Qiong Wu

List of Publications by Year in descending order

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		430442	500791
62	901	18	28
papers	citations	h-index	g-index

63	63	63	659
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	Effects of number, type and length of the alkyl-chain on the structure and property of indazole derivatives used as corrosion inhibitors. Materials Today Chemistry, 2022, 23, 100636.	1.7	8
3	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
4	Theoretical design of new bridge-ring insensitive high energy compounds by selected normal Diels-Alder reactions between NH2-substituted oxazoles and NO2/NF2/NHNO2-substituted ethylenes/acetylenes. Defence Technology, 2021, 17, 1731-1739.	2.1	2
5	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
6	Structure design and property adjustment of new cage rich-nitrogen pentazolyltetraazacubanes as potential high energy density compounds. Defence Technology, 2020, 16, 705-711.	2.1	2
7	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
8	<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
9	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
10	Preparation of fewâ€layer twoâ€dimensional polymers by selfâ€assembly of bolaâ€amphiphilic small molecules. Journal of Polymer Science Part A, 2019, 57, 1748-1755.	2.5	4
11	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
12	MOF-derived CeO₂/Au@SiO₂ hollow nanotubes and their catalytic activity toward 4-nitrophenol reduction. New Journal of Chemistry, 2019, 43, 4581-4589.	1.4	21
13	Molecular design of novel super high energy compounds by incorporating the difluoramino group, N-oxide and different bridge groups into the 1H-tetrazole. Journal of Fluorine Chemistry, 2019, 218, 21-26.	0.9	7
14	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
15	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
16	In Situ Formation of Ptâ€“Au Nanoparticles on Magnetic Composites Carriers: Tuning Catalytic Activity by Incorporation of Different Metal Oxides. Bulletin of the Korean Chemical Society, 2018, 39, 71-77.	1.0	7
17	Facile one-step synthesis of TiO2/Ag/SnO2 ternary heterostructures with enhanced visible light photocatalytic activity. Scientific Reports, 2018, 8, 10532.	1.6	69
18	Encapsulation of supported gâ€C ₃ N ₄ /Au with metalâ€“organic frameworks for enhanced stability towards photocatalytic hydrogen evolution. Micro and Nano Letters, 2018, 13, 1321-1324.	0.6	1

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19	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
20	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
21	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
22	Density Function Theory Study on Effects of Different Energetic Substituent Groups and Bridge Groups on Performance of Carbon-Linked Ditetrazole 2N-Oxides. Chinese Journal of Chemical Physics, 2017, 30, 404-410.	0.6	0
23	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
24	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
25	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
26	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
27	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
28	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
29	Theoretical study of energetic carbon-oxidized triazole and tetrazole derivatives. Canadian Journal of Chemistry, 2015, 93, 368-374.	0.6	2
30	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
31	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
32	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
33	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
34	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
35	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
36	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

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37	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
38	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
39	First-principles study of the high-pressure behavior of solid 1,7-diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazaheptane. Computational and Theoretical Chemistry, 2014, 1030, 38-43.	1.1	4
40	Computer-aided design of two novel and super-high energy cage explosives: dodecanitrohexaprismane and hexanitrohexaazaprismane. RSC Advances, 2014, 4, 3789-3797.	1.7	38
41	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
42	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
43	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
44	Pressure-induced hydrogen transfer and polymerization in crystalline furoxan. RSC Advances, 2014, 4, 15995-16004.	1.7	12
45	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
46	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
47	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
48	Pressure-induced structure and properties of crystalline Î²-FOX-7 by LDA and GGA calculations. Structural Chemistry, 2014, 25, 1625-1633.	1.0	5
49	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
50	DFT study on crystalline 1,1-diamino-2,2-dintroethylene under high pressures. Journal of Molecular Modeling, 2013, 19, 4039-4047.	0.8	25
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	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
59	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
60	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
61	Theoretical study of energetic trinitromethylâ€substituted tetrazole and tetrazine derivatives. Journal of Physical Organic Chemistry, 2013, 26, 939-947.	0.9	19
62	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