David Prendergast

List of Publications by Year in descending order

207 papers	12,003 citations	31976 53 h-index	30922 102 g-index
211 all docs	211 docs citations	211 times ranked	16780 citing authors

#	Article	IF	Citations
1	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	27.8	1,026
2	Aqueous vs. nonaqueous Zn-ion batteries: consequences of the desolvation penalty at the interface. Energy and Environmental Science, 2018, 11, 881-892.	30.8	604
3	Theory-driven design of high-valence metal sites for water oxidation confirmed using in situ soft X-ray absorption. Nature Chemistry, 2018, 10, 149-154.	13.6	476
4	Coupling between oxygen redox and cation migration explains unusual electrochemistry in lithium-rich layered oxides. Nature Communications, 2017, 8, 2091.	12.8	469
5	Nanostructured Metal Hydrides for Hydrogen Storage. Chemical Reviews, 2018, 118, 10775-10839.	47.7	461
6	Attosecond band-gap dynamics in silicon. Science, 2014, 346, 1348-1352.	12.6	415
7	The structure of interfacial water on gold electrodes studied by x-ray absorption spectroscopy. Science, 2014, 346, 831-834.	12.6	391
8	X-Ray Absorption Spectra of Water from First Principles Calculations. Physical Review Letters, 2006, 96, 215502.	7.8	327
9	Metalâ€“oxygen decoordination stabilizes anion redox in Li-rich oxides. Nature Materials, 2019, 18, 256-265.	27.5	280
10	Femtosecond x-ray spectroscopy of an electrocyclic ring-opening reaction. Science, 2017, 356, 54-59.	12.6	253
11	Experimental and theoretical investigation of the electronic structure of Cu2O and CuO thin films on Cu(110) using x-ray photoelectron and absorption spectroscopy. Journal of Chemical Physics, 2013, 138, 024704.	3.0	219
12	Mg Desolvation and Intercalation Mechanism at the Mo₆S₈ Chevrel Phase Surface. Chemistry of Materials, 2015, 27, 5932-5940.	6.7	157
13	Polysulfide-Blocking Microporous Polymer Membrane Tailored for Hybrid Li-Sulfur Flow Batteries. Nano Letters, 2015, 15, 5724-5729.	9.1	153
14	Efficient implementation of core-excitation Betheâ€“Salpeter equation calculations. Computer Physics Communications, 2015, 197, 109-117.	7.5	142
15	Phase Transformation and Lithiation Effect on Electronic Structure of Li_xFePO₄: An In-Depth Study by Soft X-ray and Simulations. Journal of the American Chemical Society, 2012, 134, 13708-13715.	13.7	136
16	X-ray Absorption Spectra of Dissolved Polysulfides in Lithiumâ€“Sulfur Batteries from First-Principles. Journal of Physical Chemistry Letters, 2014, 5, 1547-1551.	4.6	134
17	Reversible Mg-Ion Insertion in a Metastable One-Dimensional Polymorph of V2O5. CheM, 2018, 4, 564-585.	11.7	126
18	Tuning Semiconductor Band Edge Energies for Solar Photocatalysis via Surface Ligand Passivation. Nano Letters, 2012, 12, 383-388.	9.1	124

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19	On the hydration and hydrolysis of carbon dioxide. Chemical Physics Letters, 2011, 514, 187-195.	2.6	119
20	Electronic Structure of Warm Dense Copper Studied by Ultrafast X-Ray Absorption Spectroscopy. Physical Review Letters, 2011, 106, 167601.	7.8	117
21	Detecting the oxyl radical of photocatalytic water oxidation at an n-SrTiO3/aqueous interface through its subsurface vibration. Nature Chemistry, 2016, 8, 549-555.	13.6	117
22	Direct and simultaneous observation of ultrafast electron and hole dynamics in germanium. Nature Communications, 2017, 8, 15734.	12.8	117
23	Molecular understanding of polyelectrolyte binders that actively regulate ion transport in sulfur cathodes. Nature Communications, 2017, 8, 2277.	12.8	117
24	Macromolecular Design Strategies for Preventing Activeâ€Material Crossover in Nonâ€Aqueous Allâ€Organic Redoxâ€Flow Batteries. Angewandte Chemie - International Edition, 2017, 56, 1595-1599.	13.8	116
25	Mapping polaronic states and lithiation gradients in individual V2O5 nanowires. Nature Communications, 2016, 7, 12022.	12.8	115
