John J Rehr

List of Publications by Year
in descending order

133 papers	13,387 citations	109321 35 h-index	20961 115 g-index
137 all docs	137 docs citations	137 times ranked	12710 citing authors

#	Article	IF	Citations
1	Real-space multiple-scattering calculation and interpretation of x-ray-absorption near-edge structure. Physical Review B, 1998, 58, 7565-7576.	3.2	4,006
2	Theoretical approaches to x-ray absorption fine structure. Reviews of Modern Physics, 2000, 72, 621-654.	45.6	2,843
3	Parameter-free calculations of X-ray spectra with FEFF9. Physical Chemistry Chemical Physics, 2010, 12, 5503.	2.8	985
4	Scattering-matrix formulation of curved-wave multiple-scattering theory: Application to x-ray-absorption fine structure. Physical Review B, 1990, 41, 8139-8149.	3.2	598
5	Ab initio theory and calculations of X-ray spectra. Comptes Rendus Physique, 2009, 10, 548-559.	0.9	468
6	Parallel calculation of electron multiple scattering using Lanczos algorithms. Physical Review B, 2002, 65, .	3.2	466
7	Dynamic screening effects in x-ray absorption spectra. Physical Review B, 2003, 67, .	3.2	264
8	Bethe-Salpeter equation calculations of core excitation spectra. Physical Review B, 2011, 83, .	3.2	228
9	Real-time time-dependent density functional theory approach for frequency-dependent nonlinear optical response in photonic molecules. Journal of Chemical Physics, 2007, 127, 154114.	3.0	158
10	Multiple-scattering x-ray-absorption fine-structure Debye-Waller factor calculations. Physical Review B, 1999, 59, 948-957.	3.2	150
11	X-ray and Electron Spectroscopy of Water. Chemical Reviews, 2016, 116, 7551-7569.	47.7	143
12	Extended x-ray-absorption fine-structure amplitudesâ€”Wave-function relaxation and chemical effects. Physical Review B, 1978, 17, 560-565.	3.2	140
13	Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations. Physical Review B, 2014, 89, .	3.2	138
14	Theoretical x-ray absorption Debye-Waller factors. Physical Review B, 2007, 76, .	3.2	126
15	Valence Electron Photoemission Spectrum of Semiconductors:AbÂInitioDescription of Multiple Satellites. Physical Review Letters, 2011, 107, 166401.	7.8	120
16	Inelastic scattering from core electrons: A multiple scattering approach. Physical Review B, 2005, 72, .	3.2	100
17	High-throughput computational X-ray absorption spectroscopy. Scientific Data, 2018, 5, 180151.	5.3	94
18	Experimental (XAS, STEM, TPR, and XPS) and Theoretical (DFT) Characterization of Supported Rhenium Catalysts. Journal of Physical Chemistry C, 2011, 115, 5740-5755.	3.1	83

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19	Automated generation and ensemble-learned matching of X-ray absorption spectra. Npj Computational Materials, 2018, 4, .	8.7	82
20	Dynamic structure in supported Pt nanoclusters: Real-time density functional theory and x-ray spectroscopy simulations. Physical Review B, 2008, 78, .	3.2	77
21	Cumulant expansion of the retarded one-electron Green function. Physical Review B, 2014, 90, .	3.2	77
22	Many-pole model of inelastic losses in x-ray absorption spectra. Physical Review B, 2007, 76, .	3.2	68
23	Progress and challenges in the theory and interpretation of X-ray spectra. Journal of Synchrotron Radiation, 2001, 8, 61-65.	2.4	62
24	Interference between extrinsic and intrinsic losses in x-ray absorption fine structure. Physical Review B, 2002, 65, .	3.2	61
25	Dynamical effects in electron spectroscopy. Journal of Chemical Physics, 2015, 143, 184109.	3.0	57
26	Optical to UV spectra and birefringence of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu First-principles calculations with excitonic effects. Physical Review B, 2008, 78, .	3.2	56
27	Extended X-Ray Absorption Fine Structure from Hydrogen Atoms in Water. Physical Review Letters, 2000, 85, 4289-4292.	7.8	47
28	Role of inversion symmetry and multipole effects in nonresonant x-ray Raman scattering from icosahedralB4C. Physical Review B, 2004, 69, .	3.2	47
29	Theoretical optical and x-ray spectra of liquid and solid H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O. Physical Review B, 2012, 85, .	3.2	47
30	Ab initiocalculations of electron inelastic mean free paths and stopping powers. Physical Review B, 2006, 74, .	3.2	46
31	Basis set effects on the hyperpolarizability of CHCl3: Gaussian-type orbitals, numerical basis sets and real-space grids. Journal of Chemical Physics, 2010, 133, 034111.	3.0	46
32	The status of strontium in biological apatites: anÂXANES/EXAFS investigation. Journal of Synchrotron Radiation, 2014, 21, 136-142.	2.4	43
33	FinalState Rule vs the BetheSalpeter Equation for DeepCore Xray Absorption Spectra. Physica Scripta, 2005, , 207.	2.5	40
34	Multiple satellites in materials with complex plasmon spectra: From graphite to graphene. Physical Review B, 2014, 89, .	3.2	38
35	Real-time cumulant approach for charge-transfer satellites in x-ray photoemission spectra. Physical Review B, 2015, 91, .	3.2	38
36	Frequency and Solvent Dependence of Nonlinear Optical Properties of Molecules. Journal of Physical Chemistry C, 2008, 112, 8016-8021.	3.1	37

