Michael Odelius

List of Publications by Year
in descending order

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159	7,855	53794	53230
papers	citations	45 h-index	85 g-index

168	168	168	8058
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Experimental and Theoretical Core Level and Valence Band Analysis of Clean Perovskite Single Crystal Surfaces. Small, 2022, 18, e2106450.	10.0	5
2	Carbon K-edge x-ray emission spectroscopy of gas phase ethylenic molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2022, 55, 044001.	1.5	5
3	Photoinduced bond oscillations in ironpentacarbonyl give delayed synchronous bursts of carbonmonoxide release. Nature Communications, 2022, 13, 1337.	12.8	2
4	Electronic Structure Changes of an Aromatic Amine Photoacid along the FÃ¶rster Cycle. Angewandte Chemie - International Edition, 2022, 61, .	13.8	6
5	Innentitelbild: Ã„nderungen der elektronischen Struktur einer Aminoâ€PhotosÃure entlang des FÃ¶rster Zyklus (Angew. Chem. 27/2022). Angewandte Chemie, 2022, 134, .	2.0	0
6	A-site cation influence on the conduction band of lead bromide perovskites. Nature Communications, 2022, 13, .	12.8	9
7	Core-Level Binding Energy Reveals Hydrogen Bonding Configurations of Water Adsorbed on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Surfaces. Physical Review Letters, 2022, 128, 016102.	7.8	7
8	Polarization-sensitive IR-pumpâ€“x-ray-probe spectroscopy. Physical Review A, 2021, 103, .	2.5	5
9	Vibrational resonant inelastic X-ray scattering in liquid acetic acid: a ruler for molecular chain lengths. Scientific Reports, 2021, 11, 4098.	3.3	7
10	Dynamic Effects and Hydrogen Bonding in Mixed-Halide Perovskite Solar Cell Absorbers. Journal of Physical Chemistry Letters, 2021, 12, 3885-3890.	4.6	12
11	Sensitivity of Nitrogen K-Edge X-ray Absorption to Halide Substitution and Thermal Fluctuations in Methylammonium Lead-Halide Perovskites. Journal of Physical Chemistry C, 2021, 125, 8360-8368.	3.1	7
12	2p x-ray absorption spectroscopy of 3d transition metal systems. Journal of Electron Spectroscopy and Related Phenomena, 2021, 249, 147061.	1.7	44
13	Hydrogen bond effects in multimode nuclear dynamics of acetic acid observed via resonant x-ray scattering. Journal of Chemical Physics, 2021, 154, 214304.	3.0	2
14	High-resolution x-ray spectra of carbon monoxide reveal ultrafast dynamics induced by long UV pulse. New Journal of Physics, 2021, 23, 063030.	2.9	3
15	Electronic coupling between the unoccupied states of the organic and inorganic sublattices of methylammonium lead iodide: A hybrid organic-inorganic perovskite single crystal. Physical Review B, 2021, 104, .	3.2	7
16	Dynamics of resonant x-ray and Auger scattering. Reviews of Modern Physics, 2021, 93, .	45.6	48
17	Nitrogen K-Edge X-ray Absorption Spectra of Ammonium and Ammonia in Water Solution: Assessing the Performance of Polarizable Embedding Coupled Cluster Methods. Journal of Physical Chemistry Letters, 2021, 12, 8865-8871.	4.6	11
18	Photodissociation of water induced by a long UV pulse and probed by high-energy-resolution x-ray-absorption spectroscopy. Physical Review A, 2021, 104, .	2.5	5

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19	Mixedâ€Halide Double Perovskite Cs₂AgBiX₆ (X=Br, I) with Tunable Optical Properties via Anion Exchange. ChemSusChem, 2021, 14, 4507-4515.	6.8	24
20	Coupling Methylammonium and Formamidinium Cations with Halide Anions: Hybrid Orbitals, Hydrogen Bonding, and the Role of Dynamics. Journal of Physical Chemistry C, 2021, 125, 25917-25926.	3.1	4
21	Composition Related Tunability of â€œGreenâ€•Core/Shell Quantum Dots for Photovoltaic Applications from First Principles. Journal of Physical Chemistry C, 2021, 125, 27046-27057.	3.1	8
