Weihua Zhu

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2536174/publications.pdf

Version: 2024-02-01

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	First principle study and Hirshfeld surface analysis on the effect of type, number, and position of small molecules on the structural stability and optical property of a powerful energetic crystal 6-nitro-7-azido-pyrazol[3,4-d][1,2,3]triazine-2-oxide. Materials Advances, 2022, 3, 1035-1046.	2.6	1
2	Optimization and design for the curing process of solid azide propellant: Influence of typical components on the curing reactions of <scp>PBT</scp> binders with <scp>TDI</scp>. Journal of the Chinese Chemical Society, 2022, 69, 419-439.	0.8	1
3	Quantum chemical investigations of reaction mechanism. Theoretical and Computational Chemistry, 2022, , 291-345.	0.2	6
4	Tuning Nitrate Electroreduction Activity via an Equilibrium Adsorption Strategy: A Computational Study. Journal of Physical Chemistry Letters, 2022, 13, 1726-1733.	2.1	25
5	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
6	Effects of oxidizing molecules on the thermal decomposition of TTDO by ab initio molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2022, 116, 108270.	1.3	1
7	Molecular design, property prediction, and intermolecular interactions for highâ€energy cage compounds based on the skeletons of RDX and HMX. Journal of the Chinese Chemical Society, 2021, 68, 557-568.	0.8	2
8	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
9	Theoretical studies of size effects on surfacial properties for CL-20 and NTO nanoparticles. Structural Chemistry, 2021, 32, 565-580.	1.0	2
10	Theorectical Studies on Surface-Induced Energetic, Electronic, and Vibrational Properties of Triamino-trinitrobenzene Nanoparticles. Journal of Cluster Science, 2021, 32, 887-897.	1.7	2
11	Computational insights into the formation driving force of CL-20 based solvates and their desolvation process. CrystEngComm, 2021, 23, 2150-2161.	1.3	7
12	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
13	Cisâ€“Trans Isomerization and Thermal Decomposition Mechanisms of a Series of N_x (x = 4, 8, 10, 11) Chain-Catenated Energetic Crystals. Journal of Physical Chemistry A, 2021, 125, 2826-2835.	1.1	2
14	Theoretical design on a series of new cageâ€shaped high energy density compounds. Journal of the Chinese Chemical Society, 2021, 68, 1852.	0.8	0
15	Thermal decomposition mechanisms of benzotrifuroxan:2,4,6-trinitrotoluene cocrystal using quantum molecular dynamics simulations. Chemical Physics Letters, 2021, 778, 138820.	1.2	8
16	Structure, intermolecular interactions, and dynamic properties of NTO crystals with impurity defects: a computational study. CrystEngComm, 2021, 23, 2455-2468.	1.3	14
17	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
18	Computational Design of High Energy RDX-Based Derivatives: Property Prediction, Intermolecular Interactions, and Decomposition Mechanisms. Molecules, 2021, 26, 7199.	1.7	1

#	Article	IF	Citations
19	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
20	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
21	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
22	Computational study of energetic derivatives of 3,3â€²-bridged ditriazoles. Canadian Journal of Chemistry, 2020, 98, 115-127.	0.6	1
23	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
24	Computational insight into energetic cage derivatives based on hexahydroâ€1,3,5â€trinitroâ€1,3,5â€triazine. Journal of the Chinese Chemical Society, 2020, 67, 961-968.	0.8	1
25	Theoretical studies on the structure and properties of DAT/BTNAT cocrystal under high pressure. Canadian Journal of Chemistry, 2020, 98, 128-133.	0.6	1
26	Coupling effect of high temperature and pressure on the decomposition mechanism of crystalline HMX. Energetic Materials Frontiers, 2020, 1, 90-94.	1.3	9
27	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
28	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
29	Theoretical predictions on pentaerythritol tetranitrateâ€based high energy density compounds. Journal of the Chinese Chemical Society, 2020, 67, 1753-1762.	0.8	3
30	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
31	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
32	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
33	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
34	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
35	<scp>Density functional theory</scp> studies of effects of boron replacement on the structure and property of <scp>RDX</scp> and <scp>HMX</scp>. Journal of the Chinese Chemical Society, 2020, 67, 1977-1985.	0.8	2
36	Computational insight into polynitromethyl- and polydifluoroaminomethyl-substituted energetic derivatives of 2,3-dihydro pyrazino [2,3-e] [1, 2, 3, 4] tetrazine. Journal of Molecular Modeling, 2020, 26, 78.	0.8	2

