Mingli Yang

List of Publications by Year
in descending order

130	2,189	218677	315739
papers	citations	26 h-index	38 g-index

133	133	133	2417
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Understanding zinc-doped hydroxyapatite structures using first-principles calculations and convolutional neural network algorithm. Journal of Materials Chemistry B, 2022, 10, 1281-1290.	5.8	7
2	Interlayer electron flow and field shielding in twisted trilayer graphene quantum dots. Nanoscale, 2022, 14, 1310-1317.	5.6	3
3	Combining crystal graphs and domain knowledge in machine learning to predict metal-organic frameworks performance in methane adsorption. Microporous and Mesoporous Materials, 2022, 331, 111666.	4.4	16
4	Gas Adsorption Capacity of Type-II Kerogen at a Varying Burial Depth. Energy & Fuels, 2022, 36, 7472-7482.	5.1	3
5	Enhanced interlayer coupling in twisted bilayer graphene quantum dots. Applied Surface Science, 2022, 600, 154148.	6.1	5
6	Molecular simulations on the continuous methane desorption in illite nanoslits. Fuel, 2022, 328, 125207.	6.4	2
7	Effect of Mn doping on the electron injection in CdSe/TiO₂ quantum dot sensitized solar cells. Physical Chemistry Chemical Physics, 2021, 23, 647-656.	2.8	8
8	Enhanced second-order Stark effect in twisted bilayer graphene quantum dots. Nano Research, 2021, 14, 3935.	10.4	4
9	Molecular modeling on the pressure-driven methane desorption in illite nanoslits. Journal of Molecular Modeling, 2021, 27, 83.	1.8	4
10	Fast estimation on the pressure of detonation products of cyclotetramethylene tetranitramine through molecular dynamics simulations. International Journal of Modern Physics B, 2021, 35, 2150106.	2.0	2
11	First-Principles Study of the Electronâ€“Hole Recombination Rate at the Interface of the CdSe Quantum Dot and TiO₂ Substrate. Journal of Physical Chemistry C, 2021, 125, 15785-15795.	3.1	9
12	Equation of state for the detonation products of energetic materials. Materials Express, 2021, 11, 1269-1287.	0.5	0
13	Machine learning on properties of multiscale multisource hydroxyapatite nanoparticles datasets with different morphologies and sizes. Npj Computational Materials, 2021, 7, .	8.7	19
14	Interlayer polarizability in twisted bilayer graphene quantum dots. Physical Review B, 2021, 104, .	3.2	5
15	Phase separation in the supercritical mixtures of N2, H2O and CO2 through a molecular dynamics study. Journal of Molecular Liquids, 2020, 315, 113811.	4.9	2
16	Accelerating Discovery of Metalâ€“Organic Frameworks for Methane Adsorption with Hierarchical Screening and Deep Learning. ACS Applied Materials & Interfaces, 2020, 12, 52797-52807.	8.0	31
17	A Ti-MOF Decorated With a Pt Nanoparticle Cocatalyst for Efficient Photocatalytic H2 Evolution: A Theoretical Study. Frontiers in Chemistry, 2020, 8, 660.	3.6	8
18	Effect of water occupancy on the excess adsorption of methane in montmorillonites. Journal of Natural Gas Science and Engineering, 2020, 80, 103393.	4.4	13