22	Ultrafast nonadiabatic dynamics probed by nitrogen K-edge absorption spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 2667-2676.	2.8	34
23	Tuning the Bandgap in Silver Bismuth Iodide Materials by Partly Substituting Bismuth with Antimony for Improved Solar Cell Performance. ACS Applied Energy Materials, 2020, 3, 7372-7382.	5.1	30
24	Field-dependent paramagnetic relaxation enhancement in solutions of Ni(II): What happens above the NMR proton frequency of 1â€¯GHz?. Journal of Magnetic Resonance, 2020, 314, 106737.	2.1	4
25	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
26	Setting the stage for theoretical x-ray spectra of the H2S molecule with multi-configurational quantum chemical calculations of the energy landscape. Journal of Chemical Physics, 2020, 152, 094305.	3.0	4
27	Ultrafast dynamics of photo-excited 2-thiopyridone: Theoretical insights into triplet state population and proton transfer pathways. Structural Dynamics, 2020, 7, 024101.	2.3	5
28	Core-hole localization and ultra-fast dissociation in SF6. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 185101.	1.5	5
29	Deciphering Photoacidity by Following Electronic Charge Distribution Changes along the Photoacid FÃ¶rster Cycle with Time-Resolved Nitrogen K-Edge X-Ray Absorption Spectroscopy. , 2020, , .		0
30	Bandgap Tuning of Silver Bismuth Iodide via Controllable Bromide Substitution for Improved Photovoltaic Performance. ACS Applied Energy Materials, 2019, 2, 5356-5362.	5.1	23
31	A combined multi-reference pump-probe simulation method with application to XUV signatures of ultrafast methyl iodide photodissociation. Journal of Chemical Physics, 2019, 151, 124106.	3.0	12
32	Nuclear dynamics in resonant inelastic X-ray scattering and X-ray absorption of methanol. Journal of Chemical Physics, 2019, 150, 234301.	3.0	26
33	Interdependent Electronic Structure, Protonation, and Solvatization of Aqueous 2-Thiopyridone. Journal of Physical Chemistry B, 2019, 123, 5555-5567.	2.6	3
34	Probing hydrogen bond strength in liquid water by resonant inelastic X-ray scattering. Nature Communications, 2019, 10, 1013.	12.8	53
35	Ab initio simulations of complementary K-edges and solvatization effects for detection of proton transfer in aqueous 2-thiopyridone. Journal of Chemical Physics, 2019, 151, 114117.	3.0	8
36	T₁ Population as the Driver of Excitedâ€State Protonâ€Transfer in 2â€Thiopyridone. Chemistry - A European Journal, 2019, 25, 1733-1739.	3.3	14

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37	Encapsulation of small fullerenes into nitrogenated holey nanotubes: a density functional theory study. Molecular Physics, 2019, 117, 776-783.	1.7	2
38	Fingerprints of electronic, spin and structural dynamics from resonant inelastic soft X-ray scattering in transient photo-chemical species. Physical Chemistry Chemical Physics, 2018, 20, 7243-7253.	2.8	25
39	Zero-field splitting in the isoelectronic aqueous Gd(III) and Eu(II) complexes from a first principles analysis. Chemical Physics, 2018, 503, 56-64.	1.9	2
40	Structural and electronic properties of nitrogenated holey nanotubes: A density functional theory study. Diamond and Related Materials, 2018, 82, 96-101.	3.9	12
41	Ultrafast dissociation features in RIXS spectra of the water molecule. Physical Chemistry Chemical Physics, 2018, 20, 14384-14397.	2.8	24
42	Quantum dots as an electron or hole acceptor: on some factors affecting charge transfer in dyeâ€“quantum dot composites. Physical Chemistry Chemical Physics, 2018, 20, 27036-27048.	2.8	11
43	Selective negative-ion formation from core-valence doubly excited states of the water molecule. Physical Review A, 2018, 98, .	2.5	0
44	One-dimensional cuts through multidimensional potential-energy surfaces by tunable x rays. Physical Review A, 2018, 97, .	2.5	13