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37	Electronic Structures of Formic Acid (HCOOH) and Formate (HCOO^{â€“}) in Aqueous Solutions. Journal of Physical Chemistry Letters, 2012, 3, 1754-1759.	4.6	35
38	Real-space Greenâ€™s function approach to resonant inelastic x-ray scattering. Physical Review B, 2011, 83, .	3.2	34
39	Finite Temperature Greenâ€™s Function Approach for Excited State and Thermodynamic Properties of Cool to Warm Dense Matter. Physical Review Letters, 2017, 119, 176403.	7.8	34
40	Operando Effects on the Structure and Dynamics of Pt_nSn_m/Î³-Al₂O₃ from Ab Initio Molecular Dynamics and X-ray Absorption Spectra. Journal of Physical Chemistry C, 2013, 117, 12446-12457.	3.1	33
41	Multiple scattering calculations of relativistic electron energy loss spectra. Physical Review B, 2010, 81, .	3.2	32
42	Particle-hole cumulant approach for inelastic losses in x-ray spectra. Physical Review B, 2016, 94, .	3.2	32
43	Interpretation of x-ray magnetic circular dichroism and x-ray absorption near-edge structure in Ni. Physical Review B, 2000, 62, 15295-15298.	3.2	31
44	Real space calculation of optical constants from optical to x-ray frequencies. Physical Review B, 2009, 80, .	3.2	31
45	X-ray absorption Debye-Waller factors fromab initiomolecular dynamics. Physical Review B, 2012, 85, .	3.2	31
46	Cumulant expansion for phonon contributions to the electron spectral function. Physical Review B, 2014, 90, .	3.2	30
47	Order-disorder behavior in the phase transition of PbTiO3. Ferroelectrics, 1995, 164, 265-277.	0.6	29
48	Background proportional enhancement of the extended fine structure in nonresonant inelastic x-ray scattering. Physical Review B, 2006, 74, .	3.2	29
49	Characterization of Coke on a Pt-Re/Î³-Al₂O₃ Re-Forming Catalyst: Experimental and Theoretical Study. ACS Catalysis, 2017, 7, 1452-1461.	11.2	29
50	Deconvolving instrumental and intrinsic broadening in core-shell x-ray spectroscopies. Physical Review B, 2007, 75, .	3.2	28
51	Theoretical chemical contribution to the simulation of the LIII X-ray absorption edges of uranyl, neptunyl and osmyl hydrates and hydroxides. New Journal of Chemistry, 2004, 28, 929.	2.8	27
52	Plasmon satellites in valence-band photoemission spectroscopy. European Physical Journal B, 2012, 85, 1.	1.5	27
53	Advanced calculations of X-ray spectroscopies with FEFF10 and Corvus. Journal of Synchrotron Radiation, 2021, 28, 1801-1810.	2.4	27
54	Exciton spectroscopy of hexagonal boron nitride using nonresonant x-ray Raman scattering. Physical Review B, 2008, 77, .	3.2	26

