

John J Rehr

List of Publications by Year in descending order

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133
papers

13,387
citations

109321

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20961

115
g-index

137
all docs

137
docs citations

137
times ranked

12710
citing authors

#	ARTICLE	IF	CITATIONS
1	Full spectrum optical constant interface to the Materials Project. Computational Materials Science, 2022, 201, 110904.	3.0	6
2	Real-Time Equation-of-Motion CCSD Cumulant Green's Function. Journal of Chemical Theory and Computation, 2022, 18, 1799-1807.	5.3	10
3	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
4	Ab Initio Multiplet-Plus-Cumulant Approach for Correlation Effects in X-Ray Photoelectron Spectroscopy. Physical Review Letters, 2022, 128, .	7.8	6
5	Real-time equation-of-motion CC cumulant and CC Green's function simulations of photoemission spectra of water and water dimer. Journal of Chemical Physics, 2022, 157, .	3.0	4
6	Database of ab initio L-edge X-ray absorption near edge structure. Scientific Data, 2021, 8, 153.	5.3	21
7	Real-space Green's function approach for x-ray spectra at high temperature. Physical Review B, 2021, 104, .	3.2	9
8	Equation-of-Motion Coupled-Cluster Cumulant Green's Function for Excited States and X-Ray Spectra. Frontiers in Chemistry, 2021, 9, 734945.	3.6	8
9	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
10	Web-based methods for X-ray and photoelectron spectroscopies. Computational Materials Science, 2021, 200, 110814.	3.0	3
11	Advanced calculations of X-ray spectroscopies with FEFF10 and Corvus. Journal of Synchrotron Radiation, 2021, 28, 1801-1810.	2.4	27
12	Noble-metal dark-edge fermiology: Centrifugal barriers, core-hole memory, and the Zeeman Auger effect. Physical Review B, 2021, 104, .	3.2	0
13	Real-Time Coupled-Cluster Approach for the Cumulant Green's Function. Journal of Chemical Theory and Computation, 2020, 16, 6983-6992.	5.3	19
14	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
15	Equation of motion coupled-cluster cumulant approach for intrinsic losses in x-ray spectra. Journal of Chemical Physics, 2020, 152, 174113.	3.0	25
16	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
17	Probing the Local Bonding at the Pt ₃ -Al ₂ O ₃ Interface. Journal of Physical Chemistry C, 2020, 124, 9876-9885.	3.1	10
18	Charge-transfer satellites and chemical bonding in photoemission and x-ray absorption of SrTiO ₃ and rutile TiO ₂ and Expe	3.2	14

#	ARTICLE	IF	CITATIONS
19	Nonlinear response in the cumulant expansion for core-level photoemission. Physical Review Research, 2020, 2, .	3.6	9
20	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
21	Corvus: a framework for interfacing scientific software for spectroscopic and materials science applications. Journal of Synchrotron Radiation, 2019, 26, 1694-1704.	2.4	5
22	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
23	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
24	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
25	Automated generation and ensemble-learned matching of X-ray absorption spectra. Npj Computational Materials, 2018, 4, .	8.7	82
26	Correlative Structure-Bonding and Stability Studies of Pt/ γ -Al ₂ O ₃ Catalysts. Microscopy and Microanalysis, 2018, 24, 1644-1645.	0.4	1
27	Extended X-Ray Absorption Fine Structure of ZrW ₂ O ₈ : Theory vs. Experiment. Frontiers in Chemistry, 2018, 6, 356.	3.6	8
28	Coulomb-hole and screened exchange in the electron self-energy at finite temperature. Physical Review B, 2018, 98, .	3.2	10
29	Exchange and correlation in finite-temperature TDDFT. European Physical Journal B, 2018, 91, 1.	1.5	7
30	Efficient Calculation of the Negative Thermal Expansion in ZrW ₂ O ₈ . Frontiers in Chemistry, 2018, 6, 296.	3.6	13
31	A consistent path for phase determination based on transmission electron microscopy techniques and supporting simulations. Micron, 2018, 115, 41-49.	2.2	0
32	Bethe-Salpeter Equation calculations of nitrogen-vacancy defects in diamond. Journal of Physics and Chemistry of Solids, 2018, 122, 87-93.	4.0	3
33	High-throughput computational X-ray absorption spectroscopy. Scientific Data, 2018, 5, 180151.	5.3	94
34	Relativistic Dirac-Fock atom properties for Z $Z > 121$ to $Z < 138$.	2.4	4
35	Atomic Data and Nuclear Data Tables, 2017, 114, 262-280. Characterization of Coke on a Pt-Re/ γ -Al ₂ O ₃ Re-Forming Catalyst: Experimental and Theoretical Study. ACS Catalysis, 2017, 7, 1452-1461.	11.2	29
36	Quantitative first-principles calculations of valence and core excitation spectra of solid C $C < 60$	3.2	6

