Weihua Zhu

List of Publications by Year
in descending order

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163	3,395	136740	182168
papers	citations	32	51
		h-index	g-index

164	164	164	1309
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Design of 1,2,4,5-Tetrazine-Based High-Energy Density Materials. Journal of Physical Chemistry A, 2009, 113, 9404-9412.	1.1	180
2	First-principles band gap criterion for impact sensitivity of energetic crystals: a review. Structural Chemistry, 2010, 21, 657-665.	1.0	165
3	Theoretical Studies on the Structures, Thermodynamic Properties, Detonation Properties, and Pyrolysis Mechanisms of Spiro Nitramines. Journal of Physical Chemistry A, 2006, 110, 3797-3807.	1.1	144
4	Crystal density predictions for nitramines based on quantum chemistry. Journal of Hazardous Materials, 2007, 141, 280-288.	6.5	116
5	DFT study on energetic tetrazolo-[1,5-b]-1,2,4,5-tetrazine and 1,2,4-triazolo-[4,3-b]-1,2,4,5-tetrazine derivatives. Journal of Hazardous Materials, 2010, 179, 581-590.	6.5	115
6	First-Principles Study of the Four Polymorphs of Crystalline Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine. Journal of Physical Chemistry B, 2007, 111, 12715-12722.	1.2	108
7	A new design strategy for high-energy low-sensitivity explosives: combining oxygen balance equal to zero, a combination of nitro and amino groups, and N-oxide in one molecule of 1-amino-5-nitrotetrazole-3N-oxide. Journal of Materials Chemistry A, 2014, 2, 13006.	5.2	91
8	Molecular dynamics simulations of RDX and RDX-based plastic-bonded explosives. Journal of Hazardous Materials, 2009, 164, 1082-1088.	6.5	84
9	Comparative Theoretical Studies of Energetic Substituted Carbon- and Nitrogen-Bridged Difurazans. Journal of Physical Chemistry A, 2010, 114, 603-612.	1.1	76
10	First-Principles Study of Different Polymorphs of Crystalline Zirconium Hydride. Journal of Physical Chemistry C, 2010, 114, 22361-22368.	1.5	75
11	Ab initio study of electronic structure and optical properties of heavy-metal azides: TlN3, AgN3, and CuN3. Journal of Computational Chemistry, 2008, 29, 176-184.	1.5	74
12	Ab Initio Study of Energetic Solids:Â Cupric Azide, Mercuric Azide, and Lead Azide. Journal of Physical Chemistry B, 2006, 110, 18196-18203.	1.2	56
13	DFT studies of pressure effects on structural and vibrational properties of crystalline octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine. Theoretical Chemistry Accounts, 2009, 124, 179-186.	0.5	54
14	Densities, Heats of Formation, Energetic Properties, and Thermodynamics of Formation of Energetic Nitrogen-Rich Salts Containing Substituted Protonated and Methylated Tetrazole Cations: A Computational Study. Journal of Physical Chemistry C, 2010, 114, 13142-13152.	1.5	52
15	Decomposition of a 1,3,5-Triamino-2,4,6-trinitrobenzene Crystal at Decomposition Temperature Coupled with Different Pressures: An ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2015, 119, 16500-16506.	1.5	51
16	Computational studies on the heats of formation, energetic properties, and thermal stability of energetic nitrogen-rich furazano[3,4-b]pyrazine-based derivatives. Computational and Theoretical Chemistry, 2012, 992, 110-119.	1.1	50
17	Comparative First-Principles Study of Structural and Optical Properties of Alkali Metal Azides. Journal of Physical Chemistry B, 2006, 110, 9856-9862.	1.2	48
18	Molecular Design of Tetrazole- and Tetrazine-Based High-Density Energy Compounds with Oxygen Balance Equal to Zero. Journal of Chemical & Engineering Data, 2013, 58, 2748-2762.	1.0	47

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19	Theoretic design of 1,2,3,4-tetrazine-1,3-dioxide-based high-energy density compounds with oxygen balance close to zero. Structural Chemistry, 2013, 24, 1579-1590.	1.0	45
20	Design and selection of nitrogen-rich bridged di-1,3,5-triazine derivatives with high energy and reduced sensitivity. Journal of Molecular Modeling, 2012, 18, 3125-3138.	0.8	44
