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	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	7.5	698
2	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
3	Isotopic fractionation of Mg2+(aq), Ca2+(aq), and Fe2+(aq) with carbonate minerals. Geochimica Et Cosmochimica Acta, 2010, 74, 6301-6323.	3.9	190
4	Kinetic Evidence for Five-Coordination in AlOH(aq)2+ Ion. Science, 2005, 308, 1450-1453.	12.6	168
5	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
6	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	2.8	84
7	Equatorial and apical solvent shells of the UO22+ ion. Journal of Chemical Physics, 2008, 128, 124507.	3.0	79
8	LDA Predictions of C20Isomerizations:Â Neutral and Charged Species. The Journal of Physical Chemistry, 1996, 100, 6966-6972.	2.9	68
9	Molecular simulation of the magnetite-water interface. Geochimica Et Cosmochimica Acta, 2003, 67, 1001-1016.	3.9	66
10	Gaussian Basis Set and Planewave Relativistic Spinâ˜Orbit Methods in NWChem. Journal of Chemical Theory and Computation, 2009, 5, 491-499.	5.3	66
11	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
12	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
13	Water and carbon dioxide adsorption at olivine surfaces. Chemical Geology, 2013, 359, 81-89.	3.3	60
14	Calculation of boron-isotope fractionation between B(OH)3(aq) and. Geochimica Et Cosmochimica Acta, 2010, 74, 2843-2850.	3.9	58
15	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
16	Structureâ€“Activity Relationships for Rates of Aromatic Amine Oxidation by Manganese Dioxide. Environmental Science & Technology, 2016, 50, 5094-5102.	10.0	57
17	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
18	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

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19	Parallel implementation of Î³â€point pseudopotential planeâ€wave DFT with exact exchange. Journal of Computational Chemistry, 2011, 32, 54-69.	3.3	47
20	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
21	Predicting Reduction Rates of Energetic Nitroaromatic Compounds Using Calculated One-Electron Reduction Potentials. Environmental Science & Technology, 2015, 49, 3778-3786.	10.0	46
22	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
23	Structure and dynamics of the hydration shells of the Al3+ ion. Journal of Chemical Physics, 2007, 126, 104505.	3.0	44
24	Trace Uranium Partitioning in a Multiphase Nano-FeOOH System. Environmental Science & Technology, 2017, 51, 4970-4977.	10.0	44
25	Iron Vacancies Accommodate Uranyl Incorporation into Hematite. Environmental Science & Technology, 2018, 52, 6282-6290.	10.0	44
26	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
27	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
28	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
29	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
30	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
31	Parallel implementation of the projector augmented plane wave method for charged systems. Computer Physics Communications, 2002, 143, 11-28.	7.5	35
32	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
33	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
34	Importance of Counteranions on the Hydration Structure of the Curium Ion. Journal of Physical Chemistry Letters, 2013, 4, 2166-2170.	4.6	28
35	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
36	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

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37	One-Electron-Transfer Reactions of Polychlorinated Ethylenes:â€‰ Concerted and Stepwise Cleavages. Journal of Physical Chemistry A, 2008, 112, 3712-3721.	2.5	24
38	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
39	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
40	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
41	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
42	Association of Defects and Zinc in Hematite. Environmental Science & Technology, 2019, 53, 13687-13694.	10.0	20
43	Ab Initio atomic simulations of antisite pair recovery in cubic silicon carbide. Applied Physics Letters, 2007, 90, 221915.	3.3	19
44	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
45	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
46	Plane-Wave DFT Methods for Chemistry. Annual Reports in Computational Chemistry, 2017, 13, 185-228.	1.7	17
47	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
48	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
49	Ion Association in AlCl3 Aqueous Solutions from Constrained First-Principles Molecular Dynamics. Inorganic Chemistry, 2012, 51, 10856-10869.	4.0	15
50	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
51	Electron transfer calculations between edge sharing octahedra in hematite, goethite, and annite. Geochimica Et Cosmochimica Acta, 2020, 291, 79-91.	3.9	15
52	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
53	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
54	One-Electron Reduction Potentials from Chemical Structure Theory Calculations. ACS Symposium Series, 2011, , 37-64.	0.5	14

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55	Strengthening of the Coordination Shell by Counter Ions in Aqueous Th⁴⁺ Solutions. Journal of Physical Chemistry A, 2016, 120, 10216-10222.	2.5	14
56	Theoretical studies of the global minima and polarizabilities of small lithium clusters. Chemical Physics Letters, 2016, 644, 235-242.	2.6	13
57	Estimating the thermodynamics and kinetics of chlorinated hydrocarbon degradation. Theoretical Chemistry Accounts, 2006, 116, 281-296.	1.4	12
58	Bamboo -- Translating MPI applications to a latency-tolerant, data-driven form. , 2012, , .		12
59	Towards Highly scalable Ab Initio Molecular Dynamics (AIMD) Simulations on the Intel Knights Landing Manycore Processor. , 2017, , .		12
60	Bonding and Microstructural Stability in Ni₅₅Ti₄₅ Studied by Experimental and Theoretical Methods. Journal of Physical Chemistry C, 2010, 114, 19704-19713.	3.1	11
61	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
62	Time Domain Simulations of Single Molecule Raman Scattering. Journal of Physical Chemistry A, 2018, 122, 7437-7442.	2.5	10
63	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
64	Quantum Solvers for Plane-Wave Hamiltonians: Abridging Virtual Spaces Through the Optimization of Pairwise Correlations. Frontiers in Chemistry, 2021, 9, 603019.	3.6	10
65	FIRST PRINCIPLES MOLECULAR DYNAMICS SIMULATIONS USING DENSITY-FUNCTIONAL THEORY. , 2002, , 1684-1734.		9
66	Tuning Band Gap Energies in Pb3(C6X6) Extended Solid-State Structures. Journal of Physical Chemistry C, 2012, 116, 8370-8378.	3.1	9
67	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
68	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
69	NWChem: New Functionality. Lecture Notes in Computer Science, 2003, , 168-177.	1.3	7
70	Time domain simulations of chemical bonding effects in surface-enhanced spectroscopy. Journal of Chemical Physics, 2013, 139, 174303.	3.0	6
71	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
72	Resolving Configurational Disorder for Impurities in a Low-Entropy Phase. Journal of Physical Chemistry Letters, 2021, 12, 5689-5694.	4.6	6

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73	Effect of Temperature on Local Hydration of Zn in Hematite. ACS Earth and Space Chemistry, 2022, 6, 551-557.	2.7	6
74	<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
75	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
76	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
77	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
78	Transitioning NWChem to the Next Generation of Manycore Machines. , 2017, , 165-186.		5
79	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
80	Thermodynamics of Tetravalent Thorium and Uranium Complexes from First-Principles Calculations. Journal of Physical Chemistry A, 2013, 117, 4988-4995.	2.5	4
81	Computational Nanoscience with NWChem. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1297-1304.	0.4	1
82	NWChem. , 2011, , 1345-1353.		0
83	Water Structure and Dynamics at Hematite Electrodes. ECS Meeting Abstracts, 2018, , .	0.0	0
84	Reaction Roulette: Utilizing Elemental MS/MS for the Characterization of Gas Phase Ion-Molecule Interactions. , 2021, , .		0