Philippe Wernet

List of Publications by Year in descending order

111 papers	5,760 citations	94433 37 h-index	76900 74 g-index
113 all docs	113 docs citations	113 times ranked	5496 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	Structure of photosystem II and substrate binding at room temperature. Nature, 2016, 540, 453-457.	27.8	323
3	Spectroscopic probing of local hydrogen-bonding structures in liquid water. Journal of Physics Condensed Matter, 2002, 14, L213-L219.	1.8	262
4	Orbital-specific mapping of the ligand exchange dynamics of Fe(CO)5 in solution. Nature, 2015, 520, 78-81.	27.8	247
5	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
6	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.	1.7	158
7	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.	2.5	156
8	X-ray Absorption Spectroscopy Measurements of Liquid Water. Journal of Physical Chemistry B, 2005, 109, 13835-13839.	2.6	120
9	Nearest-neighbor oxygen distances in liquid water and ice observed by x-ray Raman based extended x-ray absorption fine structure. Journal of Chemical Physics, 2007, 127, 174504.	3.0	118
10	X-ray Raman spectroscopy at the oxygenKedge of water and ice:â€ƒ Implications on local structure models. Physical Review B, 2002, 66, .	3.2	101
11	A liquid flatjet system for solution phase soft-x-ray spectroscopy. Structural Dynamics, 2015, 2, 054301.	2.3	99
12	Comment on "Energetics of Hydrogen Bond Network Rearrangements in Liquid Water". Science, 2005, 308, 793a-793a.	12.6	90
13	Open shells and multi-electron interactions: core level photoionization of the 3d metal atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, R79-R125.	1.5	80
14	Spectroscopic characterization of microscopic hydrogen-bonding disparities in supercritical water. Journal of Chemical Physics, 2005, 123, 154503.	3.0	79
15	The hydrogen bond in ice probed by soft x-ray spectroscopy and density functional theory. Journal of Chemical Physics, 2005, 122, 154505.	3.0	79
16	Femtosecond Laser Excitation Drives Ferromagnetic Gadolinium out of Magnetic Equilibrium. Physical Review Letters, 2012, 109, 057401.	7.8	77
17	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
18	Isotope effects in liquid water probed by x-ray Raman spectroscopy. Physical Review B, 2007, 76, .	3.2	72

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19	A high-order harmonic generation apparatus for time- and angle-resolved photoelectron spectroscopy. Review of Scientific Instruments, 2013, 84, 075106.	1.3	71
20	A setup for resonant inelastic soft x-ray scattering on liquids at free electron laser light sources. Review of Scientific Instruments, 2012, 83, 123109.	1.3	70
21	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.	2.5	67
22	Surface structure of thin ice films. Chemical Physics Letters, 2004, 395, 161-165.	2.6	66
23	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
24	L-Edge X-ray Absorption Spectroscopy of Dilute Systems Relevant to Metalloproteins Using an X-ray Free-Electron Laser. Journal of Physical Chemistry Letters, 2013, 4, 3641-3647.	4.6	64
25	A sample holder for soft x-ray absorption spectroscopy of liquids in transmission mode. Review of Scientific Instruments, 2011, 82, 103101.	1.3	63
26	Probing the oxidation state of transition metal complexes: a case study on how charge and spin densities determine Mn L-edge X-ray absorption energies. Chemical Science, 2018, 9, 6813-6829.	7.4	60
27	Using X-ray free-electron lasers for spectroscopy of molecular catalysts and metalloenzymes. Nature Reviews Physics, 2021, 3, 264-282.	26.6	60
28	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
29	Real-Time Evolution of the Valence Electronic Structure in a Dissociating Molecule. Physical Review Letters, 2009, 103, 013001.	7.8	58
30	Suppression of the low-spin multiplet components in the3pphotoelectron spectra of atomic and solid3dmetals. Physical Review A, 2000, 62, .	2.5	54
31	Metastable state contributions to the measured 3p photoabsorption spectrum of Cr+ions in a laser-produced plasma. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, L583-L591.	1.5	49
32	The local structure of protonated water from x-ray absorption and density functional theory. Journal of Chemical Physics, 2006, 124, 194508.	3.0	49
33	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
34	Intrinsic deviations in fluorescence yield detected x-ray absorption spectroscopy: the case of the transition metal L_{2,3}edges. Journal of Physics Condensed Matter, 2012, 24, 452201.	1.8	47
35	Time-resolved soft X-ray absorption spectroscopy in transmission mode on liquids at MHz repetition rates. Structural Dynamics, 2017, 4, 054902.	2.3	47
36	Ultrafast temperature jump in liquid water studied by a novel infrared pump-x-ray probe technique. Applied Physics A: Materials Science and Processing, 2008, 92, 511-516.	2.3	46