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19	Probing the surface activity of hydroxyapatite nanoparticles through their interaction with water molecules. AIP Advances, 2020, 10, 065217.	1.3	5
20	A modified model for estimating excess adsorption of methane in moist nanoporous silica. Chemical Physics, 2020, 533, 110740.	1.9	7
21	Interfacial interaction and its influence on the mechanical performances of hydroxyapatite through a polycrystalline model. Physica B: Condensed Matter, 2020, 594, 412338.	2.7	3
22	Computational characterization of the structural and mechanical properties of Al x CoCrFeNiTi1â^'x high entropy alloys. Materials Research Express, 2019, 6, 096519.	1.6	7
23	Radiative and non-radiative decay kinetics of (CdSe)N (N = 3 and 4) clusters. Journal of Chemical Physics, 2019, 151, 064306.	3.0	1
24	Dielectric and optical properties of porous graphenes with uniform pore structures. Journal of Molecular Modeling, 2019, 25, 266.	1.8	3
25	Effect of Ta addition on the structural, thermodynamic and mechanical properties of CoCrFeNi high entropy alloys. RSC Advances, 2019, 9, 16447-16454.	3.6	6
26	Computational characterization of the structural and mechanical properties of nanoporous titania. RSC Advances, 2019, 9, 15298-15306.	3.6	5
27	A reactive force field molecular dynamics study of molecular nitrogen and water mixtures under high temperature and high pressure. Journal of Molecular Modeling, 2019, 25, 120.	1.8	3
28	Effect of Hydroxyapatite Surface on BMP-2 Biological Properties by Docking and Molecular Simulation Approaches. Journal of Physical Chemistry B, 2019, 123, 3372-3382.	2.6	22
29	Unraveling the Structure-Dependent Radiative and Nonradiative Decays in (CdSe)₁₃ Clusters through First-Principles Calculations. Journal of Physical Chemistry C, 2019, 123, 30714-30722.	3.1	11
30	First-Principles-Based Force Field for 2,6-Diamino-3,5-dinitropyrazine-1-oxide (LLM-105). ACS Omega, 2019, 4, 21054-21062.	3.5	4
31	Radiative and non-radiative exciton recombination rate constants in ZnSe clusters. European Physical Journal B, 2019, 92, 1.	1.5	7
32	Nucleation of Biomimetic Hydroxyapatite Nanoparticles on the Surface of Type I Collagen: Molecular Dynamics Investigations. Journal of Physical Chemistry C, 2019, 123, 2533-2543.	3.1	22
33	Molecular Dynamics Exploration of Ordered-to-Disordered Surface Structures of Biomimetic Hydroxyapatite Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 6691-6703.	3.1	12
34	Probing the surface structure of hydroxyapatite through its interaction with hydroxyl: a first-principles study. RSC Advances, 2018, 8, 3716-3722.	3.6	25
35	Theoretical characterization on the size-dependent electron and hole trapping activity of chloride-passivated CdSe nanoclusters. Journal of Chemical Physics, 2018, 148, 134308.	3.0	7
36	Understanding the phase separation of N2/H2O and CO2/H2O binary systems through reactive force fields-based molecular dynamics simulations. Journal of Applied Physics, 2018, 124, .	2.5	6

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37	A comparative study of the dissolubility of pure and silicon substituted hydroxyapatite from density functional theory calculations. Journal of Molecular Modeling, 2018, 24, 168.	1.8	3
38	First-principles study on the hydroxyl migration from inner to surface in hydroxyapatite. Applied Surface Science, 2018, 452, 381-388.	6.1	10
39	Coupled-cluster method for open-shell heavy-element systems with spin-orbit coupling. Journal of Chemical Physics, 2017, 146, 134108.	3.0	14
40	Hydroxyl migration disorders the surface structure of hydroxyapatite nanoparticles. Applied Surface Science, 2017, 416, 901-910.	6.1	13
41	First-principles study on structural, electronic, vibrational and thermodynamic properties of Sr₁₀(PO₄)₆X₂(X = F, Cl, Br). RSC Advances, 2017, 7, 30310-30319.	3.6	6
42	Computer simulations on the mechanical behaviors of biphasic calcium phosphates. Journal of Molecular Modeling, 2017, 23, 156.	1.8	13
43	Confinement of hydrogen and hydroxyl radicals in water cages: a density functional theory study. RSC Advances, 2017, 7, 14537-14543.	3.6	5
44	A theoretical study of molecular structure, optical properties and bond activation of energetic compound FOX-7 under intense electric fields. Chemical Physics, 2017, 483-484, 122-131.	1.9	10
45	Effect of an external electric field on the C N cleavage reactions in nitromethane and triaminotrinitrobenzene. Computational and Theoretical Chemistry, 2017, 1117, 215-219.	2.5	11
46	Stokes shifts of small ZnSe clusters from first-principles calculations. Molecular Physics, 2017, 115, 3192-3198.	1.7	6
47	Shell effect on the electron and hole reorganization energy of core-shell IIâ€“VI nanoclusters. Chemical Physics, 2017, 494, 72-77.	1.9	5
48	Polarization response of clathrate hydrates capsulated with guest molecules. Journal of Chemical Physics, 2016, 144, 204308.	3.0	11
49	Spin-orbit coupling with approximate equation-of-motion coupled-cluster method for ionization potential and electron attachment. Journal of Chemical Physics, 2016, 145, 154110.	3.0	10
50	Coreâ€“shell interaction and its impact on the optical absorption of pure and doped core-shell CdSe/ZnSe nanoclusters. Journal of Chemical Physics, 2016, 144, 134307.	3.0	10
51	First-principles study of water desorption from montmorillonite surface. Journal of Molecular Modeling, 2016, 22, 105.	1.8	10
52	Surface Structure of Hydroxyapatite from Simulated Annealing Molecular Dynamics Simulations. Langmuir, 2016, 32, 4643-4652.	3.5	31
53	A theoretical study of the activation of nitromethane under applied electric fields. RSC Advances, 2016, 6, 24712-24718.	3.6	8
54	Electronic, vibrational and thermodynamic properties of Ca10(AsO4)6(OH)2: first principles study. EPJ Applied Physics, 2015, 72, 31201.	0.7	3