21	Computational study of energetic nitrogenâ€rich derivatives of 1,1â€²â€•and 5,5â€²â€bridged ditetrazoles. Journal of Computational Chemistry, 2011, 32, 2298-2312.	1.5	43
22	Density functional theory study of the structural and optical properties of lithium azide. Chemical Physics Letters, 2006, 422, 117-121.	1.2	39
23	Computer-aided design of two novel and super-high energy cage explosives: dodecanitrohexaprismane and hexanitrohexaazaprismane. RSC Advances, 2014, 4, 3789-3797.	1.7	38
24	First-principles study of structural and vibrational properties of crystalline silver azide under high pressure. Journal of Solid State Chemistry, 2007, 180, 3521-3528.	1.4	37
25	Comparative DFT Study of Crystalline Ammonium Perchlorate and Ammonium Dinitramide. Journal of Physical Chemistry A, 2008, 112, 4688-4693.	1.1	37
26	Structural Transformations and Absorption Properties of Crystalline 7-Amino-6-nitrobenzodifuroxan under High Pressures. Journal of Physical Chemistry C, 2013, 117, 16830-16839.	1.5	36
27	A comparison of high-level theoretical methods to predict the heats of formation of azo compounds. Computational and Theoretical Chemistry, 2010, 956, 55-60.	1.5	35
28	Initial chemical events in shocked octahydro-1,3,5,7-tetranitro-1,3,5,7- tetrazocine: A new initiation decomposition mechanism. Journal of Chemical Physics, 2012, 136, 044516.	1.2	34
29	Characterization of nitrogen-bridged 1,2,4,5-tetrazine-, furazan-, and 1H-tetrazole-based polyheterocyclic compounds: heats of formation, thermal stability, and detonation properties. Journal of Molecular Modeling, 2012, 18, 3467-3479.	0.8	34
30	Theoretical studies on the structures, heats of formation, energetic properties and pyrolysis mechanisms of nitrogen-rich difurazano[3,4-b:3â€²,4â€²-e]piperazine derivatives and their analogues. Structural Chemistry, 2013, 24, 1071-1087.	1.0	34
31	Density functional theory studies of hydrostatic compression of crystalline ammonium perchlorate. Physical Chemistry Chemical Physics, 2008, 10, 7318.	1.3	33
32	First-principles study of crystalline mono-amino-2,4,6-trinitrobenzene, 1,3-diamino-2,4,6-trinitrobenzene, and 1,3,5-triamino-2,4,6-trinitrobenzene. Computational and Theoretical Chemistry, 2009, 900, 84-89.	1.5	33
33	First-Principles Study of Electronic, Absorption, and Thermodynamic Properties of Crystalline Styphnic Acid and Its Metal Salts. Journal of Physical Chemistry B, 2009, 113, 10315-10321.	1.2	30
34	Theoretical studies of furoxan-based energetic nitrogen-rich compounds. Structural Chemistry, 2011, 22, 149-159.	1.0	30
35	Effects of Noncovalent Interactions on the Impact Sensitivity of HNS-Based Cocrystals: A DFT Study. Crystal Growth and Design, 2019, 19, 756-767.	1.4	30
36	A new design strategy on cage insensitive high explosives: symmetrically replacing carbon atoms by nitrogen atoms followed by the introduction of N-oxides. RSC Advances, 2015, 5, 93607-93614.	1.7	28

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37	How does low temperature coupled with different pressures affect initiation mechanisms and subsequent decompositions in nitramine explosive HMX?. Physical Chemistry Chemical Physics, 2015, 17, 22823-22831.	1.3	27
38	Molecular design of trinitromethyl-substituted nitrogen-rich heterocycle derivatives with good oxygen balance as high-energy density compounds. Structural Chemistry, 2013, 24, 1725-1736.	1.0	26
39	First-principles study of the structural transformation, electronic structure, and optical properties of crystalline 2,6-diamino-3,5-dinitropyrazine-1-oxide under high pressure. Journal of Molecular Modeling, 2013, 19, 5159-5170.	0.8	26
40	An ab initio molecular dynamics study of thermal decomposition of 3,6-di(azido)-1,2,4,5-tetrazine. Physical Chemistry Chemical Physics, 2014, 16, 21620-21628.	1.3	25
