Quantum Effects on the Structure of Water. Physical Review Letters, 2017, 119, 075502.	2.9	26
45	Probing the OH Stretch in Different Local Environments in Liquid Water. Journal of Physical Chemistry Letters, 2017, 8, 5487-5491.	2.1	30
46	Diffusive dynamics during the high-to-low density transition in amorphous ice. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 8193-8198.	3.3	155
47	X-ray Emission Spectrum of Liquid Ethanol: Origin of Split Peaks. Journal of Physical Chemistry B, 2017, 121, 11163-11168.	1.2	15
48	Waterâ€”The Most Anomalous Liquid. Chemical Reviews, 2016, 116, 7459-7462.	23.0	124
49	Water: A Tale of Two Liquids. Chemical Reviews, 2016, 116, 7463-7500.	23.0	627
50	Combinatorial Broadening Mechanism of Oâ€“H Stretching Bands in H-Bonded Molecular Clusters. Journal of Applied Spectroscopy, 2016, 83, 350-357.	0.3	4
51	The structural validity of various thermodynamical models of supercooled water. Journal of Chemical Physics, 2016, 145, 134507.	1.2	41
52	Evaporative cooling of microscopic water droplets in vacuo: Molecular dynamics simulations and kinetic gas theory. Journal of Chemical Physics, 2016, 144, 124502.	1.2	22
53	The temperature dependence of intermediate range oxygen-oxygen correlations in liquid water. Journal of Chemical Physics, 2016, 145, 084503.	1.2	33
54	Structural Changes in RuO₂ during Electrochemical Hydrogen Evolution. Journal of Physical Chemistry C, 2016, 120, 7094-7102.	1.5	19

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55	Chemical Bond Activation Observed with an X-ray Laser. Journal of Physical Chemistry Letters, 2016, 7, 3647-3651.	2.1	21
56	X-ray and Electron Spectroscopy of Water. Chemical Reviews, 2016, 116, 7551-7569.	23.0	143
57	Probing water with X-ray lasers. Advances in Physics: X, 2016, 1, 226-245.	1.5	8
58	Structural transformations in bulk and matrix-isolated methanol from measured and computed infrared spectroscopy. Journal of Molecular Liquids, 2016, 216, 53-58.	2.3	17
59	Requirements of first-principles calculations of X-ray absorption spectra of liquid water. Physical Chemistry Chemical Physics, 2016, 18, 566-583.	1.3	30
60	Indication of non-thermal contribution to visible femtosecond laser-induced CO oxidation on Ru(0001). Journal of Chemical Physics, 2015, 143, 074701.	1.2	14
61	Optical laser-induced CO desorption from Ru(0001) monitored with a free-electron X-ray laser: DFT prediction and X-ray confirmation of a precursor state. Surface Science, 2015, 640, 80-88.	0.8	13
62	The structural origin of anomalous properties of liquid water. Nature Communications, 2015, 6, 8998.	5.8	373
63	Probing the transition state region in catalytic CO oxidation on Ru. Science, 2015, 347, 978-982.	6.0	193
64	Detection of adsorbate overlayer structural transitions using sum-frequency generation spectroscopy. Surface Science, 2015, 633, 77-81.	0.8	3
65	Long-range ionâ€“water and ionâ€“ion interactions in aqueous solutions. Physical Chemistry Chemical Physics, 2015, 17, 8427-8430.	1.3	15
66	Theoretical study of the X-ray natural circular dichroism of some crystalline amino acids. Chemical Physics, 2015, 450-451, 109-114.	0.9	12
67	Anomalous Behavior of the Homogeneous Ice Nucleation Rate in â€œNo-Manâ€™s Landâ€. Journal of Physical Chemistry Letters, 2015, 6, 2826-2832.	2.1	102
68	Strong Influence of Coadsorbate Interaction on CO Desorption Dynamics on Ru(0001) Probed by Ultrafast X-Ray Spectroscopy andAbÂInitioSimulations. Physical Review Letters, 2015, 114, 156101.	2.9	25
69	Theoretical analysis of hydrogen spillover mechanism on carbon nanotubes. Frontiers in Chemistry, 2015, 3, 2.	1.8	32
70	The electrocatalytic properties of doped TiO2. Electrochimica Acta, 2015, 180, 514-527.	2.6	34
71	X-ray emission spectroscopy of bulk liquid water in â€œno-manâ€™s landâ€. Journal of Chemical Physics, 2015, 142, 044505.	1.2	32
72	The structure of water; from ambient to deeply supercooled. Journal of Non-Crystalline Solids, 2015, 407, 399-417.	1.5	51

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73	Comparison of x-ray absorption spectra between water and ice: New ice data with low pre-edge absorption cross-section. Journal of Chemical Physics, 2014, 141, 034507.	1.2	60