26	Efficient Hydrogen Production from Methanol Using a Single-Site Pt₁/CeO₂ Catalyst. Journal of the American Chemical Society, 2019, 141, 17995-17999.	13.7	114
27	Imaging local electronic corrugations and doped regions in graphene. Nature Communications, 2011, 2, 372.	12.8	111
28	Characterization of Polysulfide Radicals Present in an Etherâ€Based Electrolyte of a Lithiumâ€“Sulfur Battery During Initial Discharge Using In Situ Xâ€Ray Absorption Spectroscopy Experiments and Firstâ€Principles Calculations. Advanced Energy Materials, 2015, 5, 1500285.	19.5	107
29	Bound Excitons in Metallic Single-Walled Carbon Nanotubes. Nano Letters, 2007, 7, 1626-1630.	9.1	105
30	Strain-Induced Band Gap Modification in Coherent Core/Shell Nanostructures. Nano Letters, 2010, 10, 3156-3162.	9.1	101
31	The electronic structure of liquid water within density-functional theory. Journal of Chemical Physics, 2005, 123, 014501.	3.0	98
32	Topochemically De-Intercalated Phases of V₂O₅ as Cathode Materials for Multivalent Intercalation Batteries: A First-Principles Evaluation. Chemistry of Materials, 2016, 28, 5611-5620.	6.7	84
33	Design Rules for Membranes from Polymers of Intrinsic Microporosity for Crossover-free Aqueous Electrochemical Devices. Joule, 2019, 3, 2968-2985.	24.0	84
34	Diversity-oriented synthesis of polymer membranes with ion solvation cages. Nature, 2021, 592, 225-231.	27.8	83
35	Electronic bonding transition in compressedSiO2glass. Physical Review B, 2007, 75, .	3.2	81
36	Exploration of the Detailed Conditions for Reductive Stability of Mg(TFSI)₂ in Diglyme: Implications for Multivalent Electrolytes. Journal of Physical Chemistry C, 2016, 120, 3583-3594.	3.1	81

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37	Atomic-Scale Perspective of Ultrafast Charge Transfer at a Dyeâ€“Semiconductor Interface. Journal of Physical Chemistry Letters, 2014, 5, 2753-2759.	4.6	79
38	Fingerprinting Lithium-Sulfur Battery Reaction Products by X-ray Absorption Spectroscopy. Journal of the Electrochemical Society, 2014, 161, A1100-A1106.	2.9	76
39	The Formation Time of Tiâ€“O^{â€¢} and Tiâ€“O^{â€¢}â€“Ti Radicals at the n-SrTiO₃/Aqueous Interface during Photocatalytic Water Oxidation. Journal of the American Chemical Society, 2017, 139, 1830-1841.	13.7	76
40	Broadband Dielectric Function of Nonequilibrium Warm Dense Gold. Physical Review Letters, 2006, 96, 255003.	7.8	74
41	Instability at the Electrode/Electrolyte Interface Induced by Hard Cation Chelation and Nucleophilic Attack. Chemistry of Materials, 2017, 29, 8504-8512.	6.7	74
42	Reversible Magnesium Intercalation into a Layered Oxyfluoride Cathode. Chemistry of Materials, 2016, 28, 17-20.	6.7	70
43	Insights into the Mechanism of Methanol Steam Reforming Tandem Reaction over CeO₂ Supported Single-Site Catalysts. Journal of the American Chemical Society, 2021, 143, 12074-12081.	13.7	70
44	The Solvation Structure of Mg Ions in Dichloro Complex Solutions from First-Principles Molecular Dynamics and Simulated X-ray Absorption Spectra. Journal of the American Chemical Society, 2014, 136, 14456-14464.	13.7	67
45	Lithium Polysulfide Radical Anions in Ether-Based Solvents. Journal of Physical Chemistry C, 2016, 120, 18403-18410.	3.1	65
46	Electronâ^'Hole Interaction in Carbon Nanotubes: Novel Screening and Exciton Excitation Spectra. Nano Letters, 2009, 9, 1330-1334.	9.1	64
47	Accurate X-Ray Spectral Predictions: An Advanced Self-Consistent-Field Approach Inspired by Many-Body Perturbation Theory. Physical Review Letters, 2017, 118, 096402.	7.8	64
48	Evaluation of Multivalent Cation Insertion in Single- and Double-Layered Polymorphs of V₂O₅. ACS Applied Materials & Interfaces, 2017, 9, 23756-23765.	8.0	64
49	Cation-cation contact pairing in water: Guanidinium. Journal of Chemical Physics, 2013, 139, 035104.	3.0	62