41	Tuning Nitrate Electroreduction Activity via an Equilibrium Adsorption Strategy: A Computational Study. Journal of Physical Chemistry Letters, 2022, 13, 1726-1733.	2.1	25
42	Density functional theory study of high-pressure behavior of crystalline hexanitrostilbene. Computational and Theoretical Chemistry, 2009, 910, 148-153.	1.5	24
43	Ab Initio Molecular Dynamics Study of Temperature Effects on the Structure and Stability of Energetic Solid Silver Azide. Journal of Physical Chemistry C, 2011, 115, 20782-20787.	1.5	24
44	Insights into the roles of two constituents CL-20 and HMX in the CL-20:HMX cocrystal at high pressure: a DFT-D study. RSC Advances, 2015, 5, 34216-34225.	1.7	24
45	Decomposition Mechanisms of Î±-Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine Nanoparticles at High Temperatures. Journal of Physical Chemistry C, 2017, 121, 7728-7740.	1.5	24
46	Prediction of the properties and thermodynamics of formation for energetic nitrogenâ€rich salts composed of triaminoguanidinium cation and 5â€nitroiminotetrazolateâ€based anions. Journal of Computational Chemistry, 2012, 33, 1781-1789.	1.5	22
47	Catalytic behavior of hydrogen radicals in the thermal decomposition of crystalline furoxan: DFT-based molecular dynamics simulations. RSC Advances, 2014, 4, 34454.	1.7	22
48	Vacancy-induced initial decomposition of condensed phase NTO via bimolecular hydrogen transfer mechanisms at high pressure: a DFT-D study. Physical Chemistry Chemical Physics, 2015, 17, 10568-10578.	1.3	21
49	Theoretical studies on heats of formation, detonation properties, and bond dissociation energies of monofurazan derivatives. International Journal of Quantum Chemistry, 2010, 110, 1549-1558.	1.0	20
50	Theoretical study of energetic trinitromethylâ€substituted tetrazole and tetrazine derivatives. Journal of Physical Organic Chemistry, 2013, 26, 939-947.	0.9	19
51	Surface-Induced Energetics, Electronic Structure, and Vibrational Properties of Î²-HMX Nanoparticles: A Computational Study. Journal of Physical Chemistry C, 2016, 120, 27182-27191.	1.5	19
52	Computational study of energetic nitrogen-rich derivatives of 1,4-bis(1-azo-2,4-dinitrobenzene)-iminotetrazole. Journal of Molecular Modeling, 2013, 19, 1853-1864.	0.8	18
53	Thermal decomposition of isolated and crystal 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane according to ab initio molecular dynamics simulations. RSC Advances, 2017, 7, 8347-8356.	1.7	18
54	Theoretical studies on new potential high energy density compounds (HEDCs) adamantyl nitrates from gas to solid. Science in China Series B: Chemistry, 2008, 51, 427-439.	0.8	16

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55	First-principles study of electronic structure, absorption spectra, and thermodynamic properties of crystalline 1H-tetrazole and its substituted derivatives. Structural Chemistry, 2010, 21, 847-854.	1.0	16
56	DFT studies on trinitromethyl- or dinitromethyl-modified derivatives of RDX and Î²-HMX. Computational and Theoretical Chemistry, 2013, 1019, 116-124.	1.1	16
57	Comparative theoretical studies of dinitromethyl- or trinitromethyl-modified derivatives of CL-20. Canadian Journal of Chemistry, 2013, 91, 1243-1251.	0.6	16
58	Comparative DFT- and DFT-D-based molecular dynamics studies of pressure effects in crystalline 1,3,5-triamino-2,4,6-trinitrobenzene at room temperature. RSC Advances, 2014, 4, 53149-53156.	1.7	16
59	Theoretical Design on a Series of Novel Bicyclic and Cage Nitramines as High Energy Density Compounds. Journal of Physical Chemistry A, 2017, 121, 9163-9171.	1.1	16
60	Interface reaction processes and reactive properties of Al/CuO nanothermite: An ab initio molecular dynamics simulation. Applied Surface Science, 2018, 459, 835-844.	3.1	16
61	Theoretical studies of a series of azaoxaisowurtzitane cage compounds with high explosive performance and low sensitivity. Computational and Theoretical Chemistry, 2017, 1114, 77-86.	1.1	15