#	Article	IF	Citations
37	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
38	Effects of boron doping on structural, electronic, elastic, and optical properties of energetic crystal 2,6-diamino-3,5-dinitropyrazine-1-oxide: a theoretical study using the first principles calculation and Hirshfeld surface analysis. Journal of Molecular Modeling, 2020, 26, 41.	0.8	1
39	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
40	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
41	Theoretical studies on the role of each component in benzotrifuroxan/2,4,6-trinitrotoluene cocrystal. Chemical Physics Letters, 2020, 753, 137608.	1.2	5
42	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
43	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
44	Application of Molecular Electrostatic Potential Surface to Predict Supramolecular Synthons for RDX/Solvent Cocrystals. Crystal Research and Technology, 2019, 54, 1900171.	0.6	6
45	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
46	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
47	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
48	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
49	Structural and Vibrational Properties of Crystalline Î² â€Octahydroâ€1,3,5,7â€tetranitroâ€1,3,5,7â€tetrazocine at High Temperatures: Ab Initio Molecular Dynamics Studies. ChemistrySelect, 2019, 4, 4244-4250.	0.7	1
50	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
51	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
52	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
53	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
54	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

#	Article	IF	Citations
55	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
56	High-nitrogen nitrotetrazole substituted tetrazole 3-N-oxides as potential high energy density compounds. Canadian Journal of Chemistry, 2018, 96, 459-465.	0.6	1
57	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
58	Preparation, characterization and compatibility studies of poly(DFAMO/AMMO). Journal of Macromolecular Science - Pure and Applied Chemistry, 2018, 55, 135-141.	1.2	8
59	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
60	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
61	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
62	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
63	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
64	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
65	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
66	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
67	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
68	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
69	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
70	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
71	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
72	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

#	Article	IF	Citations
73	Prediction of supramolecular synthons and crystal packings of supramolecular HMX/solvent assemblies. RSC Advances, 2017, 7, 55482-55488.	1.7	10
74	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
75	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
76	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
77	Density functional theory study of high-energy metal (Al, Mg, Ti, and Zr)/CuO composites. RSC Advances, 2016, 6, 90206-90211.	1.7	7
78	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
79	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
80	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
81	Comparative DFT-D studies on structural and absorption properties of crystalline 3,3â€²-dinitroamino-4,4â€²-azoxyfurazan, 3,3â€²-dinitro-4,4â€²-azoxyfurazan, and 3,4-bis(3-nitrofurazan-4-yl)furoxan under high pressures. Canadian Journal of Chemistry, 2015, 93, 1191-1198.	0.6	0
82	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
83	Theoretical study of energetic carbon-oxidized triazole and tetrazole derivatives. Canadian Journal of Chemistry, 2015, 93, 368-374.	0.6	2
84	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
85	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
86	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
87	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
88	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
89	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
90	Improving an insensitive low-energy compound, 1,3,4,6,7,9-hexaazacycl[3.3.3]azine, to be an insensitive high explosive by way of two-step structural modifications. Canadian Journal of Chemistry, 2014, 92, 1157-1161.	0.6	1