50	Building a Fast Lane for Mg Diffusion in Î±-MoO₃ by Fluorine Doping. Chemistry of Materials, 2016, 28, 6900-6908.	6.7	60
51	On chemical bonding and electronic structure of grapheneâ€“metal contacts. Chemical Science, 2013, 4, 494-502.	7.4	59
52	Probing Adsorption Interactions in Metalâ€“Organic Frameworks using X-ray Spectroscopy. Journal of the American Chemical Society, 2013, 135, 18183-18190.	13.7	56
53	NEXAFS Spectroscopy Reveals the Molecular Orientation in Blade-Coated Pyridal[2,1,3]thiadiazole-Containing Conjugated Polymer Thin Films. Macromolecules, 2015, 48, 6606-6616.	4.8	56
54	Deciphering the Oxygen Absorption Preâ€edge: A Caveat on its Application for Probing Oxygen Redox Reactions in Batteries. Energy and Environmental Materials, 2021, 4, 246-254.	12.8	56

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55	Infrared Nanospectroscopy at the Grapheneâ€“Electrolyte Interface. Nano Letters, 2019, 19, 5388-5393.	9.1	55
56	Bloch-state-based interpolation: An efficient generalization of the Shirley approach to interpolating electronic structure. Physical Review B, 2009, 80, .	3.2	52
57	Vanadium K-Edge X-ray Absorption Spectroscopy as a Probe of the Heterogeneous Lithiation of V₂O₅: First-Principles Modeling and Principal Component Analysis. Journal of Physical Chemistry C, 2016, 120, 23922-23932.	3.1	52
58	Universal Relationship between Molecular Structure and Crystal Structure in Peptoid Polymers and Prevalence of the cis Backbone Conformation. Journal of the American Chemical Society, 2018, 140, 827-833.	13.7	52
59	Effects of vibrational motion on core-level spectra of prototype organic molecules. Chemical Physics Letters, 2008, 467, 195-199.	2.6	49
60	Re-examining the Chevrel phase Mo₆S₈ cathode for Mg intercalation from an electronic structure perspective. Physical Chemistry Chemical Physics, 2015, 17, 22548-22551.	2.8	49
61	Atomic-level engineering and imaging of polypeptoid crystal lattices. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 22491-22499.	7.1	48
62	Identifying Catalytic Active Sites of Trimolybdenum Phosphide (Mo₃P) for Electrochemical Hydrogen Evolution. Advanced Energy Materials, 2019, 9, 1900516.	19.5	47
63	X-Ray absorption spectroscopy of LiBF₄ in propylene carbonate: a model lithium ion battery electrolyte. Physical Chemistry Chemical Physics, 2014, 16, 23568-23575.	2.8	46
64	Velocity-gauge real-time TDDFT within a numerical atomic orbital basis set. Computer Physics Communications, 2018, 226, 30-38.	7.5	45
65	CuBi₂O₄: Electronic Structure, Optical Properties, and Photoelectrochemical Performance Limitations of the Photocathode. Chemistry of Materials, 2021, 33, 934-945.	6.7	45
66	Finite temperature effects on the X-ray absorption spectra of lithium compounds: First-principles interpretation of X-ray Raman measurements. Journal of Chemical Physics, 2014, 140, 034107.	3.0	43
67	X-ray spectroscopy as a probe for lithium polysulfide radicals. Physical Chemistry Chemical Physics, 2015, 17, 7743-7753.	2.8	43
68	Probing the mechanism of CO₂ capture in diamine-appended metalâ€“organic frameworks using measured and simulated X-ray spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 21448-21457.	2.8	43
69	Electronic Structure and Performance Bottlenecks of CuFeO₂ Photocathodes. Chemistry of Materials, 2019, 31, 2524-2534.	6.7	43
70	Ultrafast carrier thermalization and trapping in silicon-germanium alloy probed by extreme ultraviolet transient absorption spectroscopy. Structural Dynamics, 2017, 4, 044029.	2.3	42
71	Local Effects in the X-ray Absorption Spectrum of Salt Water. Journal of Physical Chemistry B, 2010, 114, 9594-9601.	2.6	41
72	Thermodynamic origins of the solvent-dependent stability of lithium polysulfides from first principles. Physical Chemistry Chemical Physics, 2017, 19, 1441-1448.	2.8	41