62	Conformational Changes and Decomposition Mechanisms of HMX-Based Cocrystal Explosives at High Temperatures. Journal of Physical Chemistry C, 2020, 124, 25-36.	1.5	15
63	Density functional theory studies of energetic nitrogen-rich derivatives of substituted carbon-bridged diiminotetrazoles. Computational and Theoretical Chemistry, 2011, 967, 257-264.	1.1	14
64	Theoretical studies on the unimolecular decomposition of nitroglycerin. Journal of Molecular Modeling, 2013, 19, 1617-1626.	0.8	14
65	Structureâ€“property relationships of energetic nitrogen-rich salts composed of triaminoguanidinium or ammonium cation and tetrazole-based anions. Journal of Molecular Graphics and Modelling, 2013, 40, 54-63.	1.3	14
66	Structure, intermolecular interactions, and dynamic properties of NTO crystals with impurity defects: a computational study. CrystEngComm, 2021, 23, 2455-2468.	1.3	14
67	First-principles study of the structure, mechanical properties, and phase stability of crystalline zirconia under high pressure. Structural Chemistry, 2012, 23, 601-611.	1.0	13
68	Theoretical design of energetic nitrogen-rich derivatives of 1,7-diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazaheptane. Journal of Molecular Modeling, 2013, 19, 2945-2954.	0.8	13
69	A comparative theoretical study of heterocycle-functionalized tetrazolate- and tetrazolate-1-oxide-based dianionic salts. Canadian Journal of Chemistry, 2013, 91, 1233-1242.	0.6	13
70	Dispersion-corrected DFT study on the structure and absorption properties of crystalline 5-nitro-2,4-dihydro-1,2,4-triazole-3-one under compression. Structural Chemistry, 2015, 26, 477-484.	1.0	13
71	Designing and looking for novel cage compounds based on bicyclo-HMX as high energy density compounds. RSC Advances, 2018, 8, 44-52.	1.7	13
72	Possible pre-phase transition of the Î±-HMX crystal observed by the variation of hydrogen-bonding network under high pressures. CrystEngComm, 2020, 22, 330-348.	1.3	13

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73	Density functional theory study of structural, vibrational, and thermodynamic properties of crystalline 2,4-dinitrophenol, 2,4-dinitroresorcinol, and 4,6-dinitroresorcinol. Computational and Theoretical Chemistry, 2009, 895, 131-137.	1.5	12
74	Theoretical studies of energetic nitrogen-rich ionic salts composed of substituted 5-nitroiminotetrazolate anions and various cations. Journal of Molecular Modeling, 2013, 19, 3103-3118.	0.8	12
75	Pressure-induced hydrogen transfer and polymerization in crystalline furoxan. RSC Advances, 2014, 4, 15995-16004.	1.7	12
76	Designing and screening novel explosives with high energy and low sensitivity by appropriately introducing N-oxides, amino groups, and nitro groups into s-heptazine. RSC Advances, 2014, 4, 53000-53009.	1.7	12
77	Thermal decomposition mechanisms of the energetic benzotrifuroxan:1,3,3â€trinitroazetidine cocrystal using ab initio molecular dynamics simulations. Journal of the Chinese Chemical Society, 2020, 67, 218-226.	0.8	12
78	Comparative Theoretical Studies on Energetic Ionic Salts Composed of Heterocycle-Functionalized Nitraminofurazanate-Based Anions and Triaminoguanidinium Cation. Journal of Chemical & Engineering Data, 2014, 59, 295-306.	1.0	11
79	Quantum chemical studies on three novel 1,2,4-triazole N-oxides as potential insensitive high explosives. Journal of Molecular Modeling, 2014, 20, 2441.	0.8	11
80	Comparative DFT and DFT-D studies on structural, electronic, vibrational and absorption properties of crystalline ammonium perchlorate. RSC Advances, 2016, 6, 48489-48497.	1.7	11
81	Searching for a new family of modified CL-20 cage derivatives with high energy and low sensitivity. Structural Chemistry, 2018, 29, 837-845.	1.0	11
82	Insight into the roles of small molecules in CL-20 based hostâ€“guest crystals: a comparative DFT-D study. CrystEngComm, 2020, 22, 6228-6238.	1.3	11
