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	Mechanistic Advantages of Organotin Molecular EUV Photoresists. ACS Applied Materials & Interfaces, 2022, 14, 5514-5524.	8.0	11
2	Efficient basis sets for core-excited states motivated by Slater's rules. Physical Chemistry Chemical Physics, 2022, 24, 2243-2250.	2.8	6
3	Chloride-Assisted Corrosion of Copper and Protection by Benzotriazole. ACS Applied Materials & Interfaces, 2022, 14, 6093-6101.	8.0	5
4	Resolving the backbone tilt of crystalline poly(3-hexylthiophene) with resonant tender X-ray diffraction. Materials Horizons, 2022, 9, 1649-1657.	12.2	3
5	Reversible dehydrogenation and rehydrogenation of cyclohexane and methylcyclohexane by single-site platinum catalyst. Nature Communications, 2022, 13, 1092.	12.8	41
6	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
7	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
8	Nature of the Electrical Double Layer on Suspended Graphene Electrodes. Journal of the American Chemical Society, 2022, 144, 13327-13333.	13.7	8
9	Layer Edge States Stabilized by Internal Electric Fields in Two-Dimensional Hybrid Perovskites. Nano Letters, 2021, 21, 182-188.	9.1	14
10	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
11	Revealing Charge-Transfer Dynamics at Electrified Sulfur Cathodes Using Constrained Density Functional Theory. Journal of Physical Chemistry Letters, 2021, 12, 739-744.	4.6	5
12	CuBi₂O₄: Electronic Structure, Optical Properties, and Photoelectrochemical Performance Limitations of the Photocathode. Chemistry of Materials, 2021, 33, 934-945.	6.7	45
13	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
14	Understanding the Structural Evolution of a Nickel Chalcogenide Electrocatalyst Surface for Water Oxidation. Energy & Fuels, 2021, 35, 4387-4403.	5.1	33
15	Electronic structure modulation of MoS2 by substitutional Se incorporation and interfacial MoO3 hybridization: Implications of Fermi engineering for electrocatalytic hydrogen evolution and oxygen evolution. Chemical Physics Reviews, 2021, 2, .	5.7	8
16	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
17	Anion-Assisted Delivery of Multivalent Cations to Inert Electrodes. Journal of Physical Chemistry Letters, 2021, 12, 4347-4356.	4.6	17
18	Diversity-oriented synthesis of polymer membranes with ion solvation cages. Nature, 2021, 592, 225-231.	27.8	83

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19	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
20	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
21	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
22	Using cryo-TEM to study the effect of side-chain chemistry on the crystal motifs in polypeptoid nanosheets. Microscopy and Microanalysis, 2021, 27, 2894-2895.	0.4	1
23	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
24	Controlled Experiments and Optimized Theory of Absorption Spectra of Li Metal and Salts. ACS Applied Materials & Interfaces, 2021, 13, 45488-45495.	8.0	8
25	Lessons learned from FeSb2O4 on stereoactive lone pairs as a design principle for anion insertion. Cell Reports Physical Science, 2021, 2, 100592.	5.6	3
26	Exploring the Ion Solvation Environments in Solid-State Polymer Electrolytes through Free-Energy Sampling. Macromolecules, 2021, 54, 8590-8600.	4.8	3
27	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
28	Ultrafast core-excited electron dynamics in model crystalline organic semiconductors. Physical Chemistry Chemical Physics, 2020, 22, 1400-1408.	2.8	1
29	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
30	Addressing the sensitivity of signals from solid/liquid ambient pressure XPS (APXPS) measurement. Journal of Chemical Physics, 2020, 153, 044709.	3.0	16
31	Revealing Nanoscale Chemical Heterogeneities in Polycrystalline Moâ€BiVO₄ Thin Films. Small, 2020, 16, e2001600.	10.0	12
32	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
33	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
34	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
35	Revealing electronic state-switching at conical intersections in alkyl iodides by ultrafast XUV transient absorption spectroscopy. Nature Communications, 2020, 11, 4042.	12.8	40
36	Metal-Insulator Transitions in Î²â€²-Cu V2O5 Mediated by Polaron Oscillation and Cation Shuttling. Matter, 2020, 2, 1166-1186.	10.0	9