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73	Reversible dehydrogenation and rehydrogenation of cyclohexane and methylcyclohexane by single-site platinum catalyst. Nature Communications, 2022, 13, 1092.	12.8	41
74	Revealing electronic state-switching at conical intersections in alkyl iodides by ultrafast XUV transient absorption spectroscopy. Nature Communications, 2020, 11, 4042.	12.8	40
75	Gold-like activity copper-like selectivity of heteroatomic transition metal carbides for electrocatalytic carbon dioxide reduction reaction. Nature Communications, 2021, 12, 5067.	12.8	40
76	On the importance of nuclear quantum motions in near edge x-ray absorption fine structure spectroscopy of molecules. Journal of Chemical Physics, 2009, 130, 184109.	3.0	39
77	pH-dependent x-ray absorption spectra of aqueous boron oxides. Journal of Chemical Physics, 2011, 134, 154503.	3.0	39
78	Mapping Catalytically Relevant Edge Electronic States of MoS₂. ACS Central Science, 2018, 4, 493-503.	11.3	39
79	Impact of electronâ€“electron cusp on configuration interaction energies. Journal of Chemical Physics, 2001, 115, 1626-1634.	3.0	38
80	Atomically Thin Interfacial Suboxide Key to Hydrogen Storage Performance Enhancements of Magnesium Nanoparticles Encapsulated in Reduced Graphene Oxide. Nano Letters, 2017, 17, 5540-5545.	9.1	37
81	Spectroscopy of Donorâˆ’Ï€â€“Acceptor Porphyrins for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2013, 117, 13357-13364.	3.1	36
82	Improved treatment of exact exchange in Quantum ESPRESSO. Computer Physics Communications, 2017, 214, 52-58.	7.5	36
83	Imaging Unstained Synthetic Polymer Crystals and Defects on Atomic Length Scales Using Cryogenic Electron Microscopy. Macromolecules, 2018, 51, 7794-7799.	4.8	36
84	Improved Li⁺ Transport in Polyacetal Electrolytes: Conductivity and Current Fraction in a Series of Polymers. ACS Energy Letters, 2021, 6, 1886-1891.	17.4	36
85	Investigation of protein conformation and interactions with salts via X-ray absorption spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 14008-14013.	7.1	35
86	Enhanced and stabilized hydrogen production from methanol by ultrasmall Ni nanoclusters immobilized on defect-rich h-BN nanosheets. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 29442-29452.	7.1	34
87	Ligand-Mediated Modification of the Electronic Structure of CdSe Quantum Dots. Nano Letters, 2012, 12, 2763-2767.	9.1	33
88	Understanding the Structural Evolution of a Nickel Chalcogenide Electrocatalyst Surface for Water Oxidation. Energy & Fuels, 2021, 35, 4387-4403.	5.1	33
89	Molecular-Scale Structure of Electrodeâ€“Electrolyte Interfaces: The Case of Platinum in Aqueous Sulfuric Acid. Journal of the American Chemical Society, 2018, 140, 16237-16244.	13.7	32
90	Optical Properties of Silicon Clusters in the Presence of Water:Â A First Principles Theoretical Analysis. Journal of the American Chemical Society, 2004, 126, 13827-13837.	13.7	31

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91	In Situ X-ray Absorption Spectroscopy Studies of Discharge Reactions in a Thick Cathode of a Lithium Sulfur Battery. Journal of the Electrochemical Society, 2017, 164, A18-A27.	2.9	31
92	Properties of aqueous nitrate and nitrite from x-ray absorption spectroscopy. Journal of Chemical Physics, 2015, 143, 084503.	3.0	30
93	Understanding and control of bipolar self-doping in copper nitride. Journal of Applied Physics, 2016, 119, .	2.5	30
94	Synthesis of a mixed-valent tin nitride and considerations of its possible crystal structures. Journal of Chemical Physics, 2016, 144, 144201.	3.0	29
95	Warm dense matter created by isochoric laser heating. High Energy Density Physics, 2010, 6, 246-257.	1.5	28
96	Cooperative adsorption of carbon disulfide in diamine-appended metalâ€“organic frameworks. Nature Communications, 2018, 9, 5133.	12.8	28
97	Integrating Ab Initio Simulations and X-ray Photoelectron Spectroscopy: Toward A Realistic Description of Oxidized Solid/Liquid Interfaces. Journal of Physical Chemistry Letters, 2018, 9, 194-203.	4.6	27