83	Theoretical studies on the surface property, thermal behaviors, stability, and disassembly process of HMX/DMF cocrystal. Computational Materials Science, 2020, 178, 109643.	1.4	11
84	Prediction of supramolecular synthons and crystal packings of supramolecular HMX/solvent assemblies. RSC Advances, 2017, 7, 55482-55488.	1.7	10
85	DFT studies on nitrogen-rich pyrazino [2, 3-e] [1, 2, 3, 4] tetrazineâ€“based highâ€“energy density compounds. Journal of Molecular Modeling, 2019, 25, 283.	0.8	10
86	Effect of particle size on the thermal decomposition of nano Îµ-CL-20 by ReaxFF-lg molecular dynamics simulations. Chemical Physics Letters, 2020, 761, 138067.	1.2	10
87	DFT study on the structures and properties of 3-nitro-1,2,4-triazol-5-one crystals at high pressure. Journal of Molecular Graphics and Modelling, 2007, 26, 415-419.	1.3	9
88	DFT study of pressure effects in molecular crystal 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo-[5.5.0.05,903,11]-dodecane. Canadian Journal of Chemistry, 2014, 92, 616-624.	0.6	9
89	Searching for a new family of insensitive high explosives by introducing N hybridization and N-oxides into a cage cubane. Journal of Molecular Modeling, 2014, 20, 2483.	0.8	9
90	Thermal decomposition mechanisms of energetic ionic crystal dihydrazinium 3,3â€²-dinitro-5,5â€²-bis-1,2,4-triazole-1,1-diolate: An ab initio molecular dynamics study. Fuel, 2017, 202, 246-259.	3.4	9

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91	Coupling effect of high temperature and pressure on the decomposition mechanism of crystalline HMX. Energetic Materials Frontiers, 2020, 1, 90-94.	1.3	9
92	Ab initio molecular dynamics studies on the transport mechanisms of oxygen atoms in the adiabatic reaction of Al/CuO nanothermite. Chemical Physics Letters, 2020, 745, 137278.	1.2	9
93	Intermolecular interactions, vibrational spectra, and detonation performance of <scp>CL</scp>â€20/<scp>TNT</scp> cocrystal. Journal of the Chinese Chemical Society, 2020, 67, 1742-1752.	0.8	9
94	Desensitizing high energy materials HMX and CL-20 by the smallest all carbon compound cyclo[18]carbon: a DFT study. Journal of Materials Science, 2022, 57, 10197-10212.	1.7	9
95	Comparative theoretical studies on energetic substituted 1,2,4-triazole molecules and their corresponding ionic salts containing 1,2,4-triazole-based cations or anions. Structural Chemistry, 2013, 24, 1429-1442.	1.0	8
96	Searching for a new family of high energy explosives by introducing N atoms, N-oxides, and NO₂ into a cage adamantane. Canadian Journal of Chemistry, 2016, 94, 667-673.	0.6	8
97	Preparation, characterization and compatibility studies of poly(DFAMO/AMMO). Journal of Macromolecular Science - Pure and Applied Chemistry, 2018, 55, 135-141.	1.2	8
98	Molecular design of all nitrogen pentazoleâ€based high energy density compounds with oxygen balance equal to zero. Journal of the Chinese Chemical Society, 2019, 66, 377-384.	0.8	8
99	First-principle study and Hirshfeld surface analysis on the effect of H2O, NH3 and H2S on structural, electronic, elastic, optical and thermodynamic properties of a novel high-energy crystal 2,4,6-triamino-5-nitropyrimidine-1,3-dioxide. Journal of Materials Science, 2020, 55, 237-249.	1.7	8
100	Thermal decomposition mechanisms of benzotrifuroxan:2,4,6-trinitrotoluene cocrystal using quantum molecular dynamics simulations. Chemical Physics Letters, 2021, 778, 138820.	1.2	8
101	Periodic density functional theory study of the high-pressure behavior of energetic crystalline 1,4-dinitrofurazano[3, 4-b]piperazine. Journal of Molecular Modeling, 2013, 19, 305-314.	0.8	7
102	Periodic DFT study of structural, electronic, absorption, and thermodynamic properties of crystalline Î±-RDX under hydrostatic compression. Structural Chemistry, 2014, 25, 451-461.	1.0	7
103	A DFT study of the unimolecular decomposition of 1,2,4-butanetriol trinitrate. Journal of Molecular Modeling, 2014, 20, 2081.	0.8	7