45	Time-resolved electron spectroscopy for chemical analysis of photodissociation: Photoelectron spectra of Fe(CO)5, Fe(CO)4, and Fe(CO)3. Journal of Chemical Physics, 2018, 149, 044307.	3.0	20
46	Soft X-ray Spectroscopy of the Amine Group: Hydrogen Bond Motifs in Alkylamine/Alkylammonium Acidâ€“Base Pairs. Journal of Physical Chemistry B, 2018, 122, 7737-7746.	2.6	22
47	Photoelectron shake-ups as a probe of molecular symmetry: 4d XPS analysis of I₃^{â^’} in solution. Physical Chemistry Chemical Physics, 2018, 20, 19916-19921.	2.8	7
48	Anomalous polarization dependence in vibrationally resolved resonant inelastic x-ray scattering of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math>. Physical Review A, 2018, 98, .	2.5	5
49	Disentangling Transient Charge Density and Metalâ€“Ligand Covalency in Photoexcited Ferricyanide with Femtosecond Resonant Inelastic Soft X-ray Scattering. Journal of Physical Chemistry Letters, 2018, 9, 3538-3543.	4.6	42
50	Selective gating to vibrational modes through resonant X-ray scattering. Nature Communications, 2017, 8, 14165.	12.8	50
51	Quantifying covalent interactions with resonant inelastic soft X-ray scattering: Case study of Ni2+ aqua complex. Chemical Physics Letters, 2017, 669, 196-201.	2.6	4
52	Communication: Direct evidence for sequential dissociation of gas-phase Fe(CO)5 via a singlet pathway upon excitation at 266 nm. Journal of Chemical Physics, 2017, 146, 211103.	3.0	14
53	Ultrafast Independent Nâ^’H and Nâ^’C Bond Deformation Investigated with Resonant Inelastic Xâ€Ray Scattering. Angewandte Chemie - International Edition, 2017, 56, 6088-6092.	13.8	36
54	A study of the water molecule using frequency control over nuclear dynamics in resonant X-ray scattering. Physical Chemistry Chemical Physics, 2017, 19, 19573-19589.	2.8	32

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55	Infrared-pumpâ€“x-ray-probe spectroscopy of vibrationally excited molecules. Physical Review A, 2017, 95, .	2.5	14
56	Gradual collapse of nuclear wave functions regulated by frequency tuned X-ray scattering. Scientific Reports, 2017, 7, 43891.	3.3	15
57	Untersuchung unabhÃngiger Nâ€Hâ€•und Nâ€Câ€Bindungsverformungen auf ultrakurzen Zeitskalen mit resonanter inelastischer RÃ¶ntgenstreuung. Angewandte Chemie, 2017, 129, 6184-6188.	2.0	3
58	InnenrÃ¼cktitelbild: Untersuchung unabhÃngiger Nâ€Hâ€•und Nâ€Câ€Bindungsverformungen auf ultrakurzen Zeitskalen mit resonanter inelastischer RÃ¶ntgenstreuung (Angew. Chem. 22/2017). Angewandte Chemie, 2017, 129, 6441-6441.	2.0	0
59	Aqueous Solvation of Ammonia and Ammonium: Probing Hydrogen Bond Motifs with FT-IR and Soft X-ray Spectroscopy. Journal of the American Chemical Society, 2017, 139, 12773-12783.	13.7	65
60	Valence Level Character in a Mixed Perovskite Material and Determination of the Valence Band Maximum from Photoelectron Spectroscopy: Variation with Photon Energy. Journal of Physical Chemistry C, 2017, 121, 26655-26666.	3.1	98
61	Theoretical simulations of oxygen <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>K</mml:mi></mml:math> -edge resonant inelastic x-ray scattering of kaolinite. Physical Review B, 2017, 95, .	3.2	11
62	An ab initio CASSCF study of zero field splitting fluctuations in the octet ground state of aqueous [Gd(iii)(HPDO3A)(H2O)]. Journal of Chemical Physics, 2017, 147, 244306.	3.0	10
63	Cost and sensitivity of restricted activeâ€space calculations of metal Lâ€edge Xâ€ray absorption spectra. Journal of Computational Chemistry, 2016, 37, 477-486.	3.3	59
64	Elucidating the Mechanism of Zn²⁺ Sensing by a Bipyridine Probe Based on Two-Photon Absorption. Journal of Physical Chemistry B, 2016, 120, 9067-9075.	2.6	13