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55	A study of optical absorption of cysteine-capped CdSe nanoclusters using first-principles calculations. Physical Chemistry Chemical Physics, 2015, 17, 9222-9230.	2.8	29
56	Molecular dynamics simulations on the shear viscosity of Al2O3 nanofluids. Computers and Fluids, 2015, 117, 17-23.	2.5	40
57	Optical absorption of warped nanographenes tuned by five- and seven-membered carbon rings. Physical Chemistry Chemical Physics, 2015, 17, 17864-17871.	2.8	9
58	The mechanism of 2,4,6-trinitrotoluene detection with amino acid-capped quantum dots: a density functional theory study. RSC Advances, 2015, 5, 48406-48412.	3.6	12
59	Ab initio intermolecular potential energy surfaces of the Krâ€“CS2 and Xeâ€“CS2 complexes. Computational and Theoretical Chemistry, 2015, 1070, 88-93.	2.5	5
60	An interlayer expansion model for counterion-intercalated montmorillonite from first-principles calculations. Computational Materials Science, 2015, 96, 134-139.	3.0	20
61	A density functional theory study of the hydration of calcium ions confined in the interlayer space of montmorillonites. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450028.	1.8	11
62	Controllable synthesis of carbon coils and growth mechanism for twinning double-helix catalyzed by Ni nanoparticle. Composites Part B: Engineering, 2014, 61, 350-357.	12.0	20
63	Mechanistic Study of the Role of Primary Amines in Precursor Conversions to Semiconductor Nanocrystals at Low Temperature. Angewandte Chemie - International Edition, 2014, 53, 6898-6904.	13.8	24
64	Theoretical characterization of formamide on the inner surface of montmorillonite. Surface Science, 2014, 624, 37-43.	1.9	13
65	Theory Studies on Low-Lying States of Lead Chalcogenide Cations. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2014, 30, 431-438.	4.9	0
66	The structure and optical absorption of single source precursors for II-VI quantum dots. Chemical Physics Letters, 2013, 568-569, 125-129.	2.6	13
67	Micro-flowers changing to nano-bundle aggregates by translocation of the sugar moiety in Janus TA nucleosides. Chemical Communications, 2013, 49, 3742.	4.1	17
68	The Formation Mechanism of Binary Semiconductor Nanomaterials: Shared by Singleâ€Source and Dualâ€Source Precursor Approaches. Angewandte Chemie - International Edition, 2013, 52, 11034-11039.	13.8	34
69	Polarization response of methane encapsulated in water cages. Computational and Theoretical Chemistry, 2013, 1013, 52-56.	2.5	4
70	Structures and optical absorptions of PbSe clusters from ab initio calculations. Journal of Chemical Physics, 2013, 139, 094305.	3.0	16
71	Isomorphous substituted bimetallic oxide cluster as a novel strategy for single-atom catalysis. Computational and Theoretical Chemistry, 2013, 1021, 262-267.	2.5	3
72	Effect of interlayer counterions on the structures of dry montmorillonites with Si4+/Al3+ substitution. Computational Materials Science, 2013, 69, 95-99.	3.0	34

