Betsy M Rice

List of Publications by Year
in descending order

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115 papers	5,998 citations	87888 38 h-index	74163 75 g-index
116 all docs	116 docs citations	116 times ranked	3136 citing authors

#	Article	IF	Citations
1	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
2	A Quantum Mechanical Investigation of the Relation between Impact Sensitivity and the Charge Distribution in Energetic Molecules. Journal of Physical Chemistry A, 2002, 106, 1770-1783.	2.5	489
3	Predicting heats of formation of energetic materials using quantum mechanical calculations. Combustion and Flame, 1999, 118, 445-458.	5.2	332
4	Predicting trends in rate parameters for self-diffusion on FCC metal surfaces. Surface Science, 2002, 515, 21-35.	1.9	304
5	Intermolecular potential of carbon dioxide dimer from symmetry-adapted perturbation theory. Journal of Chemical Physics, 1999, 110, 3785-3803.	3.0	279
6	Density functional calculations of bond dissociation energies for NO2 scission in some nitroaromatic molecules. Computational and Theoretical Chemistry, 2002, 583, 69-72.	1.5	247
7	Accurate Predictions of Crystal Densities Using Quantum Mechanical Molecular Volumes. Journal of Physical Chemistry A, 2007, 111, 10874-10879.	2.5	175
8	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
9	Predicting Structure of Molecular Crystals from First Principles. Physical Review Letters, 2008, 101, 115503.	7.8	143
10	Ab Initioand Nonlocal Density Functional Study of 1,3,5-Trinitro-s-triazine (RDX) Conformers. Journal of Physical Chemistry A, 1997, 101, 8720-8726.	2.5	141
11	Theoretical Predictions of Energetic Molecular Crystals at Ambient and Hydrostatic Compression Conditions Using Dispersion Corrections to Conventional Density Functionals (DFT-D). Journal of Physical Chemistry C, 2010, 114, 6734-6748.	3.1	136
12	Intermolecular Potential for the Hexahydro-1,3,5-trinitro-1,3,5-s-triazine Crystal (RDX):â€‰ A Crystal Packing, Monte Carlo, and Molecular Dynamics Study. Journal of Physical Chemistry B, 1997, 101, 798-808.	2.6	119
13	Evaluation of electrostatic descriptors for predicting crystalline density. Journal of Computational Chemistry, 2013, 34, 2146-2151.	3.3	112
14	Theoretical Studies of the Hydrostatic Compression of RDX, HMX, HNIW, and PETN Crystals. Journal of Physical Chemistry B, 1999, 103, 6783-6790.	2.6	110
15	Simulations of High-Pressure Phases in RDX. Journal of Physical Chemistry B, 2011, 115, 4378-4386.	2.6	108
16	Molecular dynamics study of the melting of nitromethane. Journal of Chemical Physics, 2003, 119, 9617-9627.	3.0	103
17	Near-neighbor calculations using a modified cell-linked list method. Computer Physics Communications, 1999, 119, 135-148.	7.5	101
18	Theoretical Studies of Solid Nitromethane. Journal of Physical Chemistry B, 2000, 104, 8406-8419.	2.6	91

