Cai-Chao Ye

List of Publications by Year
in descending order

44 papers	1,087 citations	516710 16 h-index	414414 32 g-index
44 all docs	44 docs citations	44 times ranked	1287 citing authors

#	Article	IF	Citations
1	C₃Nâ€”A 2D Crystalline, Holeâ€Free, Tunableâ€Narrowâ€Bandgap Semiconductor with Ferromagnetic Properties. Advanced Materials, 2017, 29, 1605625.	21.0	350
2	Soft template-directed interlayer confinement synthesis of a Fe-Co dual single-atom catalyst for Zn-air batteries. Energy Storage Materials, 2022, 45, 805-813.	18.0	99
3	Rationalizing the interphase stability of Li|doped-Li₇La₃Zr₂O₁₂via automated reaction screening and machine learning. Journal of Materials Chemistry A, 2019, 7, 19961-19969.	10.3	59
4	Enhancing the magnetic relaxivity of MRI contrast agents via the localized superacid microenvironment of graphene quantum dots. Biomaterials, 2020, 250, 120056.	11.4	48
5	Quantum size effect of poly(o-phenylenediamine) quantum dots: From controllable fabrication to tunable photoluminescence properties. Synthetic Metals, 2014, 198, 142-149.	3.9	42
6	Initial decomposition reaction of di-tetrazine-tetroxide (DTTO) from quantum molecular dynamics: implications for a promising energetic material. Journal of Materials Chemistry A, 2015, 3, 1972-1978.	10.3	38
7	Adsorption and decomposition mechanism of hexogen (RDX) on Al(111) surface by periodic DFT calculations. Journal of Molecular Modeling, 2013, 19, 2451-2458.	1.8	37
8	Theoretical calculation based synthesis of a poly(p-phenylenediamine)â€“Fe₃O₄composite: a magnetically recyclable photocatalyst with high selectivity for acid dyes. RSC Advances, 2014, 4, 54810-54818.	3.6	30
9	Initial Decomposition of HMX Energetic Material from Quantum Molecular Dynamics and the Molecular Structure Transition of Î²-HMX to Î´-HMX. Journal of Physical Chemistry C, 2019, 123, 9231-9236.	3.1	28
10	Formation of noble-metal-free 2D/2D ZnmIn2Sm+3 (mÂ=Â1, 2, 3)/MXene Schottky heterojunction as an efficient photocatalyst for hydrogen evolution. Chemical Engineering Journal, 2021, 424, 130170.	12.7	28
11	Prediction of the crystal packing of diâ€tetrazineâ€tetroxide (DTTO) energetic material. Journal of Computational Chemistry, 2016, 37, 163-167.	3.3	24
12	ReaxFF study on combustion mechanism of ethanol/nitromethane. Fuel, 2021, 303, 121221.	6.4	24
13	Synthesis of Tostadasâ€Shaped Metalâ€Organic Frameworks for Remitting Capacity Fading of Liâ€Ion Batteries. Advanced Functional Materials, 2022, 32, .	14.9	23
14	Polarizing Graphene Quantum Dots toward Long-Acting Intracellular Reactive Oxygen Species Evaluation and Tumor Detection. ACS Applied Materials & Interfaces, 2020, 12, 10781-10790.	8.0	21
15	Adsorption and Decomposition Mechanism of 1,1â€Diaminoâ€2,2â€dinitroethylene on Al(111) Surface by Periodic DFT Calculations. Chinese Journal of Chemistry, 2012, 30, 2539-2548.	4.9	19
16	Reaction mechanism from quantum molecular dynamics for the initial thermal decomposition of 2,4,6-triamino-1,3,5-triazine-1,3,5-trioxide (MTO) and 2,4,6-trinitro-1,3,5-triazine-1,3,5-trioxide (MTO3N), promising green energetic materials. Journal of Materials Chemistry A, 2015, 3, 12044-12050.	10.3	18
17	Initial Decomposition Reactions of Bicyclo-HMX [BCHMX or cis-1,3,4,6-Tetranitrooctahydroimidazo-[4,5-d]imidazole] from Quantum Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 2290-2296.	3.1	17
18	Prediction of structures and properties of 2,4,6-triamino-1,3,5-triazine-1,3,5-trioxide (MTO) and 2,4,6-trinitro-1,3,5-triazine-1,3,5-trioxide (MTO3N) green energetic materials from DFT and ReaxFF molecular modeling. Journal of Materials Chemistry A, 2016, 4, 1264-1276.	10.3	17