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73	First-principles study of ammonium ions and their hydration in montmorillonites. Journal of Molecular Modeling, 2013, 19, 1875-1881.	1.8	15
74	Effect of Tertiary and Secondary Phosphines on Lowâ€Temperature Formation of Quantum Dots. Angewandte Chemie - International Edition, 2013, 52, 4823-4828.	13.8	55
75	First-principles study of O2 activation on ligand-protected Au32 clusters. Physical Chemistry Chemical Physics, 2013, 15, 9742.	2.8	7
76	Competition between Eleyâ€“Rideal and Langmuirâ€“Hinshelwood Pathways of CO Oxidation on Cu_n and Cu_nO (n = 6, 7) Clusters. Journal of Physical Chemistry C, 2013, 117, 8767-8773.	3.1	31
77	In silico identification of EGFR-T790M inhibitors with novel scaffolds: start with extraction of common features. Drug Design, Development and Therapy, 2013, 7, 789.	4.3	15
78	Local and nonlocal contributions to molecular first-order hyperpolarizability: A Hirshfeld partitioning analysis. Journal of Chemical Physics, 2012, 136, 224304.	3.0	9
79	First-Principles Study of AuC₆₀ Clusters. Journal of Nanoscience and Nanotechnology, 2012, 12, 6571-6575.	0.9	2
80	Gas-Induced Formation of Cu Nanoparticle as Catalyst for High-Purity Straight and Helical Carbon Nanofibers. ACS Nano, 2012, 6, 8611-8619.	14.6	50
81	Comparative ab Initio Study of CO Adsorption on Scn and ScnO (n = 2â€“13) Clusters. Journal of Physical Chemistry A, 2012, 116, 93-97.	2.5	13
82	First-principles study of the adsorption of lysine on hydroxyapatite (100) surface. Applied Surface Science, 2012, 258, 4911-4916.	6.1	38
83	Stability competition between the layered and compact Cu16 clusters. European Physical Journal D, 2012, 66, 1.	1.3	3
84	Theoretical study of static (Hyper)polarizabilities of twisted intramolecular charge transfer chromophores. International Journal of Quantum Chemistry, 2012, 112, 1086-1096.	2.0	6
85	Comparative DFT study of N₂ and no adsorption on vanadium clusters V_n (n = 2â€“13). Journal of Computational Chemistry, 2012, 33, 1854-1861.	3.3	24
86	Icosahedral to double-icosahedral shape transition of copper clusters. Journal of Chemical Physics, 2012, 136, 104501.	3.0	32
87	Correlation between biological activity and binding energy in systems of integrin with cyclic RGD-containing binders: a QM/MM molecular dynamics study. Journal of Molecular Modeling, 2012, 18, 4917-4927.	1.8	9
88	Spinâ€“orbit coupling effect on Auâ€“C60 interaction: A density functional theory study. Chemical Physics, 2012, 395, 82-86.	1.9	11
89	Comparative Study of the Interaction of O₂ and C₂H₄ with Small Vanadium Clusters from Density Functional Theory. Journal of Physical Chemistry A, 2011, 115, 10259-10265.	2.5	7
90	Theoretical Investigation of Adsorption of Molecular Oxygen on Small Copper Clusters. Journal of Physical Chemistry A, 2011, 115, 8705-8712.	2.5	28

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91	First-principles investigation on the structural stability of methane and ethane clathrate hydrates. Computational and Theoretical Chemistry, 2011, 977, 209-212.	2.5	14
92	The effect of geometry on cluster polarizability: Studies of sodium, copper, and