65	Viewing the Valence Electronic Structure of Ferric and Ferrous Hexacyanide in Solution from the Fe and Cyanide Perspectives. Journal of Physical Chemistry B, 2016, 120, 7182-7194.	2.6	76
66	Solvation structure around ruthenium(II) tris(bipyridine) in lithium halide solutions. Structural Dynamics, 2016, 3, 023607.	2.3	9
67	Anti-Stokes resonant x-ray Raman scattering for atom specific and excited state selective dynamics. New Journal of Physics, 2016, 18, 103011.	2.9	14
68	Identification of the dominant photochemical pathways and mechanistic insights to the ultrafast ligand exchange of Fe(CO)5 to Fe(CO)4EtOH. Structural Dynamics, 2016, 3, 043204.	2.3	48
69	In-Situ Probing of H2O Effects on a Ru-Complex Adsorbed on TiO2 Using Ambient Pressure Photoelectron Spectroscopy. Topics in Catalysis, 2016, 59, 583-590.	2.8	7
70	Geometrical and energetical structural changes in organic dyes for dye-sensitized solar cells probed using photoelectron spectroscopy and DFT. Physical Chemistry Chemical Physics, 2016, 18, 252-260.	2.8	28
71	Ionization and photofragmentation of Ru3(CO)12 and Os3(CO)12. Journal of Chemical Physics, 2015, 143, 154305.	3.0	8
72	Probing hydrogen bonding orbitals: resonant inelastic soft X-ray scattering of aqueous NH₃. Physical Chemistry Chemical Physics, 2015, 17, 27145-27153.	2.8	49

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73	Solventâ€Dependent Structure of the I₃^{â^'} Ion Derived from Photoelectron Spectroscopy and Ab Initio Molecular Dynamics Simulations. Chemistry - A European Journal, 2015, 21, 4049-4055.	3.3	23
74	Electronic Structure of CH₃NH₃PbX₃ Perovskites: Dependence on the Halide Moiety. Journal of Physical Chemistry C, 2015, 119, 1818-1825.	3.1	127
75	Correlating Infrared and X-ray Absorption Energies for Molecular-Level Insight into Hydrogen Bond Making and Breaking in Solution. Journal of Physical Chemistry B, 2015, 119, 8115-8124.	2.6	11
76	Orbital-specific mapping of the ligand exchange dynamics of Fe(CO)5 in solution. Nature, 2015, 520, 78-81.	27.8	247
77	Density functional investigation and some optical experiments on dye-sensitized quantum dots. Physical Chemistry Chemical Physics, 2015, 17, 28683-28696.	2.8	21
78	Systematic theoretical investigation of the zero-field splitting in Gd(III) complexes: Wave function and density functional approaches. Journal of Chemical Physics, 2015, 142, 034304.	3.0	16
79	First principles DFT study of dye-sensitized CdS quantum dots. AIP Conference Proceedings, 2014, , .	0.4	1
80	Comment on â€œState-Dependent Electron Delocalization Dynamics at the Solute-Solvent Interface: Soft-X-ray Absorption Spectroscopy and Ab Initio Calculationsâ€• Physical Review Letters, 2014, 112, 129302.	7.8	5
81	Restricted active space calculations of L-edge X-ray absorption spectra: From molecular orbitals to multiplet states. Journal of Chemical Physics, 2014, 141, 124116.	3.0	109
82	Electronic Structure of TiO₂/CH₃NH₃PbI₃ Perovskite Solar Cell Interfaces. Journal of Physical Chemistry Letters, 2014, 5, 648-653.	4.6	432
83	Spectroscopy and picosecond dynamics of aqueous NO2. Journal of Chemical Physics, 2014, 141, 064310.	3.0	3
84	Solvent Dependence of the Electronic Structure of Iâ€“ and I3â€“. Journal of Physical Chemistry B, 2014, 118, 3164-3174.	2.6	16
85	Hydration Dynamics of Aqueous Nitrate. Journal of Physical Chemistry B, 2013, 117, 3376-3388.	2.6	74
86	From Ligand Fields to Molecular Orbitals: Probing the Local Valence Electronic Structure of Ni²⁺ in Aqueous Solution with Resonant Inelastic X-ray Scattering. Journal of Physical Chemistry B, 2013, 117, 16512-16521.	2.6	36
87	Collective hydrogen-bond dynamics dictates the electronic structure of aqueous I3â^'. Physical Chemistry Chemical Physics, 2013, 15, 20189.	2.8	31