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19	Ab initio thermodynamic optimization of Ni-rich Niâ€“Coâ€“Mn oxide cathode coatings. Journal of Power Sources, 2020, 450, 227693.	7.8	15
20	Crystal Morphology Prediction and Anisotropic Evolution of 1,1-Diamino-2,2-dinitroethylene (FOX-7) by Temperature Tuning. Scientific Reports, 2020, 10, 2317.	3.3	15
21	Prediction and Classification of Formation Energies of Binary Compounds by Machine Learning: An Approach without Crystal Structure Information. ACS Omega, 2021, 6, 14533-14541.	3.5	13
22	5-IP7 is a GPCR messenger mediating neural control of synaptotagmin-dependent insulin exocytosis and glucose homeostasis. Nature Metabolism, 2021, 3, 1400-1414.	11.9	13
23	Molecular dynamics simulation on reaction and kinetics isotope effect of nano-aluminum and water. International Journal of Hydrogen Energy, 2019, 44, 19474-19483.	7.1	12
24	Machine learning assisted discovering of new M2X3-type thermoelectric materials. Rare Metals, 2022, 41, 1543-1553.	7.1	12
25	Self-Assembled NbOPO₄ Nanosheet/Reduced Graphene Oxide Heterostructure for Capacitive Desalination. ACS Applied Nano Materials, 2021, 4, 12629-12639.	5.0	11
26	Electron-induced enhanced interfacial interaction of the CuO/BiOCl heterostructure for boosted CO2 photoreduction performance under simulated sunlight. Applied Surface Science, 2022, 583, 152463.	6.1	10
27	Adsorption and decomposition of HMX and CLâ€20 on Al(111) surface by DFT investigation. Surface and Interface Analysis, 2017, 49, 441-449.	1.8	9
28	Density functional theory studies on adsorption and decomposition mechanism of FOX-7 on Al13 clusters. Canadian Journal of Chemistry, 2013, 91, 1207-1212.	1.1	8
29	Layered Hexaphenylbenzene (HPB) derivatives with pseudo-2D structure for high-performance Li ion batteries. Energy Storage Materials, 2021, 42, 109-117.	18.0	8
30	Crystal Morphology of 3,4â€Bis(3â€nitrofurazanâ€4â€yl)furoxan in Methanol and Acetic Acid/Water Solutions by Spiral Growth Mechanism. Propellants, Explosives, Pyrotechnics, 2020, 45, 1125-1136.	1.6	7
31	Structural evolution of aluminum hydride nanoparticles in water using ReaxFF molecular dynamics method. Materials Today Communications, 2021, 26, 101804.	1.9	6
32	Theoretical study on dimers of 2,6-diamino-3,5-dinitropyridine and its N-oxide. Journal of Structural Chemistry, 2012, 53, 659-664.	1.0	5
33	Ordered Element Distributed C₃N Quantum Dots Manipulated Crystallization Kinetics for 2D CsPbI₃ Solar Cells with Ultraâ€High Performance. Small, 2022, 18, e2108090.	10.0	5
34	Theoretical Study on Thermodynamic Properties and Stabilities of n-Silanes. Phosphorus, Sulfur and Silicon and the Related Elements, 2011, 186, 1948-1961.	1.6	4
35	Investigation of a Highly Sensitive Surface-Enhanced Raman Scattering Substrate Formed by a Three-Dimensional/Two-Dimensional Graphene/Germanium Heterostructure. ACS Applied Materials & Interfaces, 2022, 14, 14764-14773.	8.0	3
36	Strain Energy Calculations of Caged Silanes. Phosphorus, Sulfur and Silicon and the Related Elements, 2012, 187, 997-1002.	1.6	2

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37	Density functional theory studies of methanol adsorption and decomposition mechanism on Al₁₃ clusters. Canadian Journal of Chemistry, 2014, 92, 293-298.	1.1	2
38	Natural Graphene Plasmonic <scp>Nanoâ€Resonators</scp> for Highly Active <scp>Surfaceâ€Enhanced</scp> Raman Scattering Platforms. Energy and Environmental Materials, 2023, 6, .	12.8	2
39	A DFT study of adsorption and decomposition of hexahydro-1,3,5-trinitro-1,3,5-triazine on Mg(0001) surface. Journal of Molecular Modeling, 2013, 19, 4459-4465.	1.8	1
40	Onset of catalytic activity of graphene nanosheets in reaction with energetic materials evaluated by ReaxFF molecular dynamics simulation. Surfaces and Interfaces, 2022, 31, 102024.	3.0	1
41	Theoretical Studies on the Role of Guest in Î±-CL-20/Guest Crystals. Molecules, 2022, 27, 3266.	3.8	1
42	Molecular dynamic insight into aluminum nanoparticles self-encapsulated by CNTs and their oxygen ignition. Materials Today Communications, 2021, 28, 102628.	1.9	0
43	DFT Study for Adsorption and Decomposition Mechanism of Trimethylene Oxide on Al(111) Surface. Bulletin of the Korean Chemical Society, 2014, 35, 2013-2018.	1.9	0
44	Ordered Element Distributed C₃N Quantum Dots Manipulated Crystallization Kinetics for 2D CsPbI₃ Solar Cells with Ultraâ€High Performance (Small 15/2022). Small, 2022, 18, .	10.0	0