Eric Bylaska

List of Publications by Year
in descending order

84 papers	3,691 citations	136950 32 h-index	133252 59 g-index
90 all docs	90 docs citations	90 times ranked	4312 citing authors

#	Article	IF	Citations
1	Effect of Temperature on Local Hydration of Zn in Hematite. ACS Earth and Space Chemistry, 2022, 6, 551-557.	2.7	6
2	<scp>Gasâ€Phase Ionâ€Molecule</scp> Interactions in a Collision Reaction Cell with <scp>ICPâ€MS</scp>/<scp>MS</scp>: Investigations with <scp>CO₂</scp> as the Reaction Gas. Geostandards and Geoanalytical Research, 2022, 46, 387-399.	3.1	6
3	Toward Quantum Computing for High-Energy Excited States in Molecular Systems: Quantum Phase Estimations of Core-Level States. Journal of Chemical Theory and Computation, 2021, 17, 201-210.	5.3	16
4	Quantum Solvers for Plane-Wave Hamiltonians: Abridging Virtual Spaces Through the Optimization of Pairwise Correlations. Frontiers in Chemistry, 2021, 9, 603019.	3.6	10
5	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
6	Resolving Configurational Disorder for Impurities in a Low-Entropy Phase. Journal of Physical Chemistry Letters, 2021, 12, 5689-5694.	4.6	6
7	Gas-phase ion-molecule interactions in a collision reaction cell with triple quadrupole-inductively coupled plasma mass spectrometry: Investigations with N2O as the reaction gas. Spectrochimica Acta, Part B: Atomic Spectroscopy, 2021, 186, 106309.	2.9	15
8	Reaction Roulette: Utilizing Elemental MS/MS for the Characterization of Gas Phase Ion-Molecule Interactions. , 2021, , .		0
9	Building toward the future in chemical and materials simulation with accessible and intelligently designed web applications. Annual Reports in Computational Chemistry, 2021, , 163-208.	1.7	5
10	Using Atom Dynamics to Map the Defect Structure Around an Impurity in Nano-Hematite. Journal of Physical Chemistry Letters, 2020, 11, 10396-10400.	4.6	9
11	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
12	Reduction of 1,2,3-trichloropropane (TCP): pathways and mechanisms from computational chemistry calculations. Environmental Sciences: Processes and Impacts, 2020, 22, 606-616.	3.5	10
13	Reaction Energetics and ¹³C Fractionation of Alanine Transamination in the Aqueous and Gas Phases. Journal of Physical Chemistry A, 2020, 124, 2077-2089.	2.5	6
14	Electron transfer calculations between edge sharing octahedra in hematite, goethite, and annite. Geochimica Et Cosmochimica Acta, 2020, 291, 79-91.	3.9	15
15	A Filon-like integration strategy for calculating exact exchange in periodic boundary conditions: a plane-wave DFT implementation. Materials Theory, 2020, 4, .	4.3	5
16	Downfolding of many-body Hamiltonians using active-space models: Extension of the sub-system embedding sub-algebras approach to unitary coupled cluster formalisms. Journal of Chemical Physics, 2019, 151, 014107.	3.0	57
17	Association of Defects and Zinc in Hematite. Environmental Science & Technology, 2019, 53, 13687-13694.	10.0	20
18	Properties of perhalogenated {closo-B₁₀} and {closo-B₁₁} multiply charged anions and a critical comparison with {closo-B₁₂} in the gas and the condensed phase. Physical Chemistry Chemical Physics, 2019, 21, 5903-5915.	2.8	24