88	Zero-field splitting in nickel(II) complexes: A comparison of DFT and multi-configurational wavefunction calculations. Journal of Chemical Physics, 2013, 138, 064304.	3.0	59
89	Coherent wave packet dynamics in photo-excited NaI. EPJ Web of Conferences, 2013, 41, 02027.	0.3	1
90	The rotation of NO3â^'as a probe of molecular ion - water interactions. EPJ Web of Conferences, 2013, 41, 06002.	0.3	0

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91	Dissecting Local Atomic and Intermolecular Interactions of Transition-Metal Ions in Solution with Selective X-ray Spectroscopy. Journal of Physical Chemistry Letters, 2012, 3, 3448-3453.	4.6	59
92	Ab Initio Calculations of X-ray Spectra: Atomic Multiplet and Molecular Orbital Effects in a Multiconfigurational SCF Approach to the L-Edge Spectra of Transition Metal Complexes. Journal of Physical Chemistry Letters, 2012, 3, 3565-3570.	4.6	168
93	Ultrafast Proton Dynamics in Aqueous Amino Acid Solutions Studied by Resonant Inelastic Soft X-ray Scattering. Journal of Physical Chemistry B, 2012, 116, 13757-13764.	2.6	37
94	Cations Strongly Reduce Electron-Hopping Rates in Aqueous Solutions. Journal of the American Chemical Society, 2011, 133, 13489-13495.	13.7	7
95	Mapping the frontier electronic structures of triphenylamine based organic dyes at TiO₂interfaces. Physical Chemistry Chemical Physics, 2011, 13, 3534-3546.	2.8	10
96	H-bond switching and ligand exchange dynamics in aqueous ionic solution. Chemical Physics Letters, 2011, 504, 1-6.	2.6	38
97	Intramolecular soft modes and intermolecular interactions in liquid acetone. Physical Review B, 2011, 84, .	3.2	44
98	Large Angular Jump Mechanism Observed for Hydrogen Bond Exchange in Aqueous Perchlorate Solution. Science, 2010, 328, 1003-1005.	12.6	187
99	Photoemission core-level shifts reveal the thiolate-Au(111) interface. Physical Review B, 2010, 82, .	3.2	20
100	Spinâˆ’Orbit Coupling and Metalâˆ’Ligand Interactions in Fe(II), Ru(II), and Os(II) Complexes. Journal of Physical Chemistry C, 2010, 114, 10314-10322.	3.1	44
101	Cooperativity in Surface Bonding and Hydrogen Bonding of Water and Hydroxyl at Metal Surfaces. Journal of Physical Chemistry C, 2010, 114, 10240-10248.	3.1	51
102	Electronic and molecular structures of organic dye/TiO2 interfaces for solar cell applications: a core level photoelectron spectroscopy study. Physical Chemistry Chemical Physics, 2010, 12, 1507.	2.8	56
103	Molecular dynamics simulations of fine structure in oxygen<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>K</mml:mi></mml:math>-edge x-ray emission spectra of liquid water and ice. Physical Review B, 2009, 79, .	3.2	82
104	Real-Time Evolution of the Valence Electronic Structure in a Dissociating Molecule. Physical Review Letters, 2009, 103, 013001.	7.8	58
105	The structure of the Au(111)/methylthiolate interface: New insights from near-edge x-ray absorption spectroscopy and x-ray standing waves. Journal of Chemical Physics, 2009, 130, 124708.	3.0	30
106	Solvent dependent structural perturbations of chemical reaction intermediates visualized by time-resolved x-ray diffraction. Journal of Chemical Physics, 2009, 130, 154502.	3.0	38
107	Information Content in O[1s] K-edge X-ray Emission Spectroscopy of Liquid Water. Journal of Physical Chemistry A, 2009, 113, 8176-8181.	2.5	56
108	Ultrafast Dynamics of Hydrogen Bond Exchange in Aqueous Ionic Solutions. Journal of Physical Chemistry B, 2009, 113, 7825-7835.	2.6	119

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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.	2.6	61