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55	Intermediate-range order in water ices: Nonresonant inelastic x-ray scattering measurements and real-space full multiple scattering calculations. Physical Review B, 2009, 79, .	3.2	26
56	How Accurately Can Extended X-ray Absorption Spectra Be Predicted from First Principles? Implications for Modeling the Oxygen-Evolving Complex in Photosystem II. Journal of the American Chemical Society, 2015, 137, 12815-12834.	13.7	26
57	Equation of motion coupled-cluster cumulant approach for intrinsic losses in x-ray spectra. Journal of Chemical Physics, 2020, 152, 174113.	3.0	25
58	New developments in the theory and interpretation of X-ray spectra based on fast parallel calculations. Journal of Synchrotron Radiation, 2003, 10, 43-45.	2.4	24
59	Importance of Multiple-Scattering Phenomena in XAS Structural Determinations of [Ni(CN)4]2-in Condensed Phases. Inorganic Chemistry, 2000, 39, 3784-3790.	4.0	22
60	Cumulant Green's function calculations of plasmon satellites in bulk sodium: Influence of screening and the crystal environment. Physical Review B, 2018, 97, .	3.2	21
61	Database of ab initio L-edge X-ray absorption near edge structure. Scientific Data, 2021, 8, 153.	5.3	21
62	Real-Time Coupled-Cluster Approach for the Cumulant Greenâ€™s Function. Journal of Chemical Theory and Computation, 2020, 16, 6983-6992.	5.3	19
63	Comment on â€œOperando DRIFTS and XANES Study of Deactivating Effect of CO₂ on a Ce_{0.8}Cu_{0.2}O₂ CO-PROX Catalystâ€. Journal of Physical Chemistry C, 2011, 115, 23233-23236.	3.1	18
64	Local time-correlation approach for calculations of x-ray spectra. Physical Review B, 2012, 86, .	3.2	18
65	Resonant Inelastic X-ray Scattering of Molybdenum Oxides and Sulfides. Journal of Physical Chemistry C, 2015, 119, 2419-2426.	3.1	18
66	Anomalous Structural Disorder in Supported Pt Nanoparticles. Journal of Physical Chemistry Letters, 2017, 8, 3284-3288.	4.6	18
67	Unraveling intrinsic correlation effects with angle-resolved photoemission spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 28596-28602.	7.1	18
68	Effects of Adsorbate Coverage and Bondâ€Length Disorder on the dâ€Band Center of Carbonâ€Supported Pt Catalysts. ChemPhysChem, 2014, 15, 1569-1572.	2.1	17
69	Charge transfer satellites in x-ray spectra of transition metal oxides. Physical Review B, 2014, 89, .	3.2	17
70	Recursion method for multiple-scattering XAFS Debyeâ€“Waller factors. Journal of Synchrotron Radiation, 1999, 6, 313-314.	2.4	16
71	Modeling CoreHole Screening in CoreExcitation Spectroscopies. Physica Scripta, 2005, , 31.	2.5	16
72	Bayesâ€“Turchin approach to XAS analysis. Journal of Synchrotron Radiation, 2005, 12, 70-74.	2.4	16

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73	Many-pole model of inelastic losses applied to calculations of XANES. Journal of Physics: Conference Series, 2009, 190, 012009.	0.4	16
74	Refinement of a Model for the Nitrogenase Moï£¿Fe Cluster Using Single-Crystal Mo and Fe EXAFS. Angewandte Chemie International Edition in English, 1993, 32, 1592-1594.	4.4	14
75	Theory of dynamical scattering in near-edge electron energy loss spectroscopy. Physical Review B, 2009, 80, .	3.2	14
76	Charge-transfer satellites and chemical bonding in photoemission and x-ray absorption of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and rutile <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> : Expe	3.2	14
77	Efficient Calculation of the Negative Thermal Expansion in ZrW2O8. Frontiers in Chemistry, 2018, 6, 296.	3.6	13
78	Energy-Dependent Relative Cross Sections in Carbon 1s Photoionization: Separation of Direct Shake and Inelastic Scattering Effects in Single Molecules. Journal of Physical Chemistry A, 2019, 123, 7619-7636.	2.5	12
79	X-ray absorption near-edge spectra of overdoped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">La</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">Sr</mml:mi><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">CuO</mml:mi><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>high- xmlns:m. Physical Review B, 2011, 83, .	3.2	11
80	Molecular Dynamics Simulations of Supported Pt Nanoparticles with a Hybrid Suttonâ€“Chen Potential. Journal of Physical Chemistry C, 2016, 120, 14883-14891.	3.1	11
81	Core hole processes in x-ray absorption and photoemission by resonant Auger-electron spectroscopy and first-principles theory. Physical Review B, 2020, 101, .	3.2	11
82	Strengths of plasmon satellites in XPS: Real-time cumulant approach. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2021, 39, .	2.1	11
83	Size and Shape of Rhenium Nanoparticles. AIP Conference Proceedings, 2007, , .	0.4	10
84	XMCD Analysis Beyond Standard Procedures. AIP Conference Proceedings, 2007, , .	0.4	10
85	Coulomb-hole and screened exchange in the electron self-energy at finite temperature. Physical Review B, 2018, 98, .	3.2	10
86	Probing the Local Bonding at the Pt/Î³-Al₂O₃ Interface. Journal of Physical Chemistry C, 2020, 124, 9876-9885.	3.1	10
87	Real-Time Equation-of-Motion CCSD Cumulant Greenâ€™s Function. Journal of Chemical Theory and Computation, 2022, 18, 1799-1807.	5.3	10
88	Verfeinerung eines Modells fÃ¼r den Nitrogenase-Mo-Fe-Cluster mit Einkristall-Mo- und -Fe-EXAFS. Angewandte Chemie, 1993, 105, 1661-1663.	2.0	9
89	X-Ray Absorption Spectroscopy of Organouranium Compounds in the (+V) and (+IV) Oxidation States. Radiochimica Acta, 1997, 76, 211-218.	1.2	9
90	Rapid calculation of x-ray absorption near edge structure using parallel computation. X-Ray Spectrometry, 2001, 30, 431-434.	1.4	9