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37	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
38	Femtosecond time-resolved photoelectron spectroscopy with a vacuum-ultraviolet photon source based on laser high-order harmonic generation. Review of Scientific Instruments, 2011, 82, 063114.	1.3	37
39	Temperature dependent soft x-ray absorption spectroscopy of liquids. Review of Scientific Instruments, 2014, 85, 103102.	1.3	37
40	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
41	2pphotoelectron spectra and linear alignment dichroism of atomic Cr. Physical Review A, 2001, 64, .	2.5	35
42	Soft x-ray absorption spectroscopy of metalloproteins and high-valent metal-complexes at room temperature using free-electron lasers. Structural Dynamics, 2017, 4, 054307.	2.3	34
43	Reabsorption of Soft X-Ray Emission at High X-Ray Free-Electron Laser Fluences. Physical Review Letters, 2014, 113, 153002.	7.8	33
44	X-ray emission spectroscopy of bulk liquid water in â€œno-manâ€™s landâ€. Journal of Chemical Physics, 2015, 142, 044505.	3.0	32
45	Direct Determination of Absolute Absorption Cross Sections at the L-Edge of Dilute Mn Complexes in Solution Using a Transmission Flatjet. Inorganic Chemistry, 2018, 57, 5449-5462.	4.0	32
46	A complete photoionization experiment with polarized atoms using magnetic dichroism and phase tilt measurements. Physical Review A, 1998, 58, R3371-R3374.	2.5	31
47	Electronic structure in real time: mapping valence electron rearrangements during chemical reactions. Physical Chemistry Chemical Physics, 2011, 13, 16941.	2.8	31
48	Chemical interactions and dynamics with femtosecond X-ray spectroscopy and the role of X-ray free-electron lasers. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20170464.	3.4	31
49	Multiplet splitting and valence-shell recoupling in the core-level2pphotoelectron spectrum of atomic Mn and of Mn compounds. Physical Review A, 2001, 63, .	2.5	30
50	Compton profiles for water and mixed water-neon clusters: A measure of coordination. Physical Review B, 2004, 70, .	3.2	30
51	Time-resolved X-ray absorption spectroscopy ofÂinfrared-laser-induced temperature jumps in liquid water. Applied Physics A: Materials Science and Processing, 2009, 96, 11-18.	2.3	28
52	Dynamics of the OH group and the electronic structure of liquid alcohols. Structural Dynamics, 2014, 1, 054901.	2.3	27
53	Multiplet and lifetime effects in the4dphotoelectron spectrum of Eu. Physical Review A, 2000, 61, .	2.5	26
54	Cationic and Anionic Impact on the Electronic Structure of Liquid Water. Journal of Physical Chemistry Letters, 2017, 8, 3759-3764.	4.6	26