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37	Finite Temperature Green's Function Approach for Excited State and Thermodynamic Properties of Cool to Warm Dense Matter. <i>Physical Review Letters</i> , 2017, 119, 176403.	7.8	34
38	Comparison of Spinel and Monoclinic Crystal Structures of γ -Al ₂ O ₃ for Simulation of Electron Energy Loss Spectra. <i>Microscopy and Microanalysis</i> , 2017, 23, 2020-2021.	0.4	0
39	Probing electronic structure of stoichiometric and defective SnO_2 . <i>Physical Review B</i> , 2017, 95, .	3.2	9
40	Anomalous Structural Disorder in Supported Pt Nanoparticles. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3284-3288.	4.6	18
41	The effect of self-consistent potentials on EXAFS analysis. <i>Journal of Synchrotron Radiation</i> , 2017, 24, 1173-1179.	2.4	3
42	Particle-hole cumulant approach for inelastic losses in x-ray spectra. <i>Physical Review B</i> , 2016, 94, .	3.2	32
43	Molecular Dynamics Simulations of Supported Pt Nanoparticles with a Hybrid Sutton-Chen Potential. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14883-14891.	3.1	11
44	X-ray and Electron Spectroscopy of Water. <i>Chemical Reviews</i> , 2016, 116, 7551-7569.	47.7	143
45	Real-time cumulant approach for charge-transfer satellites in x-ray photoemission spectra. <i>Physical Review B</i> , 2015, 91, .	3.2	38
46	Dynamical effects in electron spectroscopy. <i>Journal of Chemical Physics</i> , 2015, 143, 184109.	3.0	57
47	Investigation of the Structural and Electronic Properties of Pt/ γ -Al ₂ O ₃ , a Model Catalyst System. <i>Microscopy and Microanalysis</i> , 2015, 21, 1655-1656.	0.4	0
48	Real-space multiple-scattering Hubbard model calculations for d- and f-state materials. <i>Journal of Synchrotron Radiation</i> , 2015, 22, 1042-1048.	2.4	0
49	Resonant Inelastic X-ray Scattering of Molybdenum Oxides and Sulfides. <i>Journal of Physical Chemistry C</i> , 2015, 119, 2419-2426.	3.1	18
50	Intracluster Atomic and Electronic Structural Heterogeneities in Supported Nanoscale Metal Catalysts. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25615-25627.	3.1	9
51	How Accurately Can Extended X-ray Absorption Spectra Be Predicted from First Principles? Implications for Modeling the Oxygen-Evolving Complex in Photosystem II. <i>Journal of the American Chemical Society</i> , 2015, 137, 12815-12834.	13.7	26
52	Effects of Adsorbate Coverage and Bond Length Disorder on the d-Band Center of Carbon-Supported Pt Catalysts. <i>ChemPhysChem</i> , 2014, 15, 1569-1572.	2.1	17
53	Cumulant expansion for phonon contributions to the electron spectral function. <i>Physical Review B</i> , 2014, 90, .	3.2	30
54	Dynamic structural disorder in supported nanoscale catalysts. <i>Journal of Chemical Physics</i> , 2014, 140, 134701.	3.0	9