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19	Insights on the Aluminaâ€“Water Interface Structure by Direct Comparison of Density Functional Simulations with X-ray Reflectivity. Journal of Physical Chemistry C, 2018, 122, 26934-26944.	3.1	19
20	Iron Vacancies Accommodate Uranyl Incorporation into Hematite. Environmental Science & Technology, 2018, 52, 6282-6290.	10.0	44
21	Corresponding Orbitals Derived from Periodic Bloch States for Electron Transfer Calculations of Transition Metal Oxides. Journal of Chemical Theory and Computation, 2018, 14, 4416-4426.	5.3	15
22	Time Domain Simulations of Single Molecule Raman Scattering. Journal of Physical Chemistry A, 2018, 122, 7437-7442.	2.5	10
23	Water Structure and Dynamics at Hematite Electrodes. ECS Meeting Abstracts, 2018, , .	0.0	0
24	Automatic translation of MPI source into a latency-tolerant, data-driven form. Journal of Parallel and Distributed Computing, 2017, 106, 1-13.	4.1	5
25	In silico environmental chemical science: properties and processes from statistical and computational modelling. Environmental Sciences: Processes and Impacts, 2017, 19, 188-202.	3.5	24
26	Oxidation potentials of phenols and anilines: correlation analysis of electrochemical and theoretical values. Environmental Sciences: Processes and Impacts, 2017, 19, 339-349.	3.5	65
27	Weakly bound water structure, bond valence saturation and water dynamics at the goethite (100) surface/aqueous interface: ab initio dynamical simulations. Geochemical Transactions, 2017, 18, 3.	0.7	21
28	Trace Uranium Partitioning in a Multiphase Nano-FeOOH System. Environmental Science & Technology, 2017, 51, 4970-4977.	10.0	44
29	Towards Highly scalable Ab Initio Molecular Dynamics (AIMD) Simulations on the Intel Knights Landing Manycore Processor. , 2017, , .		12
30	Plane-Wave DFT Methods for Chemistry. Annual Reports in Computational Chemistry, 2017, 13, 185-228.	1.7	17
31	Performance Evaluation of NWChem Ab-Initio Molecular Dynamics (AIMD) Simulations on the IntelÂ® Xeon Phiâ„¢ Processor. Lecture Notes in Computer Science, 2017, , 404-418.	1.3	7
32	Transitioning NWChem to the Next Generation of Manycore Machines. , 2017, , 165-186.		5
33	Strengthening of the Coordination Shell by Counter Ions in Aqueous Th⁴⁺ Solutions. Journal of Physical Chemistry A, 2016, 120, 10216-10222.	2.5	14
34	Structureâ€“Activity Relationships for Rates of Aromatic Amine Oxidation by Manganese Dioxide. Environmental Science & Technology, 2016, 50, 5094-5102.	10.0	57
35	Ab Initio Molecular Dynamics of Uranium Incorporated in Goethite (Î±-FeOOH): Interpretation of X-ray Absorption Spectroscopy of Trace Polyvalent Metals. Inorganic Chemistry, 2016, 55, 11736-11746.	4.0	42
36	Theoretical studies of the global minima and polarizabilities of small lithium clusters. Chemical Physics Letters, 2016, 644, 235-242.	2.6	13

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37	Predicting Reduction Rates of Energetic Nitroaromatic Compounds Using Calculated One-Electron Reduction Potentials. Environmental Science & Technology, 2015, 49, 3778-3786.	10.0	46
38	Electronic and Chemical State of Aluminum from the Single- (K) and Double-Electron Excitation (KL_{II&III}, KL_I) X-ray Absorption Near-Edge Spectra of Î±-Alumina, Sodium Aluminate, Aqueous Al³⁺Â·(H₂O)₆, and Aqueous Al(OH)₄^{â€“}. Journal of Physical Chemistry B, 2015, 119, 8380-8388.	2.6	20
39	Coordination and Hydrolysis of Plutonium Ions in Aqueous Solution Using Carâ€“Parrinello Molecular Dynamics Free Energy Simulations. Journal of Physical Chemistry A, 2013, 117, 12256-12267.	2.5	35
40	Water and carbon dioxide adsorption at olivine surfaces. Chemical Geology, 2013, 359, 81-89.	3.3	60
41	Mechanisms and Kinetics of Alkaline Hydrolysis of the Energetic Nitroaromatic Compounds 2,4,6-Trinitrotoluene (TNT) and 2,4-Dinitroanisole (DNAN). Environmental Science & Technology, 2013, 47, 6790-6798.	10.0	37
42	The Aqueous Ca²⁺ System, in Comparison with Zn²⁺, Fe^{3 +}, and Al^{3 +}: An Abâ€...Initio Molecular Dynamics Study. Chemistry - A European Journal, 2013, 19, 3047-3060.	3.3	45
43	Importance of Counteranions on the Hydration Structure of the Curium Ion. Journal of Physical Chemistry Letters, 2013, 4, 2166-2170.	4.6	28
44	Thermodynamics of Tetravalent Thorium and Uranium Complexes from First-Principles Calculations. Journal of Physical Chemistry A, 2013, 117, 4988-4995.	2.5	4
45	Time domain simulations of chemical bonding effects in surface-enhanced spectroscopy. Journal of Chemical Physics, 2013, 139, 174303.	3.0	6
46	Extending molecular simulation time scales: Parallel in time integrations for high-level quantum chemistry and complex force representations. Journal of Chemical Physics, 2013, 139, 074114.	3.0	18
47	Free energies and mechanisms of water exchange around Uranyl from first principles molecular dynamics. Materials Research Society Symposia Proceedings, 2012, 1383, 113.	0.1	5
48	Bamboo -- Translating MPI applications to a latency-tolerant, data-driven form. , 2012, , .		12
49	Near-Quantitative Agreement of Model-Free DFT-MD Predictions with XAFS Observations of the Hydration Structure of Highly Charged Transition-Metal Ions. Journal of Physical Chemistry Letters, 2012, 3, 2588-2593.	4.6	40
50	Ion Association in AlCl3 Aqueous Solutions from Constrained First-Principles Molecular Dynamics. Inorganic Chemistry, 2012, 51, 10856-10869.	4.0	15
51	Tuning Band Gap Energies in Pb3(C6X6) Extended Solid-State Structures. Journal of Physical Chemistry C, 2012, 116, 8370-8378.	3.1	9
52	Structure and Hydrolysis of the U(IV), U(V), and U(VI) Aqua Ions from Ab Initio Molecular Simulations. Inorganic Chemistry, 2012, 51, 3016-3024.	4.0	58
53	Hydration Shell Structure and Dynamics of Curium(III) in Aqueous Solution: First Principles and Empirical Studies. Journal of Physical Chemistry A, 2011, 115, 4665-4677.	2.5	52
54	Parallel implementation of Î³â€point pseudopotential planeâ€wave DFT with exact exchange. Journal of Computational Chemistry, 2011, 32, 54-69.	3.3	47