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19	The multiscale coarse-graining method: Assessing its accuracy and introducing density dependent coarse-grain potentials. Journal of Chemical Physics, 2010, 133, 064109.	3.0	85
20	Predicting heats of detonation using quantum mechanical calculations. Thermochimica Acta, 2002, 384, 377-391.	2.7	76
21	Isothermalâ^'Isobaric Molecular Dynamics Simulations of 1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane (HMX) Crystals. Journal of Physical Chemistry B, 1998, 102, 6692-6695.	2.6	75
22	Molecular dynamics study of the effects of voids and pressure in defect-nucleated melting simulations. Journal of Chemical Physics, 2003, 118, 9680-9688.	3.0	74
23	Potential energy surface for cyclotrimethylene trinitramine dimer from symmetry-adapted perturbation theory. Physical Chemistry Chemical Physics, 2007, 9, 5561.	2.8	69
24	Molecular Packing and NPT-Molecular Dynamics Investigation of the Transferability of the RDX Intermolecular Potential to 2,4,6,8,10,12-Hexanitrohexaazaisowurtzitane. Journal of Physical Chemistry B, 1998, 102, 948-952.	2.6	68
25	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
26	Molecular Dynamics Simulations of Liquid Nitromethane. Journal of Physical Chemistry A, 2001, 105, 9336-9346.	2.5	61
27	A Transferable Intermolecular Potential for Nitramine Crystals. Journal of Physical Chemistry A, 1998, 102, 8386-8392.	2.5	59
28	Molecular Packing and Molecular Dynamics Study of the Transferability of a Generalized Nitramine Intermolecular Potential to Non-Nitramine Crystals. Journal of Physical Chemistry A, 1999, 103, 989-998.	2.5	59
29	Particle-based multiscale coarse graining with density-dependent potentials: Application to molecular crystals (hexahydro-1,3,5-trinitro-s-triazine). Journal of Chemical Physics, 2011, 135, 044112.	3.0	52
30	Crystal structure prediction for cyclotrimethylene trinitramine (RDX) from first principles. Physical Chemistry Chemical Physics, 2009, 11, 5512.	2.8	51
31	Assessing a Generalized CHNO Intermolecular Potential through ab Initio Crystal Structure Prediction. Journal of Physical Chemistry B, 2004, 108, 17730-17739.	2.6	50
32	Reinvestigation of the Gas-Phase Structure of RDX Using Density Functional Theory Predictions of Electron-Scattering Intensities. Journal of Physical Chemistry A, 2002, 106, 10437-10443.	2.5	48
33	Computational Aspects of Nitrogen-Rich HEDMs. , 2007, , 153-194.		48
34	A molecular dynamics study of 1,1-diamino-2,2-dinitroethylene (FOX-7) crystal using a symmetry adapted perturbation theory-based intermolecular force field. Physical Chemistry Chemical Physics, 2011, 13, 16629.	2.8	48
35	Shock Hugoniot calculations of polymers using quantum mechanics and molecular dynamics. Journal of Chemical Physics, 2012, 137, 204901.	3.0	46
36	Diffusion of H atoms on a Si(111) surface with partial hydrogen coverage: Monte Carlo variational phaseâ€space theory with tunneling correction. Journal of Chemical Physics, 1988, 88, 7221-7231.	3.0	42

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37	Molecular Dynamics Simulations of Normal Mode Vibrational Energy Transfer in Liquid Nitromethane. Journal of Physical Chemistry A, 2004, 108, 532-540.	2.5	42
38	A molecular dynamics study of the role of pressure on the response of reactive materials to thermal initiation. Journal of Applied Physics, 2010, 107, .	2.5	42
39	Kinetic isotope effects for hydrogen diffusion in bulk nickel and on nickel surfaces. Journal of Chemical Physics, 1990, 92, 775-791.	3.0	38
40	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
41	Determination of the pressure dependent melting temperatures of Al and Ni using molecular dynamics. Journal of Applied Physics, 2009, 106, .	2.5	37
42	Multi-scale coarse-graining of non-conservative interactions in molecular liquids. Journal of Chemical Physics, 2014, 140, 104104.	3.0	37
43	Molecular-dynamics study of detonation. I. A comparison with hydrodynamic predictions. Physical Review E, 1996, 53, 611-622.	2.1	36
44	Molecular Dynamics Simulations of Hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX) Using a Combined Sorescuâ˜Riceâ˜Thompson AMBER Force Field. Journal of Physical Chemistry B, 2006, 110, 26185-26188.	2.6	36
45	Molecular Dynamics Simulations of the Melting of 1,3,3-Trinitroazetidine. Journal of Physical Chemistry B, 2006, 110, 5721-5726.	2.6	36
46	Role of microstructure in initiation of Niâ€“Al reactive multilayers. Applied Physics Letters, 2011, 98, .	3.3	36
47	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
48	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
49	Theoretical chemical characterization of energetic materials. Journal of Materials Research, 2006, 21, 2444-2452.	2.6	35
50	Non-equilibrium molecular dynamics simulation study of heat transport in hexahydro-1,3,5-trinitro-s-triazine (RDX). International Journal of Heat and Mass Transfer, 2011, 54, 5623-5632.	4.8	35
51	Performance of Density Functional Theory on the Potential-Energy Surface of the H + OCS System. Journal of Physical Chemistry A, 1998, 102, 6950-6956.	2.5	33
52	Assessment of Dispersion Corrected Atom Centered Pseudopotentials: Application to Energetic Molecular Crystals. Journal of Physical Chemistry B, 2011, 115, 803-810.	2.6	32
53	A molecular dynamics study of the role of relative melting temperatures in reactive Ni/Al nanolaminates. Journal of Physics Condensed Matter, 2011, 23, 275701.	1.8	30
54	Classical dynamics studies of the unimolecular decomposition of nitromethane. Journal of Chemical Physics, 1990, 93, 7986-8000.	3.0	29

