Lars G M Pettersson

List of Publications by Year
in descending order

327 papers	22,588 citations	7069 78 h-index	11581 135 g-index
334 all docs	334 docs citations	334 times ranked	15359 citing authors

#	Article	IF	Citations
1	The Structure of the First Coordination Shell in Liquid Water. Science, 2004, 304, 995-999.	6.0	1,287
2	Water: A Tale of Two Liquids. Chemical Reviews, 2016, 116, 7463-7500.	23.0	627
3	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
4	Structure and Bonding of Water on Pt(111). Physical Review Letters, 2002, 89, 276102.	2.9	512
5	Connecting Dopant Bond Type with Electronic Structure in N-Doped Graphene. Nano Letters, 2012, 12, 4025-4031.	4.5	471
6	Calculations of near-edge x-ray-absorption spectra of gas-phase and chemisorbed molecules by means of density-functional and transition-potential theory. Physical Review B, 1998, 58, 8097-8110.	1.1	467
7	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
8	Ultrafast X-ray probing of water structure below the homogeneous ice nucleation temperature. Nature, 2014, 510, 381-384.	13.7	385
9	The structural origin of anomalous properties of liquid water. Nature Communications, 2015, 6, 8998.	5.8	373
10	The electronic structure effect in heterogeneous catalysis. Catalysis Letters, 2005, 100, 111-114.	1.4	349
11	Subsurface Oxygen in Oxide-Derived Copper Electrocatalysts for Carbon Dioxide Reduction. Journal of Physical Chemistry Letters, 2017, 8, 285-290.	2.1	332
12	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
13	Perspective on the structure of liquid water. Chemical Physics, 2011, 389, 1-34.	0.9	289
14	Chemical bonding on surfaces probed by X-ray emission spectroscopy and density functional theory. Surface Science Reports, 2004, 55, 49-167.	3.8	273
15	Spectroscopic probing of local hydrogen-bonding structures in liquid water. Journal of Physics Condensed Matter, 2002, 14, L213-L219.	0.7	262
16	Detailed study of pyridine at the Câ€Š1sand Nâ€Š1sionization thresholds: The influence of the vibrational fine structure. Journal of Chemical Physics, 2001, 115, 6426-6437.	1.2	239
17	Direct, atomic orbital, static exchange calculations of photoabsorption spectra of large molecules and clusters. Chemical Physics Letters, 1994, 222, 75-81.	1.2	205
18	Separate state vs. transition state Kohn-Sham calculations of X-ray photoelectron binding energies and chemical shifts. Journal of Electron Spectroscopy and Related Phenomena, 1999, 104, 195-207.	0.8	202

#	Article	IF	Citations
19	The adsorption structure of glycine adsorbed on Cu(110); comparison with formate and. Surface Science, 1998, 407, 221-236.	0.8	200
20	Water Dissociation on Ru(001): An Activated Process. Physical Review Letters, 2004, 93, 196101.	2.9	196
21	Probing the transition state region in catalytic CO oxidation on Ru. Science, 2015, 347, 978-982.	6.0	193
22	Bonding between CO and the MgO(001) surface: A modified picture. Journal of Chemical Physics, 1994, 100, 2010-2018.	1.2	186
23	The interpretation of X-ray absorption spectra of water and ice. Chemical Physics Letters, 2002, 364, 363-370.	1.2	182
24	Real-Time Observation of Surface Bond Breaking with an X-ray Laser. Science, 2013, 339, 1302-1305.	6.0	179
25	Direct SCF direct static-exchange calculations of electronic spectra. Theoretical Chemistry Accounts, 1997, 97, 14-40.	0.5	171
26	Small Al clusters. II. Structure and binding in Aln(n=2â€“6, 13). Journal of Chemical Physics, 1987, 87, 2205-2213.	1.2	169
27	The electronic structure and surface chemistry of glycine adsorbed on Cu(110). Journal of Chemical Physics, 2000, 112, 5420-5427.	1.2	167
28	The bonding of CO to metal surfaces. Journal of Chemical Physics, 2000, 112, 1946-1958.	1.2	165
29	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
30	How Carbon Monoxide Adsorbs in Different Sites. Physical Review Letters, 2000, 85, 3309-3312.	2.9	157
31	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
32	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
33	Oxidation of Pt(111) under Near-Ambient Conditions. Physical Review Letters, 2011, 107, 195502.	2.9	151
34	Effective core potential calculations using frozen orbitals. Applications to transition metals. Chemical Physics, 1983, 80, 7-16.	0.9	145
35	Functional dependence of core-excitation energies. Journal of Chemical Physics, 2004, 121, 10339-10345.	1.2	144
36	X-ray and Electron Spectroscopy of Water. Chemical Reviews, 2016, 116, 7551-7569.	23.0	143