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55	Charge transfer satellites in x-ray spectra of transition metal oxides. <i>Physical Review B</i> , 2014, 89, .	3.2	17
56	Comment on "Electromagnetic Vortex Fields, Spin, and Spin-Orbit Interactions in Electron Vortices". <i>Physical Review Letters</i> , 2014, 113, 029501.	7.8	1
57	Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations. <i>Physical Review B</i> , 2014, 89, .	3.2	138
58	Cumulant expansion of the retarded one-electron Green function. <i>Physical Review B</i> , 2014, 90, .	3.2	77
59	Lattice Model of Resonant Inelastic X-Ray Scattering in Metals: Relation of a Strong Core Hole to the X-Ray Edge Singularity. <i>Physical Review Letters</i> , 2014, 112, 237401.	7.8	4
60	Multiple satellites in materials with complex plasmon spectra: From graphite to graphene. <i>Physical Review B</i> , 2014, 89, .	3.2	38
61	The status of strontium in biological apatites: an XANES/EXAFS investigation. <i>Journal of Synchrotron Radiation</i> , 2014, 21, 136-142.	2.4	43
62	Operando Effects on the Structure and Dynamics of Pt _n /Sn _m /Al ₂ O ₃ from Ab Initio Molecular Dynamics and X-ray Absorption Spectra. <i>Journal of Physical Chemistry C</i> , 2013, 117, 12446-12457.	3.1	33
63	Theoretical optical and x-ray spectra of liquid and solid H ₂ O. <i>Physical Review B</i> , 2012, 85, .	3.2	47
64	Local time-correlation approach for calculations of x-ray spectra. <i>Physical Review B</i> , 2012, 86, .	3.2	18
65	High-performance computing without commitment: SC2IT: A cloud computing interface that makes computational science available to non-specialists. , 2012, .		1
66	Plasmon satellites in valence-band photoemission spectroscopy. <i>European Physical Journal B</i> , 2012, 85, 1.	1.5	27
67	Electronic Structures of Formic Acid (HCOOH) and Formate (HCOO ⁻) in Aqueous Solutions. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1754-1759.	4.6	35
68	The rediscovery of the "French Blue" diamond. <i>Europhysics News</i> , 2012, 43, 22-25.	0.3	5
69	X-ray absorption Debye-Waller factors from ab initio molecular dynamics. <i>Physical Review B</i> , 2012, 85, .	3.2	31
70	Comment on "Operando DRIFTS and XANES Study of Deactivating Effect of CO ₂ on a Ce _{0.8} Cu _{0.2} O ₂ CO-PROX Catalyst". <i>Journal of Physical Chemistry C</i> , 2011, 115, 23233-23236.	3.1	18
71	X-ray absorption spectra of overdoped La _{2-x} Sr _x CuO ₄ high- <i>Physical Review B</i> , 2011, 83, .	3.2	11
72	Real-space Green's function approach to resonant inelastic x-ray scattering. <i>Physical Review B</i> , 2011, 83, .	3.2	34