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37	Investigating extreme ultraviolet radiation chemistry with first-principles quantum chemistry calculations. Journal of Micro/ Nanolithography, MEMS, and MOEMS, 2020, 19, .	0.9	4
38	Excitation selectivity in model tin-oxo resist: a computational chemistry perspective. , 2020, , .		1
39	Infrared Nanospectroscopy at the Grapheneâ€“Electrolyte Interface. Nano Letters, 2019, 19, 5388-5393.	9.1	55
40	Direct observation of delithiation as the origin of analog memristance in LixNbO2. APL Materials, 2019, 7, .	5.1	13
41	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
42	Graphene/h-BN In-Plane Heterostructures: Stability and Electronic and Transport Properties. Journal of Physical Chemistry C, 2019, 123, 18600-18608.	3.1	5
43	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
44	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
45	Design Rules for Membranes from Polymers of Intrinsic Microporosity for Crossover-free Aqueous Electrochemical Devices. Joule, 2019, 3, 2968-2985.	24.0	84
46	Runaway Carbon Dioxide Conversion Leads to Enhanced Uptake in a Nanohybrid Form of Porous Magnesium Borohydride. Advanced Materials, 2019, 31, e1904252.	21.0	10
47	Taming convergence in the determinant approach for x-ray excitation spectra. Physical Review B, 2019, 100, .	3.2	10
48	Exploring chemical speciation at electrified interfaces using detailed continuum models. Journal of Chemical Physics, 2019, 150, 041725.	3.0	13
49	Metalâ€“oxygen decoordination stabilizes anion redox in Li-rich oxides. Nature Materials, 2019, 18, 256-265.	27.5	280
50	The purported square ice in bilayer graphene is a nanoscale, monolayer object. Journal of Chemical Physics, 2019, 150, 231101.	3.0	7
51	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
52	Identifying Catalytic Active Sites of Trimolybdenum Phosphide (Mo₃P) for Electrochemical Hydrogen Evolution. Advanced Energy Materials, 2019, 9, 1900516.	19.5	47
53	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
54	Electronic Structure and Performance Bottlenecks of CuFeO₂ Photocathodes. Chemistry of Materials, 2019, 31, 2524-2534.	6.7	43

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55	Understanding the effect of thionation on naphthalene diimide using first-principles predictions of near-edge x-ray absorption fine structure spectra. Journal of Chemical Physics, 2019, 150, 104302.	3.0	4
56	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
57	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
58	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
59	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
60	Evidence of a second-order Peierls-driven metal-insulator transition in crystalline NbO2. Physical Review Materials, 2019, 3, .	2.4	18
61	Designing Catalysts for Water Splitting Based on Electronic Structure Considerations. ECS Meeting Abstracts, 2019, , .	0.0	0
62	Investigating EUV radiation chemistry with first principle quantum chemistry calculations. , 2019, , .		1
63	Mapping Catalytically Relevant Edge Electronic States of MoS₂. ACS Central Science, 2018, 4, 493-503.	11.3	39
64	Velocity-gauge real-time TDDFT within a numerical atomic orbital basis set. Computer Physics Communications, 2018, 226, 30-38.	7.5	45
65	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
66	Reversible Mg-Ion Insertion in a Metastable One-Dimensional Polymorph of V2O5. CheM, 2018, 4, 564-585.	11.7	126
67	Dual roles of f electrons in mixing Al 3p character into d -orbital conduction bands for lanthanide and actinide dialuminides. Physical Review B, 2018, 97, .	3.2	4
68	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
69	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
70	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
71	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
72	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

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73	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
74	Fundamental understanding of chemical processes in extreme ultraviolet resist materials. Journal of Chemical Physics, 2018, 149, 154305.	3.0	15
75	Probing the electric field-induced doping mechanism in YBa2Cu3O7 using computed Cu K-edge x-ray absorption spectra. Journal of Chemical Physics, 2018, 149, 234706.	3.0	8
76	Cooperative adsorption of carbon disulfide in diamine-appended metalâ€“organic frameworks. Nature Communications, 2018, 9, 5133.	12.8	28
77	Imaging Unstained Synthetic Polymer Crystals and Defects on Atomic Length Scales Using Cryogenic Electron Microscopy. Macromolecules, 2018, 51, 7794-7799.	4.8	36
78	Nanostructured Metal Hydrides for Hydrogen Storage. Chemical Reviews, 2018, 118, 10775-10839.	47.7	461
79	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
80	Hybrid DFT investigation of the energetics of Mg ion diffusion in Î±-MoO₃. Physical Chemistry Chemical Physics, 2018, 20, 24877-24884.	2.8	10
81	Quantum many-body effects in x-ray spectra efficiently computed using a basic graph algorithm. Physical Review B, 2018, 97, .	3.2	21
82	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
83	Cooperative Gas Adsorption without a Phase Transition in Metal-Organic Frameworks. Physical Review Letters, 2018, 121, 015701.	7.8	17
84	Critical Factors in Computational Characterization of Hydrogen Storage in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2018, 122, 18957-18967.	3.1	21
85	Solution-Based, Template-Assisted Realization of Large-Scale Graphitic ZnO. ACS Nano, 2018, 12, 7554-7561.	14.6	23
86	Electron dynamics in transition metal dichalcogenides utilizing attosecond transient absorption spectroscopy. , 2018, , .		0
87	(Invited) First-Principles Approaches to Modeling Electrochemical Interfaces Validated By X-Ray Spectroscopy. ECS Meeting Abstracts, 2018, , .	0.0	0
88	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
89	Determining crystal phase purity in c-BP through X-ray absorption spectroscopy. Physical Chemistry Chemical Physics, 2017, 19, 8174-8187.	2.8	7
90	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