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37	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
38	Hydroxyl-Induced Wetting of Metals by Water at Near-Ambient Conditions. Journal of Physical Chemistry C, 2007, 111, 7848-7850.	1.5	138
39	Spatially inhomogeneous bimodal inherent structure of simulated liquid water. Physical Chemistry Chemical Physics, 2011, 13, 19918.	1.3	136
40	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
41	Autocatalytic Water Dissociation on Cu(110) at Near Ambient Conditions. Journal of the American Chemical Society, 2008, 130, 2793-2797.	6.6	126
42	Theoretical spectroscopic parameters for the lowâ€lying states of the secondâ€row transition metal hydrides. Journal of Chemical Physics, 1987, 86, 268-278.	1.2	125
43	Waterâ€”The Most Anomalous Liquid. Chemical Reviews, 2016, 116, 7459-7462.	23.0	124
44	Lattice Resistance to Hydrolysis of Siâ^'Oâ^'Si Bonds of Silicate Minerals:Â Ab Initio Calculations of a Single Water Attack onto the (001) and (111) Î²-Cristobalite Surfaces. Journal of Physical Chemistry B, 2000, 104, 5779-5783.	1.2	120
45	X-ray Absorption Spectroscopy Measurements of Liquid Water. Journal of Physical Chemistry B, 2005, 109, 13835-13839.	1.2	120
46	Core-hole effects in x-ray-absorption spectra of fullerenes. Physical Review B, 1999, 60, 7956-7960.	1.1	118
47	Ultrafast Core-Hole-Induced Dynamics in Water Probed by X-Ray Emission Spectroscopy. Physical Review Letters, 2005, 94, 227401.	2.9	117
48	Probing the Electron Delocalization in Liquid Water and Ice at Attosecond Time Scales. Physical Review Letters, 2007, 99, 217406.	2.9	117
49	Structure and Bonding of the Waterâ^'Hydroxyl Mixed Phase on Pt(111). Journal of Physical Chemistry C, 2007, 111, 15003-15012.	1.5	117
50	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
51	In situ X-ray probing reveals fingerprints of surface platinum oxide. Physical Chemistry Chemical Physics, 2011, 13, 262-266.	1.3	110
52	Effective core potential parameters for firstâ€and secondâ€row atoms. Journal of Chemical Physics, 1987, 86, 2176-2184.	1.2	109
53	Positive ions of the firstâ€and secondâ€row transition metal hydrides. Journal of Chemical Physics, 1987, 87, 481-492.	1.2	106
54	Hydrogen bonding between adsorbed deprotonated glycine molecules on Cu(110). Journal of Chemical Physics, 2003, 119, 12577-12585.	1.2	103

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55	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
56	Adsorbate ionicity and surface-dipole-moment changes: Cluster-model studies of Cl/Cu(100) and F/Cu(100). Physical Review Letters, 1986, 56, 500-503.	2.9	101
57	X-ray Raman spectroscopy at the oxygenKedge of water and ice:â€ƒ Implications on local structure models. Physical Review B, 2002, 66, .	1.1	101
58	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
59	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
60	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
61	Spin uncoupling in surface chemisorption of unsaturated hydrocarbons. Journal of Chemical Physics, 1998, 108, 1193-1205.	1.2	94
62	Diffraction and IR/Raman data do not prove tetrahedral water. Journal of Chemical Physics, 2008, 129, 084502.	1.2	94
63	Electronic Structure of Sulfur Studied by X-ray Absorption and Emission Spectroscopy. Analytical Chemistry, 2009, 81, 6516-6525.	3.2	93
64	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
65	Comment on "Energetics of Hydrogen Bond Network Rearrangements in Liquid Water". Science, 2005, 308, 793a-793a.	6.0	90
66	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
67	A Molecular Perspective on the d-Band Model: Synergy Between Experiment and Theory. Topics in Catalysis, 2014, 57, 2-13.	1.3	90
68	X-ray absorption spectrum of liquid water from molecular dynamics simulations: Asymmetric model. Physical Review B, 2006, 73, .	1.1	88
69	Comparative Study on Structures and Energetics of NOx, SOx, and COx Adsorption on Alkaline-Earth-Metal Oxides. Journal of Physical Chemistry B, 2003, 107, 7795-7802.	1.2	87
70	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
71	An investigation of basis sets and basis set superposition error in transition metals using frozen core and frozen orbital techniques. Chemical Physics, 1982, 69, 185-192.	0.9	86
72	Fluctuations in ambient water. Journal of Molecular Liquids, 2012, 176, 2-16.	2.3	86

