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	The Structure of the First Coordination Shell in Liquid Water. Science, 2004, 304, 995-999.	12.6	1,287
2	Electronic Structure of TiO₂/CH₃NH₃PbI₃ Perovskite Solar Cell Interfaces. Journal of Physical Chemistry Letters, 2014, 5, 648-653.	4.6	432
3	Experimental evidence for sub-3-fs charge transfer from an aromatic adsorbate to a semiconductor. Nature, 2002, 418, 620-623.	27.8	346
4	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
5	Two Dimensional Ice Adsorbed on Mica Surface. Physical Review Letters, 1997, 78, 2855-2858.	7.8	274
6	Orbital-specific mapping of the ligand exchange dynamics of Fe(CO)5 in solution. Nature, 2015, 520, 78-81.	27.8	247
7	Large Angular Jump Mechanism Observed for Hydrogen Bond Exchange in Aqueous Perchlorate Solution. Science, 2010, 328, 1003-1005.	12.6	187
8	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
9	Mixed Molecular and Dissociative Water Adsorption on MgO[100]. Physical Review Letters, 1999, 82, 3919-3922.	7.8	153
10	Electronic Structure of CH₃NH₃PbX₃ Perovskites: Dependence on the Halide Moiety. Journal of Physical Chemistry C, 2015, 119, 1818-1825.	3.1	127
11	Ultrafast Dynamics of Hydrogen Bond Exchange in Aqueous Ionic Solutions. Journal of Physical Chemistry B, 2009, 113, 7825-7835.	2.6	119
12	Ultrafast Core-Hole-Induced Dynamics in Water Probed by X-Ray Emission Spectroscopy. Physical Review Letters, 2005, 94, 227401.	7.8	117
13	Probing the Electron Delocalization in Liquid Water and Ice at Attosecond Time Scales. Physical Review Letters, 2007, 99, 217406.	7.8	117
14	Structure and Bonding of the Waterâ^'Hydroxyl Mixed Phase on Pt(111). Journal of Physical Chemistry C, 2007, 111, 15003-15012.	3.1	117
15	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
16	Hydrogen bonding between adsorbed deprotonated glycine molecules on Cu(110). Journal of Chemical Physics, 2003, 119, 12577-12585.	3.0	103
17	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
18	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

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19	Diffraction and IR/Raman data do not prove tetrahedral water. Journal of Chemical Physics, 2008, 129, 084502.	3.0	94
20	Comment on "Energetics of Hydrogen Bond Network Rearrangements in Liquid Water". Science, 2005, 308, 793a-793a.	12.6	90
21	X-ray absorption spectrum of liquid water from molecular dynamics simulations: Asymmetric model. Physical Review B, 2006, 73, .	3.2	88
22	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
23	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
24	Hydration Dynamics of Aqueous Nitrate. Journal of Physical Chemistry B, 2013, 117, 3376-3388.	2.6	74
25	Isotope effects in liquid water probed by x-ray Raman spectroscopy. Physical Review B, 2007, 76, .	3.2	72
26	Ultrafast Molecular Dissociation of Water in Ice. Physical Review Letters, 2004, 93, 148302.	7.8	71
27	Surface structure of thin ice films. Chemical Physics Letters, 2004, 395, 161-165.	2.6	66
28	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
29	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
30	Electronic structure effects in liquid water studied by photoelectron spectroscopy and density functional theory. Chemical Physics Letters, 2008, 460, 86-92.	2.6	61
31	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
32	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
33	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
34	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
35	Real-Time Evolution of the Valence Electronic Structure in a Dissociating Molecule. Physical Review Letters, 2009, 103, 013001.	7.8	58
36	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

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37	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
38	Molecular dynamics simulation of the zeroâ€field splitting fluctuations in aqueous Ni(II). Journal of Chemical Physics, 1995, 103, 1800-1811.	3.0	55
39	Probing hydrogen bond strength in liquid water by resonant inelastic X-ray scattering. Nature Communications, 2019, 10, 1013.	12.8	53
40	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
41	Selective gating to vibrational modes through resonant X-ray scattering. Nature Communications, 2017, 8, 14165.	12.8	50
42	The local structure of protonated water from x-ray absorption and density functional theory. Journal of Chemical Physics, 2006, 124, 194508.	3.0	49
43	Probing hydrogen bonding orbitals: resonant inelastic soft X-ray scattering of aqueous NH₃. Physical Chemistry Chemical Physics, 2015, 17, 27145-27153.	2.8	49
44	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
45	Dynamics of resonant x-ray and Auger scattering. Reviews of Modern Physics, 2021, 93, .	45.6	48
46	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
47	Auger decay calculations with core-hole excited-state molecular-dynamics simulations of water. Journal of Chemical Physics, 2006, 124, 064307.	3.0	45
48	Spinâ^'Orbit Coupling and Metalâ^'Ligand Interactions in Fe(II), Ru(II), and Os(II) Complexes. Journal of Physical Chemistry C, 2010, 114, 10314-10322.	3.1	44
49	Intramolecular soft modes and intermolecular interactions in liquid acetone. Physical Review B, 2011, 84, .	3.2	44
50	2p x-ray absorption spectroscopy of 3d transition metal systems. Journal of Electron Spectroscopy and Related Phenomena, 2021, 249, 147061.	1.7	44
51	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
52	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
53	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
54	H-bond switching and ligand exchange dynamics in aqueous ionic solution. Chemical Physics Letters, 2011, 504, 1-6.	2.6	38

