Han Qin

List of Publications by Year
in descending order

25 papers	133 citations	1477746 6 h-index	1281420 11 g-index
25 all docs	25 docs citations	25 times ranked	111 citing authors

#	Article	IF	Citations
1	The doping effects on antibonding states and carriers of two-dimensional PC6. Physical Chemistry Chemical Physics, 2022, , .	1.3	2
2	The vibrational, thermodynamic and mechanical properties of four types HMX based on the first-principles study. Journal of Energetic Materials, 2021, 39, 125-169.	1.0	12
3	Electronic, optical, and vibrational properties of B3N3H6 from first-principles calculations. Journal of Molecular Modeling, 2021, 27, 241.	0.8	0
4	Judging the phase transition pressure of the unknown parent phase if the resulting state is known. Physical Chemistry Chemical Physics, 2020, 22, 624-627.	1.3	0
5	Formation of heterogeneous energetic materials to regulate sensitivity of TATB by 2D materials. Vacuum, 2020, 177, 109392.	1.6	1
6	Inversely deducing the initiation mechanism of energetic materials under pressure from possible defect states in nitromethane. Chemical Physics Letters, 2020, 749, 137470.	1.2	7
7	Theoretical study on the effect of different surfaces on structure, excess energy, electronic structure and impact sensitivity in 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane. Surface Science, 2020, 700, 121650.	0.8	1
8	The Raman and IR vibration modes of metal pentazolate hydrates [Na(H2O)(N5)]Â·2H2O and [Mg(H2O)6(N5)2]Â·4H2O. Journal of Molecular Modeling, 2020, 26, 84.	0.8	3
9	Vibrational, thermodynamic, and dielectric properties of Îµ-CL-20: first-principles calculations. Journal of Molecular Modeling, 2020, 26, 47.	0.8	0
10	First-principles study of structural, elastic, electronic and optical properties of RDX under pressure. Philosophical Magazine, 2020, 100, 1015-1031.	0.7	3
11	Structures, Elasticity, and Sensitivity Characteristics of É›â€CLâ€20 under High Pressure from Firstâ€Principles Calculations. Physica Status Solidi (B): Basic Research, 2019, 256, 1800440.	0.7	4
12	A comparative study of the vibrational and thermodynamic properties of Î±-RDX and Î³-RDX under ambient conditions. Journal of Molecular Modeling, 2019, 25, 182.	0.8	7
13	Structural, Elastic, Mechanical and Electronic Properties of NbWâ€Based Intermetallic Compounds: Firstâ€Principles Calculations. Physica Status Solidi (B): Basic Research, 2019, 256, 1800570.	0.7	1
14	A systematic study of the surface structures and energetics of CH3NO2 surfaces by first-principles calculations. Journal of Molecular Modeling, 2019, 25, 164.	0.8	4
15	Structural and electronic properties of Nb-Cr-Si based alloys: First-principles calculations. Physica B: Condensed Matter, 2019, 568, 1-5.	1.3	2
16	Influences of pressure on structural and electronic properties of four types of HMX. Journal of Molecular Modeling, 2019, 25, 63.	0.8	3
17	A new criterion for the prediction of solid-state phase transition in TMDs. Physical Chemistry Chemical Physics, 2019, 21, 24070-24076.	1.3	4
18	First-principle calculations of electronic, vibrational, and thermodynamic properties of 1,3-diamino-2,4,6-trinitrobenzene. Journal of Molecular Modeling, 2019, 25, 356.	0.8	4

#	Article	IF	Citations
19	First-principles study of structural, elastic, and electronic properties of triclinic TATB under different pressures. Physica B: Condensed Matter, 2019, 552, 151-158.	1.3	22
20	Effects of different dopant elements on structures, electronic properties, and sensitivity characteristics of nitromethane. Journal of Molecular Modeling, 2018, 24, 295.	0.8	4
21	Realizing Shallow Acceptor Levels in Delafossite CuAlO 2 () Surfaces by Chalcogen Doping. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1800381.	1.2	2
22	Vibrational assignments and thermodynamic properties of triclinic TATB. Physica B: Condensed Matter, 2018, 546, 1-9.	1.3	5
23	Influences of different surfaces on anisotropic impact sensitivity of hexahydro-1,3,5-trinitro-1,3,5-triazine. Vacuum, 2017, 139, 117-121.	1.6	4
24	Influences of pressure on methyl group, elasticity, sound velocity and sensitivity of solid nitromethane. European Physical Journal B, 2017, 90, 1.	0.6	14
25	First-principles calculations of structural, elastic, and electronic properties of trigonal ZnSnO3 under pressure. Materials Chemistry and Physics, 2016, 180, 75-81.	2.0	24