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73	Characterization of hydrogen bond acceptor molecules at the water surface using near-edge x-ray absorption fine-structure spectroscopy and density functional theory. Journal of Physics Condensed Matter, 2002, 14, L221-L226.	0.7	85
74	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
75	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
76	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
77	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
78	Mechanism of Dissolution of Neutral Silica Surfaces:Â Including Effect of Self-Healing. Journal of Physical Chemistry A, 2001, 105, 9528-9532.	1.1	81
79	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
80	Spectroscopic characterization of microscopic hydrogen-bonding disparities in supercritical water. Journal of Chemical Physics, 2005, 123, 154503.	1.2	79
81	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
82	Adsorption of CO and NO on NiO and CoO: a comparison. Surface Science, 1996, 347, 337-345.	0.8	78
83	Calculations of X-ray Emission Spectra of Molecules and Surface Adsorbates by Means of Density Functional Theory. Journal of Physical Chemistry A, 1998, 102, 10599-10607.	1.1	77
84	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	1.0	77
85	Hydrogen abstraction from methane on a magnesia (001) surface. The Journal of Physical Chemistry, 1991, 95, 7401-7405.	2.9	76
86	On the accuracy of gradient corrected density functional methods for transition metal complexes. Journal of Chemical Physics, 1995, 102, 872-878.	1.2	74
87	Comparing ab initio computed energetics with thermal experiments in surface science: CO/MgO(001). Journal of Chemical Physics, 1996, 105, 9339-9348.	1.2	74
88	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
89	Electronic and geometric structure of the copper (Cun) cluster anions (n .ltoreq. 10). The Journal of Physical Chemistry, 1990, 94, 5471-5477.	2.9	72
90	Ground-state interpretation of x-ray emission spectroscopy on adsorbates: CO adsorbed on Cu(100). Physical Review B, 2000, 61, 16229-16240.	1.1	72

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91	Isotope effects in liquid water probed by x-ray Raman spectroscopy. Physical Review B, 2007, 76, .	1.1	72
92	Ultrafast Molecular Dissociation of Water in Ice. Physical Review Letters, 2004, 93, 148302.	2.9	71
93	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
94	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
95	Direct Evidence of Orbital Mixing between Water and Solvated Transition-Metal Ions:â€‰ An Oxygen 1s XAS and DFT Study of Aqueous Systems. Journal of Physical Chemistry A, 2003, 107, 6869-6876.	1.1	67
96	Enhanced small-angle scattering connected to the Widom line in simulations of supercooled water. Journal of Chemical Physics, 2011, 134, 214506.	1.2	67
97	The bonding in FeN2, FeCO, and Fe2N2: Model systems for sideâ€on bonding of CO and N2. Journal of Chemical Physics, 1987, 87, 2129-2137.	1.2	66
98	Surface structure of thin ice films. Chemical Physics Letters, 2004, 395, 161-165.	1.2	66
99	Structure and Electronic Properties of Ca-Doped CeO2 and Implications on Catalytic Activity:â€‰ An Experimental and Theoretical Study. Journal of Physical Chemistry B, 1999, 103, 7627-7636.	1.2	65
100	The atomic states of nickel. Theoretica Chimica Acta, 1988, 74, 479-491.	0.9	64
101	On the dissociation energy of Mg2. Journal of Chemical Physics, 1990, 92, 5377-5383.	1.2	64
102	Substituted benzenes as building blocks in near-edge X-ray absorption spectra. Chemical Physics, 1997, 222, 125-137.	0.9	64
103	A computational and experimental study on the Jahn-Teller effect in the hydrated copper (II) ion. Comparisons with hydrated nickel (II) ions in aqueous solution and solid Tutton's salts. Journal of Physics Condensed Matter, 1989, 1, 2395-2408.	0.7	63
104	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
105	Electrocatalytic Glycerol Oxidation with Concurrent Hydrogen Evolution Utilizing an Efficient MoO_x/Pt Catalyst. Small, 2021, 17, e2104288.	5.2	63
106	Experimental and theoretical characterization of the structure of defects at the pyriteFeS2(100)surface. Physical Review B, 2004, 70, .	1.1	62
107	The structure of small metal clusters. Journal of Chemical Physics, 1986, 84, 2226-2232.	1.2	61
108	Nature of the surface chemical bond inN2on Ni(100) studied by x-ray-emission spectroscopy andab initiocalculations. Physical Review B, 1998, 57, 9274-9284.	1.1	61

