Edward F C Byrd

List of Publications by Year
in descending order

64	6,363	186265	123424
papers	citations	28 h-index	61 g-index

66	66	66	5603
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
2	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	3.3	617
3	Improved Prediction of Heats of Formation of Energetic Materials Using Quantum Mechanical Calculations. Journal of Physical Chemistry A, 2006, 110, 1005-1013.	2.5	494
4	Energies and analytic gradients for a coupled-cluster doubles model using variational Brueckner orbitals: Application to symmetry breaking in O4+. Journal of Chemical Physics, 1998, 109, 4171-4181.	3.0	228
5	Size-consistent wave functions for nondynamical correlation energy: The valence active space optimized orbital coupled-cluster doubles model. Journal of Chemical Physics, 1998, 109, 10669-10678.	3.0	222
6	Accurate Predictions of Crystal Densities Using Quantum Mechanical Molecular Volumes. Journal of Physical Chemistry A, 2007, 111, 10874-10879.	2.5	175
7	Ab Initio Study of Compressed 1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane (HMX), Cyclotrimethylenetrinitramine (RDX), 2,4,6,8,10,12-Hexanitrohexaazaisowurzitane (CL-20), 2,4,6-Trinitro-1,3,5-benzenetriamine (TATB), and Pentaerythritol Tetranitrate (PETN). Journal of Physical Chemistry C, 2007, 111, 2787-2796.	3.1	150
8	The Theoretical Prediction of Molecular Radical Species:â€‰a Systematic Study of Equilibrium Geometries and Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2001, 105, 9736-9747.	2.5	142
9	Harmonic Vibrational Frequencies: Approximate Global Scaling Factors for TPSS, M06, and M11 Functional Families Using Several Common Basis Sets. Journal of Physical Chemistry A, 2017, 121, 2265-2273.	2.5	141
10	An ab Initio Study of Solid Nitromethane, HMX, RDX, and CL20:Â Successes and Failures of DFT. Journal of Physical Chemistry B, 2004, 108, 13100-13106.	2.6	122
11	Evaluation of electrostatic descriptors for predicting crystalline density. Journal of Computational Chemistry, 2013, 34, 2146-2151.	3.3	112
12	Impact of Stereo- and Regiochemistry on Energetic Materials. Journal of the American Chemical Society, 2019, 141, 12531-12535.	13.7	92
13	Bis(1,2,4-oxadiazole)bis(methylene) Dinitrate: A High-Energy Melt-Castable Explosive and Energetic Propellant Plasticizing Ingredient. Organic Process Research and Development, 2018, 22, 736-740.	2.7	90
14	A perturbative correction to the quadratic coupled-cluster doubles method for higher excitations. Chemical Physics Letters, 2002, 353, 359-367.	2.6	79
15	The use of locally dense basis sets in correlated NMR chemical shielding calculations. Chemical Physics, 1996, 213, 153-158.	1.9	65
16	A Comparison of Methods To Predict Solid Phase Heats of Formation of Molecular Energetic Salts. Journal of Physical Chemistry A, 2009, 113, 345-352.	2.5	64
17	Tetrazole Azasydnone (C₂N₇O₂H) And Its Salts: Highâ€Performing Zwitterionic Energetic Materials Containing A Unique Explosophore. Chemistry - A European Journal, 2020, 26, 14530-14535.	3.3	53
18	Computational Aspects of Nitrogen-Rich HEDMs. , 2007, , 153-194.		48