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55	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
56	Methods development for diffraction and spectroscopy studies of metalloenzymes at X-ray free-electron lasers. Philosophical Transactions of the Royal Society B: Biological Sciences, 2014, 369, 20130590.	4.0	23
57	X-ray-induced sample damage at the Mn L-edge: a case study for soft X-ray spectroscopy of transition metal complexes in solution. Physical Chemistry Chemical Physics, 2018, 20, 16817-16827.	2.8	23
58	Valence satellite and 3p photoelectron spectra of atomic Fe and Cu. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 2539-2547.	1.5	22
59	Probing the Hofmeister Effect with Ultrafast Coreâ€“Hole Spectroscopy. Journal of Physical Chemistry B, 2014, 118, 9398-9403.	2.6	22
60	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
61	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
62	Term-dependent lifetime broadening effect on the 4d photoelectron spectrum of atomic thulium. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 215002.	1.5	19
63	X-ray absorption spectroscopy using a self-seeded soft X-ray free-electron laser. Optics Express, 2016, 24, 22469.	3.4	19
64	Iron L-Edge Absorption Spectroscopy of Iron Pentacarbonyl and Ferrocene in the Gas Phase. Journal of Physical Chemistry A, 2017, 121, 66-72.	2.5	19
65	Core-valence interactions in the linear dichroism of Cr2pphotoelectron spectra. Physical Review B, 2000, 62, 14331-14336.	3.2	18
66	Time resolved resonant inelastic X-ray scattering: A supreme tool to understand dynamics in solids and molecules. Journal of Electron Spectroscopy and Related Phenomena, 2013, 188, 172-182.	1.7	18
67	Cr L-Edge X-ray Absorption Spectroscopy of Cr^{III}(acac)₃ in Solution with Measured and Calculated Absolute Absorption Cross Sections. Journal of Physical Chemistry B, 2018, 122, 7375-7384.	2.6	18
68	Shot-to-shot and average absolute photon flux measurements of a femtosecond laser high-order harmonic photon source. New Journal of Physics, 2011, 13, 093003.	2.9	16
69	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
70	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
71	Ionic Solutions Probed by Resonant Inelastic X-ray Scattering. Zeitschrift Fur Physikalische Chemie, 2015, 229, 1855-1867.	2.8	13
72	Isotope effects in liquid water probed by transmission mode x-ray absorption spectroscopy at the oxygen K-edge. Journal of Chemical Physics, 2016, 145, 104502.	3.0	12

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73	Following Metal-to-Ligand Charge-Transfer Dynamics with Ligand and Spin Specificity Using Femtosecond Resonant Inelastic X-ray Scattering at the Nitrogen K-Edge. Journal of Physical Chemistry Letters, 2021, 12, 6676-6683.	4.6	12
74	Selection of a single femtosecond high-order harmonic using a zone plate based monochromator. Journal of Applied Physics, 2008, 104, .	2.5	11
75	Design and optimization of a parallel spectrometer for ultra-fast X-ray science. Optics Express, 2014, 22, 12583.	3.4	11
76	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
77	Combining high-resolution photoelectron spectroscopy and laser polarization for a study of the 4f and 5p photoionization of atomic thulium. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 3887-3900.	1.5	9
78	The confocal plane grating spectrometer at BESSY II. Journal of Electron Spectroscopy and Related Phenomena, 2013, 188, 133-139.	1.7	9
79	State-dependent fluorescence yields through the core-valence Coulomb exchange parameter. Physical Review A, 2014, 89, .	2.5	9
80	Breakdown of the three-parameter model for the dichroism in the 4f photoelectron spectrum of laser-aligned Eu atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 4079-4090.	1.5	8
81	Probing photoelectron angular distributions in molecules with polarization-controlled two-color above-threshold ionization. Physical Review A, 2015, 91, .	2.5	8
82	Magnetic dichroism in the 4f photoelectron spectra of free Eu atoms: Experimental proof of the atomic character of thin film Euâ€“Gd MCD. Journal of Electron Spectroscopy and Related Phenomena, 1999, 101-103, 179-183.	1.7	7
83	High resolution spectroscopy of 2p6â†'2p53d resonantly excited atomic Ca. Journal of Electron Spectroscopy and Related Phenomena, 1999, 101-103, 39-42.	1.7	7
84	Core-hole-induced degeneracy of the valence subshells in the5pphotoemission of atomic europium. Physical Review A, 2002, 65, .	2.5	7
85	Linear dichroism in the 4d photoionization of atomic europium. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 907-916.	1.5	7
86	Monochromatizing and focussing femtosecond high-order harmonic radiation with one optical element. Review of Scientific Instruments, 2013, 84, 103102.	1.3	7
87	vuv photoionization of uv-laser-tailored Ni-like Cu3d9atoms. Physical Review A, 1999, 60, R737-R740.	2.5	6
88	Resonant 3p photoelectron spectroscopy of free Cu atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 1563-1573.	1.5	6
89	Determination of theÎ²parameter for atomic Mn and Cr2pphotoemission: A benchmark test for core-electron photoionization theories. Physical Review A, 2003, 68, .	2.5	6
90	Capturing Atom-Specific Electronic Structural Dynamics of Transition-Metal Complexes with Ultrafast Soft X-Ray Spectroscopy. Annual Review of Physical Chemistry, 2022, 73, 187-208.	10.8	6