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55	Classical Dynamics Simulations of Unimolecular Decomposition of CH2NNO2: HONO Elimination vs N-N Bond Scission. The Journal of Physical Chemistry, 1995, 99, 5016-5028.	2.9	29
56	The dynamics of dissociative chemisorption of H2 on a Si(111) surface. Journal of Chemical Physics, 1987, 86, 1608-1615.	3.0	25
57	An ab Initio QCISD Study of the Potential Energy Surface for the Reaction HNO + NO â† ' N2O + OH. Journal of Physical Chemistry A, 1997, 101, 9430-9438.	2.5	25
58	3,6-Bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,4,2,5-dioxadiazene (BNDD): A Powerful Sensitive Explosive. Synlett, 2011, 2011, 2097-2099.	1.8	25
59	Mechanism of densification in silica glass under pressure as revealed by a bottom-up pairwise effective interaction model. Journal of Chemical Physics, 2012, 136, 134508.	3.0	22
60	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
61	Ab InitioStudy of Reactions ofsym-Triazine. The Journal of Physical Chemistry, 1996, 100, 5681-5689.	2.9	21
62	Efficient determination of Hugoniot states using classical molecular simulation techniques. Molecular Physics, 2003, 101, 3309-3322.	1.7	21
63	A semiclassical treatment of rotationally electronically inelastic scattering of NO from Ag(111). Journal of Chemical Physics, 1989, 90, 575-586.	3.0	20
64	Molecular-dynamics investigation of the desensitization of detonable material. Physical Review E, 1998, 57, 5106-5111.	2.1	19
65	Molecular simulation of shocked materials using the reactive Monte Carlo method. Physical Review E, 2002, 66, 021105.	2.1	19
66	Transferable Reactive Force Fields: Extensions of ReaxFF-lg to Nitromethane. Journal of Physical Chemistry A, 2017, 121, 2001-2013.	2.5	19
67	Comparative Study of Nonlocal Density Functional Theory andab InitioMethods:Â The Potential Energy Surface ofsym-Triazine Reactions. The Journal of Physical Chemistry, 1996, 100, 15368-15382.	2.9	18
68	Molecular-dynamics study of detonation. II. The reaction mechanism. Physical Review E, 1996, 53, 623-635.	2.1	18
69	RDX Compression, Î±â† ' Î³ Phase Transition, and Shock Hugoniot Calculations from Density-Functional-Theory-Based Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 19547-19557.	3.1	17
70	Investigation of the CH3CNâ"CO2 Potential Energy Surface Using Symmetry-Adapted Perturbation Theory. Journal of Physical Chemistry A, 1998, 102, 6981-6992.	2.5	16
71	Toward a Predictive Hierarchical Multiscale Modeling Approach for Energetic Materials. Challenges and Advances in Computational Chemistry and Physics, 2019, , 229-282.	0.6	16
72	Ab initio potential energy surface for the H+OCS reaction. Chemical Physics Letters, 1993, 211, 283-292.	2.6	15

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73	An intermolecular Hâ€“O potential for methyl rotations in solid nitromethane. Journal of Chemical Physics, 1991, 94, 7478-7485.	3.0	14
74	Vibrational mode selectivity in the unimolecular decomposition of CH2NNO2. Journal of Chemical Physics, 1995, 102, 8790-8799.	3.0	14
75	Quantum-Informed Multiscale M&S for Energetic Materials. Advances in Quantum Chemistry, 2014, 69, 171-219.	0.8	14
76	On the importance of shear dissipative forces in coarse-grained dynamics of molecular liquids. Physical Chemistry Chemical Physics, 2015, 17, 10795-10804.	2.8	14
77	Ab Initio Potential Energy Surface for H + OCS Reactions: Extended Basis Sets and Correlation Treatment. The Journal of Physical Chemistry, 1994, 98, 9488-9497.	2.9	13
78	A model for predicting the solubility of 1,3,5-trinitro-1,3,5-s-triazine (RDX) in supercritical CO2: isothermalâ€“isobaric Monte Carlo simulations. Fluid Phase Equilibria, 1999, 155, 177-191.	2.5	13
79	Models for predicting solubilities of 2,4,6-trinitrotoluene (TNT) and 1,3,5-trinitro-1,3,5-s-triazine (RDX) in supercritical CO2: isothermalâ€“isobaric Monte Carlo simulations. Fluid Phase Equilibria, 2001, 187-188, 139-153.	2.5	13
80	Free-energy based pair-additive potentials for bulk Ni-Al systems: Application to study Ni-Al reactive alloying. Journal of Chemical Physics, 2012, 137, 094704.	3.0	13
81	Dynamics of chemisorption/scattering of atomic hydrogen on partially covered Si(111) surfaces. Surface Science, 1988, 198, 360-399.	1.9	12
82	NPT-MC simulations of enhanced solubility of RDX in polar-modified supercritical CO2. Fluid Phase Equilibria, 1999, 166, 1-19.	2.5	11
83	Reaction ensemble molecular dynamics: Direct simulation of the dynamic equilibrium properties of chemically reacting mixtures. Physical Review E, 2004, 70, 061103.	2.1	11
84	Multiscale modeling of energetic materials: Easy to say, harder to do. AIP Conference Proceedings, 2012, , .	0.4	11
85	Classical trajectory study of the unimolecular dissociation of ammonia. Journal of Chemical Physics, 1986, 85, 4392-4399.	3.0	9
86	Transitioning model potentials to real systems. Molecular Physics, 1999, 97, 1085-1094.	1.7	9
87	Transitioning model potentials to real systems. II. Application to molecular oxygen. Journal of Chemical Physics, 2000, 113, 2354-2359.	3.0	9
88	Molecular Dynamics Simulations of the Melting Mechanisms of Perfect and Imperfect Crystals of Dimethylnitramine. Journal of Physical Chemistry B, 2007, 111, 2891-2895.	2.6	9
89	Equilibrium Molecular Dynamics Simulations. , 2009, , 255-290.		9
90	New form of polymeric nitrogen from dynamic shock simulation. Journal of Chemical Physics, 2013, 138, 054503.	3.0	9