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73	Bethe-Salpeter equation calculations of core excitation spectra. Physical Review B, 2011, 83, .	3.2	228
74	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
75	Valence Electron Photoemission Spectrum of Semiconductors: <i>Ab Initio</i> Description of Multiple Satellites. Physical Review Letters, 2011, 107, 166401.	7.8	120
76	Basis set effects on the hyperpolarizability of CHCl ₃ : Gaussian-type orbitals, numerical basis sets and real-space grids. Journal of Chemical Physics, 2010, 133, 034111.	3.0	46
77	Multiple scattering calculations of relativistic electron energy loss spectra. Physical Review B, 2010, 81, .	3.2	32
78	<i>Ab initio</i> analysis of the x-ray absorption spectrum of the myoglobin-carbon monoxide complex: Structure and vibrations. Physical Review B, 2010, 82, .	3.2	6
79	Parameter-free calculations of X-ray spectra with FEFF9. Physical Chemistry Chemical Physics, 2010, 12, 5503.	2.8	985
80	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
81	Real space calculation of optical constants from optical to x-ray frequencies. Physical Review B, 2009, 80, .	3.2	31
82	Theory of dynamical scattering in near-edge electron energy loss spectroscopy. Physical Review B, 2009, 80, .	3.2	14
83	Many-pole model of inelastic losses applied to calculations of XANES. Journal of Physics: Conference Series, 2009, 190, 012009.	0.4	16
84	Ab initio theory and calculations of X-ray spectra. Comptes Rendus Physique, 2009, 10, 548-559.	0.9	468
85	Frequency and Solvent Dependence of Nonlinear Optical Properties of Molecules. Journal of Physical Chemistry C, 2008, 112, 8016-8021.	3.1	37
86	Optical to UV spectra and birefringence of SiO_2 and TiO_2 . Physical Review B, 2008, 78, .	3.2	56
87	First-principles calculations with excitonic effects. Physical Review B, 2008, 78, . Ab initio Real Space Calculations of Electron Energy Loss Spectra. AIP Conference Proceedings, 2008, .	0.4	0
88	Dynamic structure in supported Pt nanoclusters: Real-time density functional theory and x-ray spectroscopy simulations. Physical Review B, 2008, 78, .	3.2	77
89	Exciton spectroscopy of hexagonal boron nitride using nonresonant x-ray Raman scattering. Physical Review B, 2008, 77, .	3.2	26
90	Magic angle in electron energy loss spectra: Relativistic and dielectric corrections. Physical Review B, 2008, 77, .	3.2	9

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91	Deconvolving instrumental and intrinsic broadening in core-shell x-ray spectroscopies. Physical Review B, 2007, 75, .	3.2	28
92	Theoretical x-ray absorption Debye-Waller factors. Physical Review B, 2007, 76, .	3.2	126
93	Size and Shape of Rhenium Nanoparticles. AIP Conference Proceedings, 2007, , .	0.4	10
94	Many-pole model of inelastic losses in x-ray absorption spectra. Physical Review B, 2007, 76, .	3.2	68
95	Inelastic Losses and Multi-Electron Excitations in X-Ray Spectra. AIP Conference Proceedings, 2007, , .	0.4	3
96	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
97	XMCD Analysis Beyond Standard Procedures. AIP Conference Proceedings, 2007, , .	0.4	10
98	Ab initio calculations of electron inelastic mean free paths and stopping powers. Physical Review B, 2006, 74, .	3.2	46
99	Chemical speciation via X-ray emission spectra. X-Ray Spectrometry, 2006, 35, 312-318.	1.4	9
100	Background proportional enhancement of the extended fine structure in nonresonant inelastic x-ray scattering. Physical Review B, 2006, 74, .	3.2	29
101	Modeling CoreHole Screening in CoreExcitation Spectroscopies. Physica Scripta, 2005, , 31.	2.5	16
102	Bayes's Turchin approach to XAS analysis. Journal of Synchrotron Radiation, 2005, 12, 70-74.	2.4	16
103	Inelastic scattering from core electrons: A multiple scattering approach. Physical Review B, 2005, 72, .	3.2	100
104	FinalState Rule vs the BetheSalpeter Equation for DeepCore Xray Absorption Spectra. Physica Scripta, 2005, , 207.	2.5	40
105	Role of inversion symmetry and multipole effects in nonresonant x-ray Raman scattering from icosahedral B4C. Physical Review B, 2004, 69, .	3.2	47
106	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
107	Failure of the Quasiparticle Picture of X-ray Absorption?. Foundations of Physics, 2003, 33, 1735-1742.	1.3	7
108	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