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91	Electronic Structure Changes of an Aromatic Amine Photoacid along the FÃ¶rster Cycle. Angewandte Chemie - International Edition, 2022, 61, .	13.8	6
92	Determination of Ca 2p ionization thresholds by high-resolution photoelectron spectroscopy. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, L289-L296.	1.5	5
93	Linear dichroism of the4fphotoemission in the giant resonance of atomic europium. Physical Review A, 2003, 67, .	2.5	5
94	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
95	Photoionization studies of the2presonances of atomic calcium. Physical Review A, 2002, 65, .	2.5	4
96	Strong influence of configuration interactions on the orientation and alignment dichroism in the3pphotoelectron spectra of free laser-polarized Fe atoms. Physical Review A, 2007, 75, .	2.5	4
97	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
98	Resonant X-ray emission spectroscopy from broadband stochastic pulses at an X-ray free electron laser. Communications Chemistry, 2021, 4, .	4.5	4
99	Resonant Inelastic X-ray Scattering (RIXS) Studies in Chemistry: Present and Future. , 2020, , 2315-2366.		3
100	Mapping chemical bonding of reaction intermediates with femtosecond X-ray laser spectroscopy. EPJ Web of Conferences, 2013, 41, 05025.	0.3	3
101	Ultrafast Temperature Jumps in Liquid Water Studied by Infrared-Pump and X-ray Absorption-Probe Spectroscopy. Springer Series in Chemical Physics, 2009, , 505-507.	0.2	2
102	Structure and dynamics in liquid water from x-ray absorption spectroscopy. Journal of Physics: Conference Series, 2009, 190, 012055.	0.4	2
103	Femtosecond VUV Photon Pulses for Time-resolved Photoelectron Spectroscopy. Springer Series in Chemical Physics, 2007, , 45-47.	0.2	2
104	Resonant Inelastic X-ray Scattering (RIXS) Studies in Chemistry: Present and Future. , 2019, , 1-52.		2
105	Photoinduced bond oscillations in ironpentacarbonyl give delayed synchronous bursts of carbonmonoxide release. Nature Communications, 2022, 13, 1337.	12.8	2
106	Coherent wave packet dynamics in photo-excited NaI. EPJ Web of Conferences, 2013, 41, 02027.	0.3	1
107	First Step Towards a Femtosecond VUV Microscope: Zone Plate Optics as Monochromator for High-Order Harmonics.. Springer Series in Chemical Physics, 2009, , 884-886.	0.2	0
108	Chemical and Bio-chemical X-ray Spectroscopy at Current and Future X-ray Lasers. , 2017, , .		0

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109	Taking snapshots of photosynthetic water oxidation with an X-ray laser. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C14-C14.	0.1	0
110	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
111	Electronic Structure Changes of an Aromatic Amine Photoacid along the FÃ¶rster Cycle. Angewandte Chemie, 0, , .	2.0	0