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55	One-Electron Reduction Potentials from Chemical Structure Theory Calculations. ACS Symposium Series, 2011, , 37-64.	0.5	14
56	NWChem. , 2011, , 1345-1353.		0
57	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	2.8	84
58	Bonding and Microstructural Stability in Ni₅₅Ti₄₅ Studied by Experimental and Theoretical Methods. Journal of Physical Chemistry C, 2010, 114, 19704-19713.	3.1	11
59	Calculation of boron-isotope fractionation between B(OH)3(aq) and. Geochimica Et Cosmochimica Acta, 2010, 74, 2843-2850.	3.9	58
60	Isotopic fractionation of Mg2+(aq), Ca2+(aq), and Fe2+(aq) with carbonate minerals. Geochimica Et Cosmochimica Acta, 2010, 74, 6301-6323.	3.9	190
61	Structure and dynamics of the hydration shells of the Zn2+ ion from ab initio molecular dynamics and combined ab initio and classical molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 194502.	3.0	95
62	First Principles Simulation of the Bonding, Vibrational, and Electronic Properties of the Hydration Shells of the High-Spin Fe³⁺ Ion in Aqueous Solutions. Journal of Physical Chemistry A, 2010, 114, 2189-2200.	2.5	26
63	Free Energies for Degradation Reactions of 1,2,3-Trichloropropane from ab Initio Electronic Structure Theory. Journal of Physical Chemistry A, 2010, 114, 12269-12282.	2.5	10
64	Computational Nanoscience with NWChem. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1297-1304.	0.4	1
65	Adaptive Finite Element Method for Solving the Exact Kohnâ^'Sham Equation of Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 937-948.	5.3	46
66	Gaussian Basis Set and Planewave Relativistic Spinâ^'Orbit Methods in NWChem. Journal of Chemical Theory and Computation, 2009, 5, 491-499.	5.3	66
67	Hard scaling challenges forab initiomolecular dynamics capabilities in NWChem: Using 100,000 CPUs per second. Journal of Physics: Conference Series, 2009, 180, 012028.	0.4	16
68	One-Electron-Transfer Reactions of Polychlorinated Ethylenes:â€‰ Concerted and Stepwise Cleavages. Journal of Physical Chemistry A, 2008, 112, 3712-3721.	2.5	24
69	Combined Quantum Mechanical and Molecular Mechanics Studies of the Electron-Transfer Reactions Involving Carbon Tetrachloride in Solution. Journal of Physical Chemistry A, 2008, 112, 2713-2720.	2.5	36
70	Equatorial and apical solvent shells of the UO22+ ion. Journal of Chemical Physics, 2008, 128, 124507.	3.0	79
71	Structure and dynamics of the hydration shells of the Al3+ ion. Journal of Chemical Physics, 2007, 126, 104505.	3.0	44
72	Ab Initio Calculation of Isotopic Fractionation in B(OH)3(aq) and BOH4-(aq). Journal of the American Chemical Society, 2007, 129, 2222-2223.	13.7	64

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73	Ab Initio atomic simulations of antisite pair recovery in cubic silicon carbide. Applied Physics Letters, 2007, 90, 221915.	3.3	19
74	Electron, hole and exciton self-trapping in germanium doped silica glass from DFT calculations with self-interaction correction. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 188-194.	1.4	14
75	Estimating the thermodynamics and kinetics of chlorinated hydrocarbon degradation. Theoretical Chemistry Accounts, 2006, 116, 281-296.	1.4	12
76	New development of self-interaction corrected DFT for extended systems applied to the calculation of native defects in 3Câ€“SiC. Physica Scripta, 2006, T124, 86-90.	2.5	31
77	Kinetic Evidence for Five-Coordination in AlOH(aq)2+ Ion. Science, 2005, 308, 1450-1453.	12.6	168
78	Molecular simulation of the magnetite-water interface. Geochimica Et Cosmochimica Acta, 2003, 67, 1001-1016.	3.9	66
79	NWChem: New Functionality. Lecture Notes in Computer Science, 2003, , 168-177.	1.3	7
80	FIRST PRINCIPLES MOLECULAR DYNAMICS SIMULATIONS USING DENSITY-FUNCTIONAL THEORY. , 2002, , 1684-1734.		9
81	Parallel implementation of the projector augmented plane wave method for charged systems. Computer Physics Communications, 2002, 143, 11-28.	7.5	35
82	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	7.5	698
83	From small to large behavior: The transition from the aromatic to the Peierls regime in carbon rings. Journal of Chemical Physics, 2000, 113, 6096-6106.	3.0	25
84	LDA Predictions of C20Isomerizations:Â Neutral and Charged Species. The Journal of Physical Chemistry, 1996, 100, 6966-6972.	2.9	68