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19	Shock Hugoniot calculations of polymers using quantum mechanics and molecular dynamics. Journal of Chemical Physics, 2012, 137, 204901.	3.0	46
20	4,4â€²,5,5â€²-Tetraamino-3,3â€²-azo-bis-1,2,4-triazole and the electrosynthesis of high-performing insensitive energetic materials. Journal of Materials Chemistry A, 2020, 8, 19337-19347.	10.3	43
21	Development of quantitative structureâ€“property relationships for predictive modeling and design of energetic materials. Journal of Molecular Graphics and Modelling, 2008, 27, 349-355.	2.4	38
22	An Investigation of KS-DFT Electron Densities used in Atoms-in-Molecules Studies of Energetic Molecules. Journal of Physical Chemistry A, 2009, 113, 6166-6171.	2.5	38
23	Synthesis of bisâ€Isoxazoleâ€bisâ€Methylene Dinitrate: A Potential Nitrate Plasticizer and Meltâ€Castable Energetic Material. ChemPlusChem, 2017, 82, 195-198.	2.8	37
24	Parameterizing Complex Reactive Force Fields Using Multiple Objective Evolutionary Strategies (MOES): Part 2: Transferability of ReaxFF Models to Câ€“Hâ€“Nâ€“O Energetic Materials. Journal of Chemical Theory and Computation, 2015, 11, 392-405.	5.3	36
25	Parameterizing Complex Reactive Force Fields Using Multiple Objective Evolutionary Strategies (MOES). Part 1: ReaxFF Models for Cyclotrimethylene Trinitramine (RDX) and 1,1-Diamino-2,2-dinitroethene (FOX-7). Journal of Chemical Theory and Computation, 2015, 11, 381-391.	5.3	36
26	Theoretical chemical characterization of energetic materials. Journal of Materials Research, 2006, 21, 2444-2452.	2.6	35
27	Bis(Nitroxymethylisoxazolyl) Furoxan: A Promising Standalone Meltâ€Castable Explosive. ChemPlusChem, 2020, 85, 237-239.	2.8	34
28	Assessment of Dispersion Corrected Atom Centered Pseudopotentials: Application to Energetic Molecular Crystals. Journal of Physical Chemistry B, 2011, 115, 803-810.	2.6	32
29	Synthesis of Biisoxazoletetrakis(methyl nitrate): A Potential Nitrate Plasticizer and Highly Explosive Material. European Journal of Organic Chemistry, 2017, 2017, 1765-1768.	2.4	29
30	Tailoring Energetic Sensitivity and Classification through Regioisomerism. Organic Letters, 2020, 22, 9114-9117.	4.6	29
31	Synthesis of Erythritol Tetranitrate Derivatives: Functional Group Tuning of Explosive Sensitivity. Journal of Organic Chemistry, 2020, 85, 4619-4626.	3.2	28
32	Structural and electrical analysis of epitaxial 2D/3D vertical heterojunctions of monolayer MoS2 on GaN. Applied Physics Letters, 2017, 111, .	3.3	27
33	Bis(1,2,4â€oxadiazolyl) Furoxan: A Promising Meltâ€Castable Eutectic Material of Low Sensitivity. ChemPlusChem, 2019, 84, 319-322.	2.8	27
34	Complete basis set extrapolations for low-lying triplet electronic states of acetylene and vinylidene. Journal of Chemical Physics, 2000, 113, 1447-1454.	3.0	24
35	Quadratic Coupled-Cluster Doubles:Â Implementation and Assessment of Perfect Pairing Optimized Geometriesâ€. Journal of Physical Chemistry B, 2002, 106, 8070-8077.	2.6	22
36	Assessing the Performances of Dispersion-Corrected Density Functional Methods for Predicting the Crystallographic Properties of High Nitrogen Energetic Salts. Journal of Chemical Theory and Computation, 2014, 10, 4982-4994.	5.3	22