98	Revealing electronic structure changes in Chevrel phase cathodes upon Mg insertion using X-ray absorption spectroscopy. Physical Chemistry Chemical Physics, 2016, 18, 17326-17329.	2.8	26
99	Ion-Pair Dissociation on Î±-MoO₃ Surfaces: Focus on the Electrolyteâ€“Cathode Compatibility Issue in Mg Batteries. Journal of Physical Chemistry C, 2018, 122, 398-405.	3.1	26
100	Edge-Functionalized Graphene Nanoribbon Encapsulation To Enhance Stability and Control Kinetics of Hydrogen Storage Materials. Chemistry of Materials, 2019, 31, 2960-2970.	6.7	26
101	Potentialâ€Induced Electronic Structure Changes in Supercapacitor Electrodes Observed by In Operando Soft Xâ€Ray Spectroscopy. Advanced Materials, 2015, 27, 1512-1518.	21.0	25
102	Macromolecular Design Strategies for Preventing Activeâ€Material Crossover in Nonâ€Aqueous Allâ€Organic Redoxâ€Flow Batteries. Angewandte Chemie, 2017, 129, 1617-1621.	2.0	25
103	â€œIon Solvation Spectraâ€• Free Energy Analysis of Solvation Structures of Multivalent Cations in Aprotic Solvents. Journal of Physical Chemistry Letters, 2019, 10, 4920-4928.	4.6	25
104	Nonlinear variations in the electronic structure of IIâ€“VI and IIIâ€“V wurtzite semiconductors with biaxial strain. Applied Physics Letters, 2011, 98, .	3.3	24
105	Mitigating Cation Diffusion Limitations and Intercalation-Induced Framework Transitions in a 1D Tunnel-Structured Polymorph of V₂O₅. Chemistry of Materials, 2017, 29, 10386-10397.	6.7	24
106	Ultrathin Free-Standing Oxide Membranes for Electron and Photon Spectroscopy Studies of Solidâ€“Gas and Solidâ€“Liquid Interfaces. Nano Letters, 2020, 20, 6364-6371.	9.1	24
107	Ion Solvation Engineering: How to Manipulate the Multiplicity of the Coordination Environment of Multivalent Ions. Journal of Physical Chemistry Letters, 2020, 11, 9336-9343.	4.6	24
108	Determining Atomic-Scale Structure and Composition of Organo-Lead Halide Perovskites by Combining High-Resolution X-ray Absorption Spectroscopy and First-Principles Calculations. ACS Energy Letters, 2017, 2, 1183-1189.	17.4	23

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109	Solution-Based, Template-Assisted Realization of Large-Scale Graphitic ZnO. ACS Nano, 2018, 12, 7554-7561.	14.6	23
110	Atomic Hourglass and Thermometer Based on Diffusion of a Mobile Dopant in VO₂. Journal of the American Chemical Society, 2020, 142, 15513-15526.	13.7	23
111	The hydration structure of aqueous carbonic acid from X-ray absorption spectroscopy. Chemical Physics Letters, 2014, 614, 282-286.	2.6	22
112	Adsorption Behavior of Organic Molecules: A Study of Benzotriazole on Cu(111) with Spectroscopic and Theoretical Methods. Langmuir, 2019, 35, 882-893.	3.5	22
113	Importance of Electronic Relaxation for Inter-Coulombic Decay in Aqueous Systems. Physical Review Letters, 2010, 105, 198102.	7.8	21
114	Theory and X-ray Absorption Spectroscopy for Aluminum Coordination Complexes â€“ Al K-Edge Studies of Charge and Bonding in (BDI)Al, (BDI)AlR₂, and (BDI)AlX₂ Complexes. Journal of the American Chemical Society, 2015, 137, 10304-10316.	13.7	21
115	Quantum many-body effects in x-ray spectra efficiently computed using a basic graph algorithm. Physical Review B, 2018, 97, .	3.2	21
116	Critical Factors in Computational Characterization of Hydrogen Storage in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2018, 122, 18957-18967.	3.1	21
117	Backbonding contributions to small molecule chemisorption in a metalâ€“organic framework with open copper(<scp>i</scp>) centers. Chemical Science, 2021, 12, 2156-2164.	7.4	21
118	Modifying Li⁺ and Anion Diffusivities in Polyacetal Electrolytes: A Pulsed-Field-Gradient NMR Study of Ion Self-Diffusion. Chemistry of Materials, 2021, 33, 4915-4926.	6.7	21