110	Valence electronic structure of ruthenium based complexes probed by photoelectron spectroscopy at high kinetic energy (HIKE) and modeled by DFT calculations. Chemical Physics Letters, 2008, 464, 192-197.	2.6	16
111	Diffraction and IR/Raman data do not prove tetrahedral water. Journal of Chemical Physics, 2008, 129, 084502.	3.0	94
112	Interface electronic states and molecular structure of a triarylamine based hole conductor on rutile TiO2(110). Journal of Chemical Physics, 2008, 128, 184709.	3.0	20
113	Isotope quantum effects in the electron momentum density of water. Journal of Chemical Physics, 2007, 126, 154508.	3.0	25
114	Frontier electronic structures of Ru(tcterpy)(NCS)3 and Ru(dcbpy)2(NCS)2: A photoelectron spectroscopy study. Journal of Chemical Physics, 2007, 126, 244303.	3.0	25
115	Isotope effects in liquid water probed by x-ray Raman spectroscopy. Physical Review B, 2007, 76, .	3.2	72
116	Dynamical core-hole screening in the x-ray absorption spectra of hydrogenated carbon nanotubes and graphene. Physical Review B, 2007, 76, .	3.2	19
117	Probing the Electron Delocalization in Liquid Water and Ice at Attosecond Time Scales. Physical Review Letters, 2007, 99, 217406.	7.8	117
118	Electronic and Molecular Surface Structure of a Polyeneâ^'Diphenylaniline Dye Adsorbed from Solution onto Nanoporous TiO2. Journal of Physical Chemistry C, 2007, 111, 8580-8586.	3.1	61
119	Utility of High Performance Computing Facilities for the Calculation of the Theoretical X-ray Absorption Spectra of Solids. , 2007, , .		0
120	Theoretical X-ray absorption investigation of the uniaxial compression of hexagonal graphite. Canadian Journal of Chemistry, 2007, 85, 837-842.	1.1	1
121	Structure and Bonding of the Waterâ^'Hydroxyl Mixed Phase on Pt(111). Journal of Physical Chemistry C, 2007, 111, 15003-15012.	3.1	117
122	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.	3.0	60
123	The local structure of protonated water from x-ray absorption and density functional theory. Journal of Chemical Physics, 2006, 124, 194508.	3.0	49
124	X-ray absorption spectrum of liquid water from molecular dynamics simulations: Asymmetric model. Physical Review B, 2006, 73, .	3.2	88
125	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.	3.0	21
126	Auger decay calculations with core-hole excited-state molecular-dynamics simulations of water. Journal of Chemical Physics, 2006, 124, 064307.	3.0	45

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127	Comment on "Energetics of Hydrogen Bond Network Rearrangements in Liquid Water". Science, 2005, 308, 793a-793a.	12.6	90
128	Ultrafast Core-Hole-Induced Dynamics in Water Probed by X-Ray Emission Spectroscopy. Physical Review Letters, 2005, 94, 227401.	7.8	117
129	Half or full core hole in density functional theory X-ray absorption spectrum calculations of water?. Physical Chemistry Chemical Physics, 2005, 7, 2854.	2.8	96
130	Photodissociation of diiodomethane in acetonitrile solution and fragment recombination into iso-diiodomethane studied with ab initio molecular dynamics simulations. Journal of Chemical Physics, 2004, 121, 2208-2214.	3.0	36
131	Ultrafast Molecular Dissociation of Water in Ice. Physical Review Letters, 2004, 93, 148302.	7.8	71
132	X-ray absorption spectra of water within a plane-wave Car-Parrinello molecular dynamics framework. Journal of Chemical Physics, 2004, 121, 10065-10075.	3.0	45
133	Surface structure of thin ice films. Chemical Physics Letters, 2004, 395, 161-165.	2.6	66
134	s-Tetrazine in Aqueous Solution:Â A Density Functional Study of Hydrogen Bonding and Electronic Excitations. Journal of Physical Chemistry A, 2004, 108, 2044-2052.	2.5	33
135	The Structure of the First Coordination Shell in Liquid Water. Science, 2004, 304, 995-999.	12.6	1,287