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37	Special quasirandom structures of alon. Computational Materials Science, 2015, 96, 312-318.	3.0	22
38	Simple and Efficient Synthesis of Explosive Cocrystals containing 3,5â€Dimethylpyrazolâ€1â€ylâ€substitutedâ€1,2,4,5â€tetrazines. Chemistry - A European Journal, 2017, 23, 16466-16471.	3.3	21
39	1,5-Diaminotetrazole-4N-oxide (SYX-9): a new high-performing energetic material with a calculated detonation velocity over 10 km s^{â^1}. Journal of Materials Chemistry A, 2022, 10, 1876-1884.	10.3	21
40	The inclusion of correlation in the calculation of phosphorus NMR chemical shieldings. Heteroatom Chemistry, 1996, 7, 307-312.	0.7	20
41	Synthesis and Characterization of Salts of the 3,6â€Dinitroâ€[1,2,4]triazolo[4,3â€b][1,2,4]triazolate Anion: Insensitive Energetic Materials Available From Economical Precursors. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2019, 645, 1197-1204.	1.2	16
42	Toward a Predictive Hierarchical Multiscale Modeling Approach for Energetic Materials. Challenges and Advances in Computational Chemistry and Physics, 2019, , 229-282.	0.6	16
43	Heterocyclic Nitrilimines and Their Use in the Synthesis of Complex High-Nitrogen Materials. Inorganic Chemistry, 2021, 60, 7607-7611.	4.0	12
44	Development of quantitative structure property relationships for predicting the melting point of energetic materials. Journal of Molecular Graphics and Modelling, 2015, 62, 190-201.	2.4	11
45	Sensitive Energetics from the Nâ€Amination of 4â€Nitroâ€1,2,3â€Triazole. ChemistryOpen, 2020, 9, 806-811.	1.9	11
46	Synthesis and Characterization of the Energetic 3â€Azidoâ€5â€aminoâ€6â€nitroâ€1,2,4â€triazine. Propellants, Explosives, Pyrotechnics, 2021, 46, 214-221.	1.6	11
47	Density Functional Theory and Experimental Studies of the Molecular, Vibrational, and Crystal Structure of Bis-Oxadiazole-Bis-Methylene Dinitrate (BODN). Journal of Physical Chemistry A, 2018, 122, 9043-9053.	2.5	9
48	1,3,4,5-Tetraamino-1,2,4-triazolium Cation: An Energetic Moiety. Inorganic Chemistry, 2021, 60, 9645-9652.	4.0	9
49	4,4â€²-Dinitrimino-5,5â€²-diamino-3,3â€²-azo-bis-1,2,4-triazole: A High-Performing Zwitterionic Energetic Material. Inorganic Chemistry, 2021, 60, 16204-16212.	4.0	9
50	Heuristics for chemical species identification in dense systems. Journal of Chemical Physics, 2020, 153, 064102.	3.0	8
51	Coupled Cluster Methods for Bond-Breaking. ACS Symposium Series, 2002, , 93-108.	0.5	6
52	Methyl sydnone imine and its energetic salts. New Journal of Chemistry, 2021, 45, 2228-2236.	2.8	6
53	Theoretical Study of Shocked Formic Acid: Bornâ€“Oppenheimer MD Calculations of the Shock Hugoniot and Early-Stage Chemistry. Journal of Physical Chemistry B, 2016, 120, 1711-1719.	2.6	5
54	Synthesis and Characterization of the Potential Meltâ€Castable Explosive 3â€(1,2,4â€Oxadiazolyl)â€5â€Nitratomethyl Isoxazole. ChemPlusChem, 2021, 86, 875-878.	2.8	5

#	Article	IF	Citations
55	Title is missing!. Journal of Computational Chemistry, 1996, 17, 1431.	3.3	5
56	Effect of a core-softened Oâ€“O interatomic interaction on the shock compression of fused silica. Journal of Chemical Physics, 2018, 148, .	3.0	3
57	3-Methyl-1,2,3-triazolium-1N-dinitromethylylide and the strategy of zwitterionic dinitromethyl groups in energetic materials design. RSC Advances, 2021, 11, 17710-17714.	3.6	3
58	Energetic triazinium salts from N-amination of 3,5-diamino-6-nitro-1,2,4-triazine. Energetic Materials Frontiers, 2022, 3, 128-136.	3.2	3
59	Challenges and opportunities in integration of 2D materials on 3D substrates: Materials and device perspectives. , 2018, , .		2
60	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
61	Ray tracing calculations in simulated propellant flames with detailed chemistry. Applied Optics, 2019, 58, 1451.	1.8	2
62	Titanium Superoxide for the Oxidation of Amines: Synthesis of bis(3â€nitroâ€1Hâ€1,2,4â€triazolâ€5â€yl)methane and its Metal Salts. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 0, , .	1.2	2
63	Theoretical Chemical Characterization of Energetic Materials. Materials Research Society Symposia Proceedings, 2005, 896, 11.	0.1	1
64	General quantitative structureâ€“property relationships and machine learning correlations to energetic material sensitivities. Theoretical and Computational Chemistry, 2022, , 139-156.	0.4	1