119	Auto-oligomerization and hydration of pyrrole revealed by x-ray absorption spectroscopy. Journal of Chemical Physics, 2009, 131, 114509.	3.0	20
120	First-Principles Predictions of Near-Edge X-ray Absorption Fine Structure Spectra of Semiconducting Polymers. Journal of Physical Chemistry C, 2017, 121, 9142-9152.	3.1	20
121	Rate Constants of Electrochemical Reactions in a Lithium-Sulfur Cell Determined by Operando X-ray Absorption Spectroscopy. Journal of the Electrochemical Society, 2018, 165, A3487-A3495.	2.9	20
122	Stabilized open metal sites in bimetallic metalâ€“organic framework catalysts for hydrogen production from alcohols. Journal of Materials Chemistry A, 2021, 9, 10869-10881.	10.3	20
123	An analysis of the NEXAFS spectra of a molecular crystal: Î±-glycine. Journal of Chemical Physics, 2010, 133, 044507.	3.0	19
124	Extreme ultraviolet transient absorption of solids from femtosecond to attosecond timescales. Journal of the Optical Society of America B: Optical Physics, 2016, 33, C57.	2.1	19
125	Identifying the Role of Dynamic Surface Hydroxides in the Dehydrogenation of Ti-Doped NaAlH₄. ACS Applied Materials & Interfaces, 2019, 11, 4930-4941.	8.0	19
126	Optimization of inhomogeneous electron correlation factors in periodic solids. Physical Review B, 2002, 66, .	3.2	18

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127	Improving Continuum Models to Define Practical Limits for Molecular Models of Electrified Interfaces. Journal of the Electrochemical Society, 2017, 164, E3438-E3447.	2.9	18
128	Effect of processing and end groups on the crystal structure of polypeptoids studied by cryogenic electron microscopy at atomic length scales. Soft Matter, 2019, 15, 4723-4736.	2.7	18
129	Mapping wave packet bifurcation at a conical intersection in CH3I by attosecond XUV transient absorption spectroscopy. Journal of Chemical Physics, 2021, 154, 234301.	3.0	18
130	Evidence of a second-order Peierls-driven metal-insulator transition in crystalline NbO2. Physical Review Materials, 2019, 3, .	2.4	18
131	Toward Equatorial Planarity about Uranyl: Synthesis and Structure of Tridentate Nitrogen-Donor {UO₂}²⁺ Complexes. Inorganic Chemistry, 2014, 53, 2506-2515.	4.0	17
132	Combining theory and experiment for X-ray absorption spectroscopy and resonant X-ray scattering characterization of polymers. Polymer, 2016, 99, 782-796.	3.8	17
133	Electronic structure study of the CdS buffer layer in CIGS solar cells by X-ray absorption spectroscopy: Experiment and theory. Solar Energy Materials and Solar Cells, 2016, 149, 275-283.	6.2	17
134	The importance of inner-shell electronic structure for enhancing the EUV absorption of photoresist materials. Journal of Chemical Physics, 2017, 146, 164106.	3.0	17
135	Cooperative Gas Adsorption without a Phase Transition in Metal-Organic Frameworks. Physical Review Letters, 2018, 121, 015701.	7.8	17
136	Anion-Assisted Delivery of Multivalent Cations to Inert Electrodes. Journal of Physical Chemistry Letters, 2021, 12, 4347-4356.	4.6	17
137	The hydration structure of dissolved carbon dioxide from X-ray absorption spectroscopy. Chemical Physics Letters, 2015, 633, 214-217.	2.6	16
138	Liquid Sulfur Impregnation of Microporous Carbon Accelerated by Nanoscale Interfacial Effects. Nano Letters, 2017, 17, 2517-2523.	9.1	16
139	Probing ultrafast Câ€“Br bond fission in the UV photochemistry of bromoform with core-to-valence transient absorption spectroscopy. Structural Dynamics, 2019, 6, 054304.	2.3	16
140	Addressing the sensitivity of signals from solid/liquid ambient pressure XPS (APXPS) measurement. Journal of Chemical Physics, 2020, 153, 044709.	3.0	16
141	Bonding and Charge Transfer in Nitrogen-Donor Uranyl Complexes: Insights from NEXAFS Spectra. Inorganic Chemistry, 2014, 53, 11415-11425.	4.0	15
142	Fundamental understanding of chemical processes in extreme ultraviolet resist materials. Journal of Chemical Physics, 2018, 149, 154305.	3.0	15