74	Operando Characterization of an Amorphous Molybdenum Sulfide Nanoparticle Catalyst during the Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2014, 118, 29252-29259.	1.5	87
75	Reabsorption of Soft X-Ray Emission at High X-Ray Free-Electron Laser Fluences. Physical Review Letters, 2014, 113, 153002.	2.9	33
76	A Molecular Perspective on the d-Band Model: Synergy Between Experiment and Theory. Topics in Catalysis, 2014, 57, 2-13.	1.3	90
77	Ti atoms in Ru0.3Ti0.7O2 mixed oxides form active and selective sites for electrochemical chlorine evolution. Electrochimica Acta, 2014, 146, 733-740.	2.6	44
78	Ultrafast X-ray probing of water structure below the homogeneous ice nucleation temperature. Nature, 2014, 510, 381-384.	13.7	385
79	A different view of structure-making and structure-breaking in alkali halide aqueous solutions through x-ray absorption spectroscopy. Journal of Chemical Physics, 2014, 140, 244506.	1.2	70
80	Highly Compressed Two-Dimensional Form of Water at Ambient Conditions. Scientific Reports, 2013, 3, 1074.	1.6	31
81	Stability of Pt-Modified Cu(111) in the Presence of Oxygen and Its Implication on the Overall Electronic Structure. Journal of Physical Chemistry C, 2013, 117, 16371-16380.	1.5	5
82	Resonant inelastic X-ray scattering of liquid water. Journal of Electron Spectroscopy and Related Phenomena, 2013, 188, 84-100.	0.8	45
83	Benchmark oxygen-oxygen pair-distribution function of ambient water from x-ray diffraction measurements with a wide Q-range. Journal of Chemical Physics, 2013, 138, 074506.	1.2	407
84	Real-Time Observation of Surface Bond Breaking with an X-ray Laser. Science, 2013, 339, 1302-1305.	6.0	179
85	Radical water. Nature Chemistry, 2013, 5, 553-554.	6.6	5
86	Solvation structures of protons and hydroxide ions in water. Journal of Chemical Physics, 2013, 138, 154506.	1.2	19
87	The Boson peak in supercooled water. Scientific Reports, 2013, 3, 1980.	1.6	47
88	Unique water-water coordination tailored by a metal surface. Journal of Chemical Physics, 2013, 138, 234708.	1.2	1
89	Selective Probing of the OH or OD Stretch Vibration in Liquid Water Using Resonant Inelastic Soft-X-Ray Scattering. Physical Review Letters, 2013, 111, 193001.	2.9	90
90	Selective Ultrafast Probing of Transient Hot Chemisorbed and Precursor States of CO on Ru(0001). Physical Review Letters, 2013, 110, 186101.	2.9	51

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91	Microscopic probing of the size dependence in hydrophobic solvation. Journal of Chemical Physics, 2012, 136, 074507.	1.2	30
92	X-ray emission spectroscopy and density functional study of CO/Fe(100). Journal of Chemical Physics, 2012, 136, 034702.	1.2	21
93	Polarization dependent resonant x-ray emission spectroscopy of D2O and H2O water: Assignment of the local molecular orbital symmetry. Journal of Chemical Physics, 2012, 136, 044517.	1.2	42
94	Fluctuations in ambient water. Journal of Molecular Liquids, 2012, 176, 2-16.	2.3	86
95	Adsorption and Cyclotrimerization Kinetics of C₂H₂ at a Cu(110) Surface. Journal of Physical Chemistry C, 2012, 116, 9550-9560.	1.5	20
96	Connecting Dopant Bond Type with Electronic Structure in N-Doped Graphene. Nano Letters, 2012, 12, 4025-4031.	4.5	471
97	In situ X-ray probing reveals fingerprints of surface platinum oxide. Physical Chemistry Chemical Physics, 2011, 13, 262-266.	1.3	110
98	Spatially inhomogeneous bimodal inherent structure of simulated liquid water. Physical Chemistry Chemical Physics, 2011, 13, 19918.	1.3	136
99	Enhanced small-angle scattering connected to the Widom line in simulations of supercooled water. Journal of Chemical Physics, 2011, 134, 214506.	1.2	67
100	Ab Initio van der Waals Interactions in Simulations of Water Alter Structure from Mainly Tetrahedral to High-Density-Like. Journal of Physical Chemistry B, 2011, 115, 14149-14160.	1.2	83
101	Wide-angle X-ray diffraction and molecular dynamics study of medium-range order in ambient and hot water. Physical Chemistry Chemical Physics, 2011, 13, 19997.	1.3	63