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55	Intermolecular Dipole-Dipole Relaxation. A Molecular Dynamics Simulation. Journal of Magnetic Resonance Series A, 1993, 105, 289-294.	1.6	37
56	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
57	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
58	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
59	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
60	Bi-isonicotinic acid on rutile (110): calculated molecular and electronic structure. Surface Science, 2003, 529, 47-58.	1.9	35
61	Ultrafast nonadiabatic dynamics probed by nitrogen K-edge absorption spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 2667-2676.	2.8	34
62	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
63	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
64	Collective hydrogen-bond dynamics dictates the electronic structure of aqueous I3â^'. Physical Chemistry Chemical Physics, 2013, 15, 20189.	2.8	31
65	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
66	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
67	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
68	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
69	Nuclear dynamics in resonant inelastic X-ray scattering and X-ray absorption of methanol. Journal of Chemical Physics, 2019, 150, 234301.	3.0	26
70	Isotope quantum effects in the electron momentum density of water. Journal of Chemical Physics, 2007, 126, 154508.	3.0	25
71	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
72	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

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73	Ultrafast dissociation features in RIXS spectra of the water molecule. Physical Chemistry Chemical Physics, 2018, 20, 14384-14397.	2.8	24
74	Mixedâ€Halide Double Perovskite Cs₂AgBiX₆ (X=Br, I) with Tunable Optical Properties via Anion Exchange. ChemSusChem, 2021, 14, 4507-4515.	6.8	24
75	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
76	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
77	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
78	Excited state geometries within time-dependent and restricted open-shell density functional theories. Computational and Theoretical Chemistry, 2003, 630, 163-175.	1.5	21
79	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
80	Density functional investigation and some optical experiments on dye-sensitized quantum dots. Physical Chemistry Chemical Physics, 2015, 17, 28683-28696.	2.8	21
81	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
82	Photoemission core-level shifts reveal the thiolate-Au(111) interface. Physical Review B, 2010, 82, .	3.2	20
83	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
84	Dynamical core-hole screening in the x-ray absorption spectra of hydrogenated carbon nanotubes and graphene. Physical Review B, 2007, 76, .	3.2	19
85	Simple non-empirical calculations of the zero field splitting in transition metal systems. Molecular Physics, 1991, 74, 1299-1314.	1.7	16
86	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
87	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
88	Solvent Dependence of the Electronic Structure of Iâ€“ and I3â€“. Journal of Physical Chemistry B, 2014, 118, 3164-3174.	2.6	16
89	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
90	Gradual collapse of nuclear wave functions regulated by frequency tuned X-ray scattering. Scientific Reports, 2017, 7, 43891.	3.3	15

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91	Molecular Dynamics Simulation of Sucrose in Aqueous and Dimethyl Sulfoxide Solution.. Acta Chemica Scandinavica, 1994, 48, 792-799.	0.7	15
92	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
93	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
94	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
95	Infrared-pumpâ€“x-ray-probe spectroscopy of vibrationally excited molecules. Physical Review A, 2017, 95, .	2.5	14
96	T₁ Population as the Driver of Excitedâ€State Protonâ€Transfer in 2â€Thiopyridone. Chemistry - A European Journal, 2019, 25, 1733-1739.	3.3	14
97	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
98	One-dimensional cuts through multidimensional potential-energy surfaces by tunable x rays. Physical Review A, 2018, 97, .	2.5	13
99	Molecular dynamics simulations of quadrupolar relaxation of131Xe in carbon tetrachloride, acetonitrile, and methanol. Molecular Physics, 1994, 82, 487-501.	1.7	12
100	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
101	Structural and electronic properties of nitrogenated holey nanotubes: A density functional theory study. Diamond and Related Materials, 2018, 82, 96-101.	3.9	12
102	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
103	Dynamic Effects and Hydrogen Bonding in Mixed-Halide Perovskite Solar Cell Absorbers. Journal of Physical Chemistry Letters, 2021, 12, 3885-3890.	4.6	12
104	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
105	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
106	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
107	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
108	Molecular dynamics simulation of nuclear spin relaxation of 7Li+ in water. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 215.	1.7	10