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109	Electronic structure effects in liquid water studied by photoelectron spectroscopy and density functional theory. Chemical Physics Letters, 2008, 460, 86-92.	1.2	61
110	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
111	Bonding of Saturated Hydrocarbons to Metal Surfaces. Physical Review Letters, 2003, 91, 046102.	2.9	60
112	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
113	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
114	Theoretical Study on the Decomposition of N2O over Alkaline Earth Metal-Oxides:Â MgOâ^'BaO. Journal of Physical Chemistry A, 2002, 106, 7868-7875.	1.1	59
115	Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics. Nature Communications, 2018, 9, 1917.	5.8	59
116	Nearâ€edge core photoabsorption in polyenes. Journal of Chemical Physics, 1995, 102, 5589-5597.	1.2	57
117	Hydrogen Dissociation on Reconstructed ZnO Surfaces. The Journal of Physical Chemistry, 1996, 100, 9054-9063.	2.9	57
118	Core-valence correlation effects in calcium hydride. Chemical Physics, 1983, 82, 355-368.	0.9	56
119	Sulfur-Metal Orbital Hybridization in Sulfur-Bearing Compounds Studied by X-ray Emission Spectroscopy. Inorganic Chemistry, 2010, 49, 6468-6473.	1.9	56
120	Correlation of hydrogen bond lengths and angles in liquid water based on Compton scattering. Journal of Chemical Physics, 2006, 125, 084504.	1.2	55
121	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
122	A theoretical study of atomic fluorine chemisorption on the Ni(100) surface. Journal of Chemical Physics, 1991, 94, 4024-4030.	1.2	52
123	Direct Experimental Measurement of Donation/Back-Donation in Unsaturated Hydrocarbon Bonding to Metals. Journal of the American Chemical Society, 2000, 122, 12310-12316.	6.6	52
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	Selective Ultrafast Probing of Transient Hot Chemisorbed and Precursor States of CO on Ru(0001). Physical Review Letters, 2013, 110, 186101.	2.9	51
126	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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127	Theoretical study of water-exchange reactions for the divalent ions of the first transition period. The Journal of Physical Chemistry, 1993, 97, 3765-3774.	2.9	50
128	The structure of mixed H2Oâ€“OH monolayer films on Ru(0001). Journal of Chemical Physics, 2008, 129, 154109.	1.2	50
129	Benzene adsorbed on Cu(110): theoretical X-ray absorption, emission and shake calculations. Surface Science, 1998, 408, 1-20.	0.8	49
130	The local structure of protonated water from x-ray absorption and density functional theory. Journal of Chemical Physics, 2006, 124, 194508.	1.2	49
131	Low O2 dissociation barrier on Pt(111) due to adsorbateâ€“adsorbate interactions. Journal of Chemical Physics, 2010, 133, 224701.	1.2	49
132	Small Al clusters. I. The effect of basis set and correlation on the geometry of small Al clusters. Journal of Chemical Physics, 1987, 87, 2198-2204.	1.2	47
133	Assembly and decomposition of building blocks to analyze polymer NEXAFS spectra. International Journal of Quantum Chemistry, 1997, 63, 749-765.	1.0	47
134	The Boson peak in supercooled water. Scientific Reports, 2013, 3, 1980.	1.6	47
135	The bonding of simple carboxylic acids on Cu(110). Journal of Chemical Physics, 2000, 112, 8146-8155.	1.2	46
136	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
137	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
138	Auger decay calculations with core-hole excited-state molecular-dynamics simulations of water. Journal of Chemical Physics, 2006, 124, 064307.	1.2	45
139	Resonant inelastic X-ray scattering of liquid water. Journal of Electron Spectroscopy and Related Phenomena, 2013, 188, 84-100.	0.8	45
140	Intra- and intermolecular effects in the Compton profile of water. Physical Review B, 2006, 73, .	1.1	44
141	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
142	Evidence for Fe²⁺ in Wurtzite Coordination: Iron Doping Stabilizes ZnO Nanoparticles. Small, 2011, 7, 2879-2886.	5.2	44
143	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
144	Probing chemical bonding in adsorbates using X-ray emission spectroscopy. Journal of Electron Spectroscopy and Related Phenomena, 2000, 110-111, 15-39.	0.8	43