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91	Improved treatment of exact exchange in Quantum ESPRESSO. Computer Physics Communications, 2017, 214, 52-58.	7.5	36
92	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
93	Detection of defect populations in superhard semiconductor boron subphosphide B₁₂P₂ through X-ray absorption spectroscopy. Journal of Materials Chemistry A, 2017, 5, 5737-5749.	10.3	7
94	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
95	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
96	Chemical and Morphological Inhomogeneity of Aluminum Metal and Oxides from Soft X-ray Spectromicroscopy. Inorganic Chemistry, 2017, 56, 5710-5719.	4.0	12
97	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
98	Thermodynamic origins of the solvent-dependent stability of lithium polysulfides from first principles. Physical Chemistry Chemical Physics, 2017, 19, 1441-1448.	2.8	41
99	Direct and simultaneous observation of ultrafast electron and hole dynamics in germanium. Nature Communications, 2017, 8, 15734.	12.8	117
100	Ultrafast carrier thermalization and trapping in silicon-germanium alloy probed by extreme ultraviolet transient absorption spectroscopy. Structural Dynamics, 2017, 4, 044029.	2.3	42
101	Femtosecond x-ray spectroscopy of an electrocyclic ring-opening reaction. Science, 2017, 356, 54-59.	12.6	253
102	Coordination Characteristics of Uranyl BBP Complexes: Insights from an Electronic Structure Analysis. ACS Omega, 2017, 2, 1055-1062.	3.5	6
103	Liquid Sulfur Impregnation of Microporous Carbon Accelerated by Nanoscale Interfacial Effects. Nano Letters, 2017, 17, 2517-2523.	9.1	16
104	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
105	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
106	Instability at the Electrode/Electrolyte Interface Induced by Hard Cation Chelation and Nucleophilic Attack. Chemistry of Materials, 2017, 29, 8504-8512.	6.7	74
107	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
108	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

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109	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
110	Coupling between oxygen redox and cation migration explains unusual electrochemistry in lithium-rich layered oxides. Nature Communications, 2017, 8, 2091.	12.8	469
111	Evaluation of Multivalent Cation Insertion in Single- and Double-Layered Polymorphs of V₂O₅. ACS Applied Materials & Interfaces, 2017, 9, 23756-23765.	8.0	64
112	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
113	Monitoring Deformation in Graphene Through Hyperspectral Synchrotron Spectroscopy to Inform Fabrication. Journal of Physical Chemistry C, 2017, 121, 15653-15664.	3.1	3
114	Soft X-ray absorption spectroscopy investigation of the surface chemistry and treatments of copper indium gallium diselenide (CIGS). Solar Energy Materials and Solar Cells, 2017, 160, 390-397.	6.2	0
115	Identifying anthropogenic uranium compounds using soft X-ray near-edge absorption spectroscopy. Spectrochimica Acta, Part B: Atomic Spectroscopy, 2017, 127, 20-27.	2.9	7
116	Molecular understanding of polyelectrolyte binders that actively regulate ion transport in sulfur cathodes. Nature Communications, 2017, 8, 2277.	12.8	117
117	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
118	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
119	Synthesis of a mixed-valent tin nitride and considerations of its possible crystal structures. Journal of Chemical Physics, 2016, 144, 144201.	3.0	29
120	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
121	Understanding and control of bipolar self-doping in copper nitride. Journal of Applied Physics, 2016, 119, .	2.5	30
122	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
123	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
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	Lithium Polysulfide Radical Anions in Ether-Based Solvents. Journal of Physical Chemistry C, 2016, 120, 18403-18410.	3.1	65
126	Building a Fast Lane for Mg Diffusion in Î±-MoO₃ by Fluorine Doping. Chemistry of Materials, 2016, 28, 6900-6908.	6.7	60