102	The structure of water in the hydration shell of cations from x-ray Raman and small angle x-ray scattering measurements. Journal of Chemical Physics, 2011, 134, 064513.	1.2	111
103	Increased fraction of low-density structures in aqueous solutions of fluoride. Journal of Chemical Physics, 2011, 134, 224507.	1.2	18
104	An implementation of core level spectroscopies in a real space Projector Augmented Wave density functional theory code. Journal of Electron Spectroscopy and Related Phenomena, 2011, 184, 427-439.	0.8	61
105	Perspective on the structure of liquid water. Chemical Physics, 2011, 389, 1-34.	0.9	289
106	Evidence for Fe²⁺ in Wurtzite Coordination: Iron Doping Stabilizes ZnO Nanoparticles. Small, 2011, 7, 2879-2886.	5.2	44
107	Doped Nanoparticles: Evidence for Fe2+ in Wurtzite Coordination: Iron Doping Stabilizes ZnO Nanoparticles (Small 20/2011). Small, 2011, 7, 2878-2878.	5.2	1
108	Oxidation of Pt(111) under Near-Ambient Conditions. Physical Review Letters, 2011, 107, 195502.	2.9	151

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109	Vibrational interference effects in x-ray emission of a model water dimer: Implications for the interpretation of the liquid spectrum. Journal of Chemical Physics, 2011, 134, 044513.	1.2	46
110	X-ray Raman scattering provides evidence for interfacial acetonitrile-water dipole interactions in aqueous solutions. Journal of Chemical Physics, 2011, 135, 164509.	1.2	19
111	Theoretical approximations to X-ray absorption spectroscopy of liquid water and ice. Journal of Electron Spectroscopy and Related Phenomena, 2010, 177, 135-157.	0.8	132
112	X-ray absorption spectroscopy and X-ray Raman scattering of water and ice; an experimental view. Journal of Electron Spectroscopy and Related Phenomena, 2010, 177, 99-129.	0.8	158
113	High resolution X-ray emission spectroscopy of water and its assignment based on two structural motifs. Journal of Electron Spectroscopy and Related Phenomena, 2010, 177, 192-205.	0.8	100
114	Chemical bonding of water to metal surfaces studied with core-level spectroscopies. Journal of Electron Spectroscopy and Related Phenomena, 2010, 177, 85-98.	0.8	55
115	Semiclassical description of nuclear dynamics in x-ray emission of water. Physical Review B, 2010, 82, .	1.1	34
116	Reply to Soper et al.: Fluctuations in water around a bimodal distribution of local hydrogen-bonded structural motifs. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, .	3.3	44
117	Oxygen-oxygen correlations in liquid water: Addressing the discrepancy between diffraction and extended x-ray absorption fine-structure using a novel multiple-data set fitting technique. Journal of Chemical Physics, 2010, 132, 104513.	1.2	37
118	The role of substrate electrons in the wetting of a metal surface. Journal of Chemical Physics, 2010, 132, 094701.	1.2	39
119	SpecSwap-RMC: a novel reverse Monte Carlo approach using a discrete set of local configurations and pre-computed properties. Journal of Physics Condensed Matter, 2010, 22, 135001.	0.7	12
120	Functional Groups and Sulfur K-Edge XANES Spectra: Divalent Sulfur and Disulfides. Journal of Physical Chemistry A, 2010, 114, 9523-9528.	1.1	20
121	Low O2 dissociation barrier on Pt(111) due to adsorbateâ€“adsorbate interactions. Journal of Chemical Physics, 2010, 133, 224701.	1.2	49
122	Increasing correlation length in bulk supercooled H2O, D2O, and NaCl solution determined from small angle x-ray scattering. Journal of Chemical Physics, 2010, 133, 134504.	1.2	84
123	Chemical Bonding on Metal Surfaces. , 2010, , 253-274.		3
124	Cooperativity in Surface Bonding and Hydrogen Bonding of Water and Hydroxyl at Metal Surfaces. Journal of Physical Chemistry C, 2010, 114, 10240-10248.	1.5	51
125	Sulfur-Metal Orbital Hybridization in Sulfur-Bearing Compounds Studied by X-ray Emission Spectroscopy. Inorganic Chemistry, 2010, 49, 6468-6473.	1.9	56
126	Complementarity between high-energy photoelectron and L-edge spectroscopy for probing the electronic structure of 5d transition metal catalysts. Physical Chemistry Chemical Physics, 2010, 12, 5694.	1.3	23