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145	The computed spectrum of AlC. Journal of Chemical Physics, 1988, 89, 5747-5752.	1.2	42
146	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
147	Coreâ€“valence correlation effects using approximate operators. Journal of Chemical Physics, 1991, 94, 2968-2976.	1.2	41
148	Quantum chemical studies of the effects on silicate mineral dissolution rates by adsorption of alkali metals. Geochimica Et Cosmochimica Acta, 1997, 61, 2577-2587.	1.6	41
149	Orbital rehybridization in n-octane adsorbed on Cu(110). Journal of Chemical Physics, 2003, 118, 3782-3789.	1.2	41
150	The structural validity of various thermodynamical models of supercooled water. Journal of Chemical Physics, 2016, 145, 134507.	1.2	41
151	Theoretical spectrum of AlN. Journal of Chemical Physics, 1988, 89, 7354-7362.	1.2	40
152	Massively parallel direct SCF calculations on large metal clusters: Ni5-Ni481. Theoretica Chimica Acta, 1993, 85, 345-361.	0.9	40
153	Ab initio model potential study of pressure effects on K2NaGaF6:Cr3+. Journal of Chemical Physics, 1993, 98, 4041-4046.	1.2	40
154	XPS and XAS investigation of condensed and adsorbed n-octane on a Cu(110) surface. Journal of Electron Spectroscopy and Related Phenomena, 2003, 128, 179-191.	0.8	40
155	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
156	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
157	ContractedCI calculations of models for catalytic reactions involving transition metals. International Journal of Quantum Chemistry, 1983, 23, 855-863.	1.0	39
158	Resonant soft-x-ray emission spectroscopy of surface adsorbates:â€,â€,Theory, computations, and measurements of ethylene and benzene on Cu(110). Physical Review B, 1999, 59, 5189-5200.	1.1	39
159	The role of substrate electrons in the wetting of a metal surface. Journal of Chemical Physics, 2010, 132, 094701.	1.2	39
160	A proposal for the structure of high- and low-density fluctuations in liquid water. Journal of Chemical Physics, 2019, 151, 034508.	1.2	39
161	The effect of 3d shell back bonding on the binding of chlorine containing molecules. Journal of Chemical Physics, 1985, 83, 3538-3546.	1.2	38
162	H2O Interaction with the Polar Cu2O(100) Surface:Â A Theoretical Study. The Journal of Physical Chemistry, 1996, 100, 1874-1878.	2.9	38

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163	Ammonia adsorbed on Cu(110): An angle resolved x-ray spectroscopic and ab initio study. Journal of Chemical Physics, 1999, 110, 4880-4890.	1.2	38
164	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
165	Effective core potential calculations on small molecules containing transition metal atoms. Chemical Physics, 1982, 66, 459-464.	0.9	37
166	Theoretical investigation of the addition of molecular hydrogen to palladium and diaquapalladium ((H2O)2Pd). The Journal of Physical Chemistry, 1984, 88, 4617-4621.	2.9	37
167	Theoretical modelling of metal oxides. Influence of field strength on atomic oxygen adsorption and a simple model reaction: Oads+CO â† ' CO2. Chemical Physics Letters, 1994, 230, 456-462.	1.2	37
168	Comment on â€œFirst-principles determination of the bonding mechanism and adsorption energy for CO/MgO(001)â€•[Chem. Phys. Lett. 290 (1998) 255]. Chemical Physics Letters, 1999, 306, 202-204.	1.2	37
169	Sensitivity of x-ray absorption spectroscopy to hydrogen bond topology. Physical Review B, 2009, 80, .	1.1	37
170	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
171	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
172	Hydrogen Evolution Linked to Selective Oxidation of Glycerol over CoMoO₄â€"A Theoretically Predicted Catalyst. Advanced Energy Materials, 2022, 12, .	10.2	37
173	Theoretical electric dipole moments and dissociation energies for the ground states of GaHâ€"BrH. Journal of Chemical Physics, 1986, 85, 3130-3131.	1.2	35
174	Cu 3d covalency in chemisorption?. Journal of Chemical Physics, 1989, 90, 4613-4616.	1.2	35
175	On the character of the O2+2Aâ€‰3âˆ'u state. Journal of Chemical Physics, 1991, 94, 818-819.	1.2	34
176	The xâ€•ray excited Auger electron spectrum of NO and potential curves and photodissociation of the NO2+ ion. Journal of Chemical Physics, 1992, 96, 4884-4895.	1.2	34
177	Static exchange and quantum defect analysis of x-ray absorption spectra of carbonyl compounds. Physica Scripta, 1996, 54, 614-624.	1.2	34
178	The Bonding and Electronic Structure Changes upon Adsorption of Important Functional Groups:Â Glycine on Copper. Journal of Physical Chemistry B, 2000, 104, 11480-11483.	1.2	34
179	Physisorption-Induced C-H Bond Elongation in Methane. Physical Review Letters, 2006, 96, 146104.	2.9	34
180	Semiclassical description of nuclear dynamics in x-ray emission of water. Physical Review B, 2010, 82, .	1.1	34

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