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91	A new parameter-free soft-core potential for silica and its application to simulation of silica anomalies. Journal of Chemical Physics, 2015, 143, 244506.	3.0	9
92	Bottom-up coarse-grain modeling of plasticity and nanoscale shear bands in Î±-RDX. Journal of Chemical Physics, 2021, 155, 064503.	3.0	9
93	Heuristics for chemical species identification in dense systems. Journal of Chemical Physics, 2020, 153, 064102.	3.0	8
94	Effects of surface structure and of embedded-atom pair functionals on adatom diffusion on fcc metallic surfaces. Surface Science, 1992, 276, 226-240.	1.9	7
95	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
96	A perspective on modeling the multiscale response of energetic materials. AIP Conference Proceedings, 2017, , .	0.4	5
97	Bottom-up coarse-grain modeling of nanoscale shear bands in shocked Î±-RDX. Journal of Materials Science, 2022, 57, 10627-10648.	3.7	5
98	A comparative study of the reaction dynamics of a model system using different criteria in parameterizing the potential enegy function. Chemical Physics Letters, 1991, 184, 335-342.	2.6	4
99	Simulating Polymorphic Phase Behavior Using Reaction Ensemble Monte Carlo. Journal of Physical Chemistry C, 2007, 111, 365-373.	3.1	4
100	Molecular Dynamics Simulations of Energetic Materials. Theoretical and Computational Chemistry, 2003, , 125-184.	0.4	3
101	Ab Initio and DFT Potential Energy Surfaces for Cyanuric Chloride Reactions. Journal of Physical Chemistry A, 1997, 101, 3400-3407.	2.5	2
102	Direct Quantum Mechanical Simulations of Shocked Energetic Materials Supporting Future Force Insensitive Munitions (IM) Requirements. , 2008, , .		2
103	Machine learning transition temperatures from 2D structure. Journal of Molecular Graphics and Modelling, 2021, 105, 107848.	2.4	2
104	Relationships with oxygen balance and bond dissociation energies. Theoretical and Computational Chemistry, 2022, , 67-79.	0.4	2
105	Theoretical Chemical Characterization of Energetic Materials. Materials Research Society Symposia Proceedings, 2005, 896, 11.	0.1	1
106	Modeling of a random network of extended co solids. , 2012, , .		1
107	General quantitative structureâ€“property relationships and machine learning correlations to energetic material sensitivities. Theoretical and Computational Chemistry, 2022, , 139-156.	0.4	1
108	Toward Addressing the Challenge to Predict the Heat Capacities of RDX and HMX Energetic Materials. Propellants, Explosives, Pyrotechnics, 0, , .	1.6	1

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109	MONTE CARLO CALCULATIONS OF THE PROPERTIES OF SOLID NITROMETHANE. , 1992, , 139-142.		0
110	Chemical Reactions in Highly Non-ideal Environments: Reactive Monte Carlo Simulations. AIP Conference Proceedings, 2003, , .	0.4	0
111	Crystal Structures from Nonempirical Force Fields. , 2008, , .		0
112	Nonequilibrium molecular dynamics simulations of aluminum oxynitride. , 2012, , .		0
113	Evaluation of ReaxFF-lg force fields for use in molecular dynamics simulations of sucrose. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	0
114	MOLECULAR SIMULATIONS OF DYNAMIC PROCESSES OF SOLID EXPLOSIVES. , 2006, , .		0
115	NOVEL SIMULATIONS OF ENERGETIC MATERIALS: CIRCUMVENTING LIMITATIONS IN EXISTING METHODOLOGIES. , 2006, , .		0