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127	Sensitivity of x-ray absorption spectroscopy to hydrogen bond topology. Physical Review B, 2009, 80, .	1.1	37
128	Assessing the electric-field approximation to IR and Raman spectra of dilute HOD in D2O. Journal of Chemical Physics, 2009, 131, 034501.	1.2	11
129	Increased fraction of weakened hydrogen bonds of water in aerosol OT reverse micelles. Journal of Chemical Physics, 2009, 131, 031103.	1.2	19
130	The inhomogeneous structure of water at ambient conditions. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15214-15218.	3.3	526
131	The Interpretation of Sulfur K-Edge XANES Spectra: A Case Study on Thiophenic and Aliphatic Sulfur Compounds. Journal of Physical Chemistry A, 2009, 113, 2750-2756.	1.1	38
132	Electronic Structure of Sulfur Studied by X-ray Absorption and Emission Spectroscopy. Analytical Chemistry, 2009, 81, 6516-6525.	3.2	93
133	On the Range of Water Structure Models Compatible with X-ray and Neutron Diffraction Data. Journal of Physical Chemistry B, 2009, 113, 6246-6255.	1.2	81
134	Theoretical and experimental sulfur K-edge X-ray absorption spectroscopic study of cysteine, cystine, homocysteine, penicillamine, methionine and methionine sulfoxide. Dalton Transactions, 2009, , 3542.	1.6	40
135	High resolution X-ray emission spectroscopy of liquid water: The observation of two structural motifs. Chemical Physics Letters, 2008, 460, 387-400.	1.2	328
136	Electronic structure effects in liquid water studied by photoelectron spectroscopy and density functional theory. Chemical Physics Letters, 2008, 460, 86-92.	1.2	61
137	Spectroscopic evidence for the formation of 3-D crystallites during isothermal heating of amorphous ice on Pt(111). Surface Science, 2008, 602, 2004-2008.	0.8	15
138	Autocatalytic Water Dissociation on Cu(110) at Near Ambient Conditions. Journal of the American Chemical Society, 2008, 130, 2793-2797.	6.6	126
139	The structure of mixed H2Oâ€“OH monolayer films on Ru(0001). Journal of Chemical Physics, 2008, 129, 154109.	1.2	50
140	Diffraction and IR/Raman data do not prove tetrahedral water. Journal of Chemical Physics, 2008, 129, 084502.	1.2	94
141	Adsorbate Electronic Structure and Bonding on Metal Surfaces. , 2008, , 57-142.		32
142	Comment on â€œIsotope and Temperature Effects in Liquid Water Probed by X-Ray Absorption and Resonant X-Ray Emission Spectroscopyâ€. Physical Review Letters, 2008, 100, 249801; author reply 249802.	2.9	40
143	Geometric and electronic structure of methane adsorbed on a Pt surface. Journal of Chemical Physics, 2007, 127, 144702.	1.2	21
144	Isotope effects in liquid water probed by x-ray Raman spectroscopy. Physical Review B, 2007, 76, .	1.1	72

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145	Probing the Electron Delocalization in Liquid Water and Ice at Attosecond Time Scales. Physical Review Letters, 2007, 99, 217406.	2.9	117
146	Sulfur X-ray Absorption and Vibrational Spectroscopic Study of Sulfur Dioxide, Sulfite, and Sulfonate Solutions and of the Substituted Sulfonate Ions X₃CSO₃⁻ (X = H,) Tj ETQq0 1 0 rgBT /Overlock 1	1.9	67
147	Bridging the Pressure Gap in Water and Hydroxyl Chemistry on Metal Surfaces:â€‰ The Cu(110) Case. Journal of Physical Chemistry C, 2007, 111, 14493-14499.	1.5	68
148	Hydroxyl-Induced Wetting of Metals by Water at Near-Ambient Conditions. Journal of Physical Chemistry C, 2007, 111, 7848-7850.	1.5	138
149	Structure and Bonding of the Waterâ^'Hydroxyl Mixed Phase on Pt(111). Journal of Physical Chemistry C, 2007, 111, 15003-15012.	1.5	117
150	Are recent water models obtained by fitting diffraction data consistent with infrared/Raman and x-ray absorption spectra?. Journal of Chemical Physics, 2006, 125, 244510.	1.2	60
151	Bonding in metalâ€“carbonyls: A comparison with experiment and calculations on adsorbed CO. Computational and Theoretical Chemistry, 2006, 762, 123-132.	1.5	20
152	Intra- and intermolecular effects in the Compton profile of water. Physical Review B, 2006, 73, .	1.1	44