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91	Chemical speciation via X-ray emission spectra. X-Ray Spectrometry, 2006, 35, 312-318.	1.4	9
92	Magic angle in electron energy loss spectra: Relativistic and dielectric corrections. Physical Review B, 2008, 77, .	3.2	9
93	Dynamic structural disorder in supported nanoscale catalysts. Journal of Chemical Physics, 2014, 140, 134701.	3.0	9
94	Intracluster Atomic and Electronic Structural Heterogeneities in Supported Nanoscale Metal Catalysts. Journal of Physical Chemistry C, 2015, 119, 25615-25627.	3.1	9
95	Probing electronic structure of stoichiometric and defective <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Sn</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2017, 95, .	3.2	9
96	Exchange-correlation contributions to thermodynamic properties of the homogeneous electron gas from a cumulant Green's function approach. Physical Review B, 2019, 100, .	3.2	9
97	Real-space Green's function approach for x-ray spectra at high temperature. Physical Review B, 2021, 104, .	3.2	9
98	Nonlinear response in the cumulant expansion for core-level photoemission. Physical Review Research, 2020, 2, .	3.6	9
99	Extended X-Ray Absorption Fine Structure of ZrW2O8: Theory vs. Experiment. Frontiers in Chemistry, 2018, 6, 356.	3.6	8
100	Equation-of-Motion Coupled-Cluster Cumulant Greenâ€™s Function for Excited States and X-Ray Spectra. Frontiers in Chemistry, 2021, 9, 734945.	3.6	8
101	Failure of the Quasiparticle Picture of X-ray Absorption?. Foundations of Physics, 2003, 33, 1735-1742.	1.3	7
102	Exchange and correlation in finite-temperature TDDFT. European Physical Journal B, 2018, 91, 1.	1.5	7
103	Magnetic extended x-ray absorption fine structure at the L3,2 edges of Fe and Co on Cu(001). Journal of Applied Physics, 1998, 83, 7025-7027.	2.5	6
104	Time-dependent density functional theory calculations of X-ray absorption. International Journal of Quantum Chemistry, 2003, 95, 487-492.	2.0	6
105	Ab initioanalysis of the x-ray absorption spectrum of the myoglobinâ€“carbon monoxide complex: Structure and vibrations. Physical Review B, 2010, 82, .	3.2	6
106	Quantitative first-principles calculations of valence and core excitation spectra of solid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>. Physical Review B, 2017, 95, .	3.2	6
107	Full spectrum optical constant interface to the Materials Project. Computational Materials Science, 2022, 201, 110904.	3.0	6
108	AbÂInitio Multiplet-Plus-Cumulant Approach for Correlation Effects in X-Ray Photoelectron Spectroscopy. Physical Review Letters, 2022, 128, .	7.8	6