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127	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
128	Selective gas capture via kinetic trapping. Physical Chemistry Chemical Physics, 2016, 18, 21760-21766.	2.8	5
129	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
130	Reprint of: Combining theory and experiment for X-ray absorption spectroscopy and resonant X-ray scattering characterization of polymers. Polymer, 2016, 105, 342-356.	3.8	8
131	Self-healing in B₁₂P₂ through Mediated Defect Recombination. Chemistry of Materials, 2016, 28, 8415-8428.	6.7	9
132	Mapping polaronic states and lithiation gradients in individual V2O5 nanowires. Nature Communications, 2016, 7, 12022.	12.8	115
133	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
134	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
135	Reversible Magnesium Intercalation into a Layered Oxyfluoride Cathode. Chemistry of Materials, 2016, 28, 17-20.	6.7	70
136	Properties of aqueous nitrate and nitrite from x-ray absorption spectroscopy. Journal of Chemical Physics, 2015, 143, 084503.	3.0	30
137	Communication: On the difficulty of reproducibly measuring PbCl2 X-ray absorption spectra. Journal of Chemical Physics, 2015, 143, 111102.	3.0	1
138	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
139	Attosecond Spectroscopy of Band-gap Dynamics. , 2015, , .		0
140	Exploring the time-scale of photo-initiated interfacial electron transfer through first-principles interpretation of ultrafast X-ray spectroscopy (Presentation Recording). Proceedings of SPIE, 2015, , .	0.8	0
141	Efficient implementation of core-excitation Betheâ€“Salpeter equation calculations. Computer Physics Communications, 2015, 197, 109-117.	7.5	142
142	Chemically directing d-block heterometallics to nanocrystal surfaces as molecular beacons of surface structure. Chemical Science, 2015, 6, 6295-6304.	7.4	1
143	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
144	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	27.8	1,026

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145	The hydration structure of dissolved carbon dioxide from X-ray absorption spectroscopy. Chemical Physics Letters, 2015, 633, 214-217.	2.6	16
146	Polysulfide-Blocking Microporous Polymer Membrane Tailored for Hybrid Li-Sulfur Flow Batteries. Nano Letters, 2015, 15, 5724-5729.	9.1	153
147	Chemical doping enhances electronic transport in networks of hexabenzocoronenes assembled in non-aqueous electrolyte. Polymer Chemistry, 2015, 6, 5560-5564.	3.9	2
148	X-ray spectroscopy as a probe for lithium polysulfide radicals. Physical Chemistry Chemical Physics, 2015, 17, 7743-7753.	2.8	43
149	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
150	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
151	Mg Desolvation and Intercalation Mechanism at the Mo₆S₈ Chevrel Phase Surface. Chemistry of Materials, 2015, 27, 5932-5940.	6.7	157
152	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
153	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
154	Electrokinetic detection for X-ray spectra of weakly interacting liquids: n-decane and n-nonane. Journal of Chemical Physics, 2014, 140, 234202.	3.0	7
155	Attosecond band-gap dynamics in silicon. Science, 2014, 346, 1348-1352.	12.6	415
156	The structure of interfacial water on gold electrodes studied by x-ray absorption spectroscopy. Science, 2014, 346, 831-834.	12.6	391
157	Bonding and Charge Transfer in Nitrogen-Donor Uranyl Complexes: Insights from NEXAFS Spectra. Inorganic Chemistry, 2014, 53, 11415-11425.	4.0	15
158	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
159	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
160	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
161	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
162	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

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163	The hydration structure of aqueous carbonic acid from X-ray absorption spectroscopy. Chemical Physics Letters, 2014, 614, 282-286.	2.6	22
164	Atomic-Scale Perspective of Ultrafast Charge Transfer at a Dyeâ€“Semiconductor Interface. Journal of Physical Chemistry Letters, 2014, 5, 2753-2759.	4.6	79
165	Toward Equatorial Planarity about Uranyl: Synthesis and Structure of Tridentate Nitrogen-Donor {UO₂}²⁺ Complexes. Inorganic Chemistry, 2014, 53, 2506-2515.	4.0	17
166	Fingerprinting Lithium-Sulfur Battery Reaction Products by X-ray Absorption Spectroscopy. Journal of the Electrochemical Society, 2014, 161, A1100-A1106.	2.9	76
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