153	The local structure of protonated water from x-ray absorption and density functional theory. Journal of Chemical Physics, 2006, 124, 194508.	1.2	49
154	Structure of water adsorbed on the open Cu(110) surface: H-up, H-down, or both?. Chemical Physics Letters, 2006, 429, 415-419.	1.2	82
155	Physisorption-Induced C-H Bond Elongation in Methane. Physical Review Letters, 2006, 96, 146104.	2.9	34
156	Fluorescence Emission of Excited Hydrogen Atoms after Core Excitation of Water Vapor. Physical Review Letters, 2006, 96, 063003.	2.9	25
157	Compton scattering study of water versus iceIh: Intra- and intermolecular structure. Physical Review E, 2006, 74, 031503.	0.8	27
158	X-ray absorption spectrum of liquid water from molecular dynamics simulations: Asymmetric model. Physical Review B, 2006, 73, .	1.1	88
159	Theoretical study of ion desorption from poly-(methyl methacrylate) and poly-(isopropenyl acetate) thin films through core excitation. Journal of Chemical Physics, 2006, 124, 124901.	1.2	21
160	Correlation of hydrogen bond lengths and angles in liquid water based on Compton scattering. Journal of Chemical Physics, 2006, 125, 084504.	1.2	55
161	Auger decay calculations with core-hole excited-state molecular-dynamics simulations of water. Journal of Chemical Physics, 2006, 124, 064307.	1.2	45
162	Molecularly intact and dissociative adsorption of water on clean Cu(110): A comparison with the water/Ru(001) system. Surface Science, 2005, 585, L183-L189.	0.8	84

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163	Studies of the X-ray absorption spectra of some methylcyano esters. Journal of Electron Spectroscopy and Related Phenomena, 2005, 142, 113-119.	0.8	8
164	The electronic structure effect in heterogeneous catalysis. Catalysis Letters, 2005, 100, 111-114.	1.4	349
165	Comment on "Energetics of Hydrogen Bond Network Rearrangements in Liquid Water". Science, 2005, 308, 793a-793a.	6.0	90
166	Spectroscopic characterization of microscopic hydrogen-bonding disparities in supercritical water. Journal of Chemical Physics, 2005, 123, 154503.	1.2	79
167	Ultrafast Core-Hole-Induced Dynamics in Water Probed by X-Ray Emission Spectroscopy. Physical Review Letters, 2005, 94, 227401.	2.9	117
168	The hydrogen bond in ice probed by soft x-ray spectroscopy and density functional theory. Journal of Chemical Physics, 2005, 122, 154505.	1.2	79
169	Half or full core hole in density functional theory X-ray absorption spectrum calculations of water?. Physical Chemistry Chemical Physics, 2005, 7, 2854.	1.3	96
170	X-ray Absorption Spectroscopy Study of the Hydrogen Bond Network in the Bulk Water of Aqueous Solutions. Journal of Physical Chemistry A, 2005, 109, 5995-6002.	1.1	156
171	X-ray Absorption Spectroscopy Measurements of Liquid Water. Journal of Physical Chemistry B, 2005, 109, 13835-13839.	1.2	120
172	CO2 Sorption on MgO and CaO Surfaces:â€‰ A Comparative Quantum Chemical Cluster Study. Journal of Physical Chemistry B, 2005, 109, 16774-16781.	1.2	142
173	X-ray Absorption Spectroscopy of Liquid Methanol Microjets:Â Bulk Electronic Structure and Hydrogen Bonding Network. Journal of Physical Chemistry B, 2005, 109, 10194-10203.	1.2	74
174	Sulfur KEdge XRay Absorption Spectra for Dimethyl Sulfoxide in the Solvated ThalliumIII, IndiumIII, GalliumIII and AluminumIII Ions. Physica Scripta, 2005, , 1077.	1.2	10
175	Water Dissociation on Ru(001): An Activated Process. Physical Review Letters, 2004, 93, 196101.	2.9	196
176	Ultrafast Molecular Dissociation of Water in Ice. Physical Review Letters, 2004, 93, 148302.	2.9	71
177	Compton profiles for water and mixed water-neon clusters: A measure of coordination. Physical Review B, 2004, 70, .	1.1	30
178	X-ray absorption spectra of water within a plane-wave Car-Parrinello molecular dynamics framework. Journal of Chemical Physics, 2004, 121, 10065-10075.	1.2	45
179	Experimental and theoretical characterization of the structure of defects at the pyriteFeS2(100)surface. Physical Review B, 2004, 70, .	1.1	62
180	Functional dependence of core-excitation energies. Journal of Chemical Physics, 2004, 121, 10339-10345.	1.2	144

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