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109	The rediscovery of the â€˜French Blueâ€™ diamond. Europhysics News, 2012, 43, 22-25.	0.3	5
110	Corvus: a framework for interfacing scientific software for spectroscopic and materials science applications. Journal of Synchrotron Radiation, 2019, 26, 1694-1704.	2.4	5
111	Lattice Model of Resonant Inelastic X-Ray Scattering in Metals: Relation of a Strong Core Hole to the X-Ray Edge Singularity. Physical Review Letters, 2014, 112, 237401.	7.8	4
112	Relativistic Diracâ€“Fock atom properties for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si25.gif" display="inline" overflow="scroll"><mml:mi>Z</mml:mi><mml:mo>=</mml:mo><mml:mn>121</mml:mn></mml:math> to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si26.gif" display="inline" overflow="scroll"><mml:mi>Z</mml:mi><mml:mo>=</mml:mo><mml:mn>138</mml:mn></mml:math>. Atomic Data and Nuclear Data Tables, 2017, 114, 262-280.	2.4	4
113	Real-time equation-of-motion CC cumulant and CC Greenâ€™s function simulations of photoemission spectra of water and water dimer. Journal of Chemical Physics, 2022, 157, .	3.0	4
114	Crystal effects in Î²-decay. Nature, 1991, 354, 436-437.	27.8	3
115	Inelastic Losses and Multi-Electron Excitations in X-Ray Spectra. AIP Conference Proceedings, 2007, , .	0.4	3
116	The effect of self-consistent potentials on EXAFS analysis. Journal of Synchrotron Radiation, 2017, 24, 1173-1179.	2.4	3
117	Bethe-Salpeter Equation calculations of nitrogen-vacancy defects in diamond. Journal of Physics and Chemistry of Solids, 2018, 122, 87-93.	4.0	3
118	Web-based methods for X-ray and photoelectron spectroscopies. Computational Materials Science, 2021, 200, 110814.	3.0	3
119	Ab initio calculation of X-ray and related core-level spectroscopies: Green's function approaches. Physical Chemistry Chemical Physics, 2022, 24, 13461-13473.	2.8	3
120	Calculation of X-ray absorption structure above K-edge of laser shock-compressed aluminum. Laser and Particle Beams, 1990, 8, 319-325.	1.0	2
121	HIGH ORDER MULTIPLE SCATTERING THEORY OF XAFS. Advanced Series in Physical Chemistry, 2002, , 1213-1227.	1.5	1
122	High-performance computing without commitment: SC2IT: A cloud computing interface that makes computational science available to non-specialists. , 2012, , .		1
123	Comment on â€œElectromagnetic Vortex Fields, Spin, and Spin-Orbit Interactions in Electron Verticesâ€• Physical Review Letters, 2014, 113, 029501.	7.8	1
124	Correlative Structure-Bonding and Stability Studies of Pt/Î³-Al2O3 Catalysts. Microscopy and Microanalysis, 2018, 24, 1644-1645.	0.4	1
125	Determination of the Crystal Structure of Gamma-Alumina by Electron Diffraction and Electron Energy-Loss Spectroscopy. Microscopy and Microanalysis, 2019, 25, 2036-2037.	0.4	1
126	Calculation and interpretation of X-ray spectroscopies with Greenâ€™s function multiple scattering theory. AIP Conference Proceedings, 2000, , .	0.4	0

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127	Ab initio Real Space Calculations of Electron Energy Loss Spectra. AIP Conference Proceedings, 2008, , .	0.4	0
128	Investigation of the Structural and Electronic Properties of Pt/Î³-Al2O3, a Model Catalyst System. Microscopy and Microanalysis, 2015, 21, 1655-1656.	0.4	0
129	Real-space multiple-scattering Hubbard model calculations ford- andf-state materials. Journal of Synchrotron Radiation, 2015, 22, 1042-1048.	2.4	0
130	Comparison of Spinel and Monoclinic Crystal Structures of Î³-Al2O3 for Simulation of Electron Energy Loss Spectra. Microscopy and Microanalysis, 2017, 23, 2020-2021.	0.4	0
131	A consistent path for phase determination based on transmission electron microscopy techniques and supporting simulations. Micron, 2018, 115, 41-49.	2.2	0
132	Noble-metal dark-edge fermiology: Centrifugal barriers, core-hole memory, and the Zeeman Auger effect. Physical Review B, 2021, 104, .	3.2	0
133	Greenâ€™s function methods for excited states and x-ray spectra of functional materials. Electronic Structure, 0, , .	2.8	0