143	Electronic structure of aqueous borohydride: a potential hydrogen storage medium. Physical Chemistry Chemical Physics, 2011, 13, 17077.	2.8	14
144	Layer Edge States Stabilized by Internal Electric Fields in Two-Dimensional Hybrid Perovskites. Nano Letters, 2021, 21, 182-188.	9.1	14

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145	Nuclear quantum effects in the structure and lineshapes of the N2 near-edge x-ray absorption fine structure spectrum. Journal of Chemical Physics, 2010, 132, 094302.	3.0	13
146	Monopeptide versus Monopeptoid: Insights on Structure and Hydration of Aqueous Alanine and Sarcosine via X-ray Absorption Spectroscopy. Journal of Physical Chemistry B, 2010, 114, 4702-4709.	2.6	13
147	Near-edge x-ray absorption fine structure spectroscopy studies of charge redistribution at graphene/dielectric interfaces. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2012, 30, 041205.	1.2	13
148	Direct observation of ring-opening dynamics in strong-field ionized selenophene using femtosecond inner-shell absorption spectroscopy. Journal of Chemical Physics, 2016, 145, 234313.	3.0	13
149	Direct observation of delithiation as the origin of analog memristance in LixNbO2. APL Materials, 2019, 7, .	5.1	13
150	Exploring chemical speciation at electrified interfaces using detailed continuum models. Journal of Chemical Physics, 2019, 150, 041725.	3.0	13
151	Chemical and Morphological Inhomogeneity of Aluminum Metal and Oxides from Soft X-ray Spectromicroscopy. Inorganic Chemistry, 2017, 56, 5710-5719.	4.0	12
152	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
153	Revealing Nanoscale Chemical Heterogeneities in Polycrystalline Moâ€“BiVO₄ Thin Films. Small, 2020, 16, e2001600.	10.0	12
154	Experiments and Theory of In situ and Operando Soft X-ray Spectroscopy for Energy Storage. Synchrotron Radiation News, 2014, 27, 4-13.	0.8	11
155	Strain and Bond Length Dynamics upon Growth and Transfer of Graphene by NEXAFS Spectroscopy from First-Principles and Experiment. Langmuir, 2018, 34, 1783-1794.	3.5	11
156	Mechanistic Advantages of Organotin Molecular EUV Photoresists. ACS Applied Materials & Interfaces, 2022, 14, 5514-5524.	8.0	11
157	Exploiting the P L_2,3 absorption edge for optics: spectroscopic and structural characterization of cubic boron phosphide thin films. Optical Materials Express, 2016, 6, 3946.	3.0	10
158	Hybrid DFT investigation of the energetics of Mg ion diffusion in Î±-MoO₃. Physical Chemistry Chemical Physics, 2018, 20, 24877-24884.	2.8	10
159	Runaway Carbon Dioxide Conversion Leads to Enhanced Uptake in a Nanohybrid Form of Porous Magnesium Borohydride. Advanced Materials, 2019, 31, e1904252.	21.0	10
160	Taming convergence in the determinant approach for x-ray excitation spectra. Physical Review B, 2019, 100, .	3.2	10
161	Conical intersection and coherent vibrational dynamics in alkyl iodides captured by attosecond transient absorption spectroscopy. Journal of Chemical Physics, 2022, 156, 114304.	3.0	10
162	Self-healing in B₁₂P₂ through Mediated Defect Recombination. Chemistry of Materials, 2016, 28, 8415-8428.	6.7	9

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163	Temperature and radiation effects at the fluorine K-edge in LiF. Journal of Electron Spectroscopy and Related Phenomena, 2017, 218, 30-34.	1.7	9
164	Two-photon absorption of soft X-ray free electron laser radiation by graphite near the carbon K-absorption edge. Chemical Physics Letters, 2018, 703, 112-116.	2.6	9
165	Metal-Insulator Transitions in Î²â€²-Cu V2O5 Mediated by Polaron Oscillation and Cation Shuttling. Matter, 2020, 2, 1166-1186.	10.0	9
166	Importance of the Positively Charged Ïƒ-Hole in Crystal Engineering of Halogenated Polypeptoids. Journal of Physical Chemistry B, 2022, 126, 4152-4159.	2.6	9
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