Yi Yu

List of Publications by Year
in descending order

18	560	687363 13	839539 18
papers	citations	h-index	g-index

18	18	18	447
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	How Stable and Powerful Can Metal cyclo-Pentazolate Salts Be? An Answer through Theoretical Crystal Design. Crystal Growth and Design, 2020, 20, 4794-4801.	3.0	6
2	Mechanism and Functionality of Pnictogen Dual Aromaticity in Pentazolate Crystals. ChemPhysChem, 2019, 20, 2525-2530.	2.1	14
3	A Study of the Shock Sensitivity of Energetic Single Crystals by Large-Scale Ab Initio Molecular Dynamics Simulations. Nanomaterials, 2019, 9, 1251.	4.1	15
4	Stabilization of the Dual-Aromatic cyclo-N₅^{â€“} Anion by Acidic Entrapment. Journal of Physical Chemistry Letters, 2019, 10, 2378-2385.	4.6	48
5	Revealing Solid Properties of High-energy-density Molecular Cocrystals from the Cooperation of Hydrogen Bonding and Molecular Polarizability. Scientific Reports, 2019, 9, 1257.	3.3	15
6	Formation of a disordered region at the grain boundary during migration with He atoms. Science China: Physics, Mechanics and Astronomy, 2017, 60, 1.	5.1	2
7	Structural, mechanical properties, and vibrational spectra of LLM-105 under high pressures from a first-principles study. Journal of Molecular Modeling, 2017, 23, 275.	1.8	21
8	From intermolecular interactions to structures and properties of a novel cocrystal explosive: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 26960-26969.	2.8	29
9	Phase Transition in Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) under Static Compression: An Application of the First-Principles Method Specialized for CHNO Solid Explosives. Journal of Physical Chemistry B, 2016, 120, 11510-11522.	2.6	51
10	Molecular Statics Simulation of Hydrogen Defect Interaction in Tungsten. Plasma Science and Technology, 2015, 17, 524-528.	1.5	4
11	Effect of hydrogen on grain boundary migration in tungsten. Science China: Physics, Mechanics and Astronomy, 2015, 58, 1-9.	5.1	11
12	Hydrogen diffusion in tungsten: A molecular dynamics study. Journal of Nuclear Materials, 2014, 455, 676-680.	2.7	21
13	Molecular dynamics simulation of hydrogen dissolution and diffusion in a tungsten grain boundary. Journal of Nuclear Materials, 2014, 455, 91-95.	2.7	31
14	Molecular dynamics simulation of helium cluster diffusion and bubble formation in bulk tungsten. Journal of Nuclear Materials, 2014, 455, 544-548.	2.7	58
15	Helium defects interactions and mechanism of helium bubble growth in tungsten: A molecular dynamics simulation. Journal of Nuclear Materials, 2014, 451, 356-360.	2.7	70
16	Helium diffusion in tungsten: A molecular dynamics study. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 84-86.	1.4	48
17	Mechanism of vacancy formation induced by hydrogen in tungsten. AIP Advances, 2013, 3, .	1.3	40
18	Analytical Wâ€“He and Hâ€“He interatomic potentials for a Wâ€“Hâ€“He system. Journal of Nuclear Materials, 2012, 426, 31-37.	2.7	76