#	Article	IF	Citations
91	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
92	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
93	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
94	A DFT study of the unimolecular decomposition of 1,2,4-butanetriol trinitrate. Journal of Molecular Modeling, 2014, 20, 2081.	0.8	7
95	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
96	Computer-aided design of two novel and super-high energy cage explosives: dodecanitrohexaprismane and hexanitrohexaazaprismane. RSC Advances, 2014, 4, 3789-3797.	1.7	38
97	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
98	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
99	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
100	Pressure-induced hydrogen transfer and polymerization in crystalline furoxan. RSC Advances, 2014, 4, 15995-16004.	1.7	12
101	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
102	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
103	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
104	Pressure-induced structure and properties of crystalline Î²-FOX-7 by LDA and GGA calculations. Structural Chemistry, 2014, 25, 1625-1633.	1.0	5
105	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
106	DFT studies on trinitromethyl- or dinitromethyl-modified derivatives of RDX and Î²-HMX. Computational and Theoretical Chemistry, 2013, 1019, 116-124.	1.1	16
107	Theoretical studies on the unimolecular decomposition of nitroglycerin. Journal of Molecular Modeling, 2013, 19, 1617-1626.	0.8	14
108	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

#	Article	IF	Citations
109	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
110	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
111	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
112	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
113	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
114	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
115	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
116	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
117	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
118	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
119	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
120	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
121	Comparative theoretical studies of dinitromethyl- or trinitromethyl-modified derivatives of CL-20. Canadian Journal of Chemistry, 2013, 91, 1243-1251.	0.6	16
122	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
123	Theoretical study of energetic trinitromethylâ€substituted tetrazole and tetrazine derivatives. Journal of Physical Organic Chemistry, 2013, 26, 939-947.	0.9	19
124	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
125	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
126	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

#	Article	IF	Citations
127	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
128	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
129	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
130	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
131	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
132	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
133	Theoretical studies of furoxan-based energetic nitrogen-rich compounds. Structural Chemistry, 2011, 22, 149-159.	1.0	30
134	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
135	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
136	First-principles band gap criterion for impact sensitivity of energetic crystals: a review. Structural Chemistry, 2010, 21, 657-665.	1.0	165
137	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
138	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
139	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
140	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
141	First-Principles Study of Different Polymorphs of Crystalline Zirconium Hydride. Journal of Physical Chemistry C, 2010, 114, 22361-22368.	1.5	75
142	Comparative Theoretical Studies of Energetic Substituted Carbon- and Nitrogen-Bridged Difurazans. Journal of Physical Chemistry A, 2010, 114, 603-612.	1.1	76
143	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
144	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

#	Article	IF	Citations
145	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
146	Density functional theory study of high-pressure behavior of crystalline hexanitrostilbene. Computational and Theoretical Chemistry, 2009, 910, 148-153.	1.5	24
147	Molecular dynamics simulations of RDX and RDX-based plastic-bonded explosives. Journal of Hazardous Materials, 2009, 164, 1082-1088.	6.5	84
148	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
149	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
150	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
151	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
152	Density functional theory studies of hydrostatic compression of crystalline ammonium perchlorate. Physical Chemistry Chemical Physics, 2008, 10, 7318.	1.3	33
153	Comparative DFT Study of Crystalline Ammonium Perchlorate and Ammonium Dinitramide. Journal of Physical Chemistry A, 2008, 112, 4688-4693.	1.1	37
154	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
155	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
156	Crystal density predictions for nitramines based on quantum chemistry. Journal of Hazardous Materials, 2007, 141, 280-288.	6.5	116
157	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
158	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
159	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
160	Density functional theory study of the structural and optical properties of lithium azide. Chemical Physics Letters, 2006, 422, 117-121.	1.2	39
161	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
162	Insight into the interaction mechanisms of N 2 / H 2 O / CO 2 /C mixture at extreme conditions by reactive molecular dynamic simulations. Journal of the Chinese Chemical Society, 0, , .	0.8	0

#	Article	IF	Citations
163	Prediction of the crystal structure and properties of energetic <scp>LLM</scp> â€105:oxidant cocrystals: A theoretical study. Journal of the Chinese Chemical Society, 0, , .	0.8	0