136	Bi-isonicotinic acid on rutile (110): calculated molecular and electronic structure. Surface Science, 2003, 529, 47-58.	1.9	35
137	Excited state geometries within time-dependent and restricted open-shell density functional theories. Computational and Theoretical Chemistry, 2003, 630, 163-175.	1.5	21
138	Hydrogen bonding between adsorbed deprotonated glycine molecules on Cu(110). Journal of Chemical Physics, 2003, 119, 12577-12585.	3.0	103
139	Experimental evidence for sub-3-fs charge transfer from an aromatic adsorbate to a semiconductor. Nature, 2002, 418, 620-623.	27.8	346
140	Electronic structure effects from hydrogen bonding in the liquid phase and in chemisorption: an integrated theory and experimental effort. Journal of Synchrotron Radiation, 2001, 8, 136-140.	2.4	7
141	Mixed Molecular and Dissociative Water Adsorption on MgO[100]. Physical Review Letters, 1999, 82, 3919-3922.	7.8	153
142	Combined MD simulation - NMR relaxation studies of molecular motion and intermolecular interactions. Theoretical and Computational Chemistry, 1999, 7, 281-324.	0.4	7
143	Two Dimensional Ice Adsorbed on Mica Surface. Physical Review Letters, 1997, 78, 2855-2858.	7.8	274
144	Quadrupolar Relaxation of21Ne,83Kr, and131Xe Dissolved in Acetonitrile. A Molecular Dynamics Study. Journal of Physical Chemistry A, 1997, 101, 9537-9544.	2.5	8

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145	Spin dynamics under the Hamiltonian varying with time in discrete steps: Molecular dynamicsâ€based simulation of electron and nuclear spin relaxation in aqueous nickel(II). Journal of Chemical Physics, 1996, 104, 3181-3188.	3.0	40
146	A Model Glycosidic Linkage: An ab Initio Geometry Optimization Study of 2-Cyclohexoxytetrahydropyran. The Journal of Physical Chemistry, 1995, 99, 12686-12692.	2.9	12
147	Molecular dynamics simulation of nuclear spin relaxation of 7Li+ in water. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 215.	1.7	10
148	Molecular dynamics simulation of the zeroâ€field splitting fluctuations in aqueous Ni(II). Journal of Chemical Physics, 1995, 103, 1800-1811.	3.0	55
149	Simple non-empirical calculations of the zero-field splitting in bis(aquo) bis(malonato) nickel(II). Theoretica Chimica Acta, 1994, 87, 307-312.	0.8	6
150	Molecular dynamics simulations of quadrupolar relaxation of131Xe in carbon tetrachloride, acetonitrile, and methanol. Molecular Physics, 1994, 82, 487-501.	1.7	12
151	Molecular Dynamics Simulations of Quadrupolar Relaxation of 131Xe in Methanol. An Ellipsoidal Picture of the Electric Field Gradient Tensor. The Journal of Physical Chemistry, 1994, 98, 12108-12116.	2.9	16
152	Molecular Dynamics Simulation of Sucrose in Aqueous and Dimethyl Sulfoxide Solution.. Acta Chemica Scandinavica, 1994, 48, 792-799.	0.7	15
153	Intermolecular Dipole-Dipole Relaxation. A Molecular Dynamics Simulation. Journal of Magnetic Resonance Series A, 1993, 105, 289-294.	1.6	37
154	Magnetic relaxation of xenonâ€131 dissolved in benzene. A study by molecular dynamics and Monte Carlo simulations. Journal of Chemical Physics, 1993, 98, 1566-1578.	3.0	29
155	Normal coordinate analysis of the zero-field splitting in octahedral NiF4-6. Molecular Physics, 1993, 78, 1259-1266.	1.7	7
156	Simple non-empirical calculations of the zero field splitting in transition metal systems. Molecular Physics, 1991, 74, 1299-1314.	1.7	16
157	Simple nonempirical calculations of the zero-field splitting in transition metal systems: I. The Ni(II)-Water complexes. International Journal of Quantum Chemistry, 1990, 38, 295-309.	2.0	14
158	Electronic Structure Changes of an Aromatic Amine Photoacid along the FÃ¶rster Cycle. Angewandte Chemie, 0, , .	2.0	0
159	Core level and valence band analysis of in-situ cleaved perovskite single crystals. , 0, , .		0