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109	Mapping the frontier electronic structures of triphenylamine based organic dyes at TiO₂interfaces. Physical Chemistry Chemical Physics, 2011, 13, 3534-3546.	2.8	10
110	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
111	Solvation structure around ruthenium(II) tris(bipyridine) in lithium halide solutions. Structural Dynamics, 2016, 3, 023607.	2.3	9
112	A-site cation influence on the conduction band of lead bromide perovskites. Nature Communications, 2022, 13, .	12.8	9
113	Quadrupolar Relaxation of21Ne,83Kr, and131Xe Dissolved in Acetonitrile. A Molecular Dynamics Study. Journal of Physical Chemistry A, 1997, 101, 9537-9544.	2.5	8
114	Ionization and photofragmentation of Ru3(CO)12 and Os3(CO)12. Journal of Chemical Physics, 2015, 143, 154305.	3.0	8
115	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
116	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
117	Normal coordinate analysis of the zero-field splitting in octahedral NiF4-6. Molecular Physics, 1993, 78, 1259-1266.	1.7	7
118	Combined MD simulation - NMR relaxation studies of molecular motion and intermolecular interactions. Theoretical and Computational Chemistry, 1999, 7, 281-324.	0.4	7
119	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
120	Cations Strongly Reduce Electron-Hopping Rates in Aqueous Solutions. Journal of the American Chemical Society, 2011, 133, 13489-13495.	13.7	7
121	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
122	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
123	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:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 172 Td (stretchy="false">)</mml:mo></mml:mrow></mml:math> 016102.	2.8	7
124	Vibrational resonant inelastic X-ray scattering in liquid acetic acid: a ruler for molecular chain lengths. Scientific Reports, 2021, 11, 4098.	3.3	7
125	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
126	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

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127	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
128	Electronic Structure Changes of an Aromatic Amine Photoacid along the FÃ¶rster Cycle. Angewandte Chemie - International Edition, 2022, 61, .	13.8	6
129	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
130	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
131	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
132	Polarization-sensitive IR-pumpâ€“x-ray-probe spectroscopy. Physical Review A, 2021, 103, .	2.5	5
133	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
134	Core-hole localization and ultra-fast dissociation in SF6. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 185101.	1.5	5
135	Experimental and Theoretical Core Level and Valence Band Analysis of Clean Perovskite Single Crystal Surfaces. Small, 2022, 18, e2106450.	10.0	5
136	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
137	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
138	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
139	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
140	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
141	Spectroscopy and picosecond dynamics of aqueous NO2. Journal of Chemical Physics, 2014, 141, 064310.	3.0	3
142	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
143	Interdependent Electronic Structure, Protonation, and Solvatization of Aqueous 2-Thiopyridone. Journal of Physical Chemistry B, 2019, 123, 5555-5567.	2.6	3
144	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

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145	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
146	Encapsulation of small fullerenes into nitrogenated holey nanotubes: a density functional theory study. Molecular Physics, 2019, 117, 776-783.	1.7	2
147	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
148	Photoinduced bond oscillations in ironpentacarbonyl give delayed synchronous bursts of carbonmonoxide release. Nature Communications, 2022, 13, 1337.	12.8	2
149	Theoretical X-ray absorption investigation of the uniaxial compression of hexagonal graphite. Canadian Journal of Chemistry, 2007, 85, 837-842.	1.1	1
150	Coherent wave packet dynamics in photo-excited NaI. EPJ Web of Conferences, 2013, 41, 02027.	0.3	1
151	First principles DFT study of dye-sensitized CdS quantum dots. AIP Conference Proceedings, 2014, , .	0.4	1
152	Utility of High Performance Computing Facilities for the Calculation of the Theoretical X-ray Absorption Spectra of Solids. , 2007, , .		0
153	The rotation of NO3â˜as a probe of molecular ion - water interactions. EPJ Web of Conferences, 2013, 41, 06002.	0.3	0
154	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
155	Selective negative-ion formation from core-valence doubly excited states of the water molecule. Physical Review A, 2018, 98, .	2.5	0
156	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
157	Electronic Structure Changes of an Aromatic Amine Photoacid along the FÃ¶rster Cycle. Angewandte Chemie, 0, , .	2.0	0
158	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
159	Core level and valence band analysis of in-situ cleaved perovskite single crystals. , 0, , .		0