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109	Time-dependent density functional theory calculations of X-ray absorption. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 487-492.	2.0	6
110	Dynamic screening effects in x-ray absorption spectra. <i>Physical Review B</i> , 2003, 67, .	3.2	264
111	Interference between extrinsic and intrinsic losses in x-ray absorption fine structure. <i>Physical Review B</i> , 2002, 65, .	3.2	61
112	Parallel calculation of electron multiple scattering using Lanczos algorithms. <i>Physical Review B</i> , 2002, 65, .	3.2	466
113	HIGH ORDER MULTIPLE SCATTERING THEORY OF XAFS. <i>Advanced Series in Physical Chemistry</i> , 2002, , 1213-1227.	1.5	1
114	Progress and challenges in the theory and interpretation of X-ray spectra. <i>Journal of Synchrotron Radiation</i> , 2001, 8, 61-65.	2.4	62
115	Rapid calculation of x-ray absorption near edge structure using parallel computation. <i>X-Ray Spectrometry</i> , 2001, 30, 431-434.	1.4	9
116	Theoretical approaches to x-ray absorption fine structure. <i>Reviews of Modern Physics</i> , 2000, 72, 621-654.	45.6	2,843
117	Calculation and interpretation of X-ray spectroscopies with Greenâ€™s function multiple scattering theory. <i>AIP Conference Proceedings</i> , 2000, , .	0.4	0
118	Extended X-Ray Absorption Fine Structure from Hydrogen Atoms in Water. <i>Physical Review Letters</i> , 2000, 85, 4289-4292.	7.8	47
119	Interpretation of x-ray magnetic circular dichroism and x-ray absorption near-edge structure in Ni. <i>Physical Review B</i> , 2000, 62, 15295-15298.	3.2	31
120	Importance of Multiple-Scattering Phenomena in XAS Structural Determinations of [Ni(CN) ₄] ²⁻ in Condensed Phases. <i>Inorganic Chemistry</i> , 2000, 39, 3784-3790.	4.0	22
121	Multiple-scattering x-ray-absorption fine-structure Debye-Waller factor calculations. <i>Physical Review B</i> , 1999, 59, 948-957.	3.2	150
122	Recursion method for multiple-scattering XAFS Debyeâ€™Waller factors. <i>Journal of Synchrotron Radiation</i> , 1999, 6, 313-314.	2.4	16
123	Real-space multiple-scattering calculation and interpretation of x-ray-absorption near-edge structure. <i>Physical Review B</i> , 1998, 58, 7565-7576.	3.2	4,006
124	Magnetic extended x-ray absorption fine structure at the L _{3,2} edges of Fe and Co on Cu(001). <i>Journal of Applied Physics</i> , 1998, 83, 7025-7027.	2.5	6
125	X-Ray Absorption Spectroscopy of Organouranium Compounds in the (+V) and (+IV) Oxidation States. <i>Radiochimica Acta</i> , 1997, 76, 211-218.	1.2	9
126	Order-disorder behavior in the phase transition of PbTiO ₃ . <i>Ferroelectrics</i> , 1995, 164, 265-277.	0.6	29

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127	Refinement of a Model for the Nitrogenase Mo ₂ Fe Cluster Using Single-Crystal Mo and Fe EXAFS. <i>Angewandte Chemie International Edition in English</i> , 1993, 32, 1592-1594.	4.4	14
128	Verfeinerung eines Modells für den Nitrogenase-Mo-Fe-Cluster mit Einkristall-Mo- und -Fe-EXAFS. <i>Angewandte Chemie</i> , 1993, 105, 1661-1663.	2.0	9
129	Crystal effects in \hat{I}^2 -decay. <i>Nature</i> , 1991, 354, 436-437.	27.8	3
130	Scattering-matrix formulation of curved-wave multiple-scattering theory: Application to x-ray-absorption fine structure. <i>Physical Review B</i> , 1990, 41, 8139-8149.	3.2	598
131	Calculation of X-ray absorption structure above K-edge of laser shock-compressed aluminum. <i>Laser and Particle Beams</i> , 1990, 8, 319-325.	1.0	2
132	Extended x-ray-absorption fine-structure amplitudes—Wave-function relaxation and chemical effects. <i>Physical Review B</i> , 1978, 17, 560-565.	3.2	140
133	Green's function methods for excited states and x-ray spectra of functional materials. <i>Electronic Structure</i> , 0, , .	2.8	0