104	Formation and growth mechanisms of natural metastable twin boundary in crystalline Î²-octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine: a computational study. RSC Advances, 2015, 5, 86041-86049.	1.7	7
105	Density functional theory study of high-energy metal (Al, Mg, Ti, and Zr)/CuO composites. RSC Advances, 2016, 6, 90206-90211.	1.7	7
106	Molecular design and property prediction of a series of novel cyclotetramethylene tetranitramine derivatives as high energy density compounds. Structural Chemistry, 2018, 29, 1457-1463.	1.0	7
107	Ab initio molecular dynamics simulations study on initial decompositions of Î²â€HMX at high temperature coupled with high pressures. Journal of the Chinese Chemical Society, 2019, 66, 1429-1435.	0.8	7
108	Designing and looking for novel low-sensitivity and high-energy cage derivatives based on the skeleton of nonanitro nonaaza pentadecane framework. Structural Chemistry, 2020, 31, 1387-1402.	1.0	7

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109	External electric field induced conformational changes as a buffer to increase the stability of CL-20/HMX cocrystal and its pure components. Materials Today Communications, 2021, 26, 101696.	0.9	7
110	Computational insights into the formation driving force of CL-20 based solvates and their desolvation process. CrystEngComm, 2021, 23, 2150-2161.	1.3	7
111	Pressure effects on structural, electronic, absorption, and thermodynamic properties of crystalline 2,4,6-triamino-3,5-dinitropyridine-1-oxide: A DFT study. Journal of Physical Organic Chemistry, 2013, 26, 589-595.	0.9	6
112	Cooperative effects of different temperatures and pressures on the initial and subsequent decomposition reactions of the nitrogen-rich energetic crystal 3,3â€²-dinitroamino-4,4â€²-azoxyfurazan. Physical Chemistry Chemical Physics, 2016, 18, 7093-7099.	1.3	6
113	Application of Molecular Electrostatic Potential Surface to Predict Supramolecular Synthons for RDX/Solvent Cocrystals. Crystal Research and Technology, 2019, 54, 1900171.	0.6	6
114	Molecular design on a new family of azaoxaadamantane cage compounds as potential high-energy density compounds. Canadian Journal of Chemistry, 2019, 97, 86-93.	0.6	6
115	Î²â€‰â†’â€‰Î´ phase transition and initial decomposition of HMX nanoparticle from reactive molecular dynamics simulations. Journal of Nanoparticle Research, 2020, 22, 1.	0.8	6
116	Effectively improving the energy of monocyclic imidazoles to a high level by the introduction of bridge-rings and nitro groups through different kinds of Dielsâ€“Alder reactions: a DFT study. Molecular Systems Design and Engineering, 2020, 5, 1679-1690.	1.7	6
117	Quantum chemical investigations of reaction mechanism. Theoretical and Computational Chemistry, 2022, , 291-345.	0.2	6
118	DFT study of structural, electronic, and absorption properties of crystalline Î²-RDX under pressures. Canadian Journal of Chemistry, 2013, 91, 968-973.	0.6	5
119	DFT-D studies on structural variation and absorption properties of crystalline benzotrifuroxan under high pressure. Canadian Journal of Chemistry, 2014, 92, 1131-1137.	0.6	5
120	Pressure-induced structure and properties of crystalline Î²-FOX-7 by LDA and GGA calculations. Structural Chemistry, 2014, 25, 1625-1633.	1.0	5
121	Comparative theoretical studies of differently bridged nitramino-substituted ditetrazole 2-N-oxides with high detonation performance and an oxygen balance of around zero. Journal of Molecular Modeling, 2017, 23, 186.	0.8	5
122	The search for new powerful energetic transition metal complexes based on 3,3â€²-dinitro-5,5â€²-bis-1,2,4-triazole-1,1â€²-diolate anion: a DFT study. Journal of Molecular Modeling, 2017, 23, 254.	0.8	5
123	Adiabatic and constant volume decomposition process of condensed phase Î´-1,3,5,7-tetranitro-1,3,5,7-tetrazocane at high temperatures: Quantum molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2018, 85, 68-74.	1.3	5
124	Pressure-induced structure, vibrational properties, and initial decomposition mechanisms of Î´-HMX crystal: A periodic DFT study. Journal of Molecular Graphics and Modelling, 2019, 90, 144-152.	1.3	5
125	Theoretical studies on the role of each component in benzotrifuroxan/2,4,6-trinitrotoluene cocrystal. Chemical Physics Letters, 2020, 753, 137608.	1.2	5
126	Pressure-induced changes in the structural and absorption properties of crystalline 5-nitramino-3,4-dinitropyrazole. Journal of Chemical Sciences, 2015, 127, 1777-1784.	0.7	4

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127	Coupling of temperature with pressure induced initial decomposition mechanisms of two molecular crystals: An ab initio molecular dynamics study. Journal of Chemical Sciences, 2016, 128, 695-705.	0.7	4
128	New concept for the design of zero-hydrogen energetic materials with high energy and low sensitivity: achieving a good balance among parent compounds, nitro groups, and N-oxides. Canadian Journal of Chemistry, 2017, 95, 505-511.	0.6	4
129	A DFT study of the structureâ€“property relationships of bistetrazole-based high-nitrogen energetic metal complexes. Journal of Molecular Modeling, 2018, 24, 119.	0.8	4
130	Thermal decomposition of energetic MOFs nickel hydrazine nitrate crystals from an ab initio molecular dynamics simulation. Computational Materials Science, 2018, 143, 170-181.	1.4	4
131	Mechanisms and kinetics of initial pyrolysis and combustion reactions of 1,1-diamino-2,2-dinitroethylene from density functional tight-binding molecular dynamics simulations. Canadian Journal of Chemistry, 2019, 97, 795-804.	0.6	4
132	Theoretical Studies on Energetic Nitrogenâ€Rich Heterocyclic Substituted Derivatives of Pyrazino [2, 3â€e] [1, 2, 3, 4] Tetrazineâ€1, 3â€diâ€N â€oxide. ChemistrySelect, 2019, 4, 13646-13655.	0.7	4
133	Coupling effects of high temperature and pressure on the decomposition mechanisms of 1,1â€diaminoâ€2,2â€dinitroehethe crystal: Ab initio molecular dynamics simulations. Journal of the Chinese Chemical Society, 2020, 67, 1571-1578.	0.8	4
134	Ab initio molecular dynamics studies on the ignition and combustion mechanisms, twice exothermic characteristics, and mass transport properties of Al/NiO nanothermite. Journal of Materials Science, 2021, 56, 11364-11376.	1.7	4
135	Theoretical design of novel high energy metal complexes based on two complementary oxygen-rich mixed ligands of 4-amino-4H-1,2,4-triazole-3,5-diol and 1,1â€²-dinitramino-5,5â€²-bistetrazole. Journal of Molecular Modeling, 2019, 25, 340.	0.8	3
136	Insight into interaction mechanisms of binary mixture systems of explosion products (H2O, CO2, and) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.2	3
137	Environmental degradability of 1,2,3,4-tetrazine-1,3-dioxide-functionalized FOX-7 derivatives with high energy and low sensitivity: a computational evaluation. Structural Chemistry, 2019, 30, 327-340.	1.0	3
138	Theoretical predictions on pentaerythritol tetranitrateâ€based high energy density compounds. Journal of the Chinese Chemical Society, 2020, 67, 1753-1762.	0.8	3
139	Computer-aided design and property prediction of novel insensitive high-energy heterocycle-substituted derivatives of cage NNNAHP. Journal of Molecular Modeling, 2020, 26, 239.	0.8	3
140	Using a Thin ZnO Film as an Intermediate Layer to Tune the Performance of Mg-Based Nanolaminates: A First-Principles Study. Langmuir, 2021, 37, 12548-12556.	1.6	3
141	Theoretical study of energetic carbon-oxidized triazole and tetrazole derivatives. Canadian Journal of Chemistry, 2015, 93, 368-374.	0.6	2
142	An Ab Initio Molecular Dynamics study of Low Temperature Effects in Crystalline Î±â€HMX. Physica Status Solidi (B): Basic Research, 2019, 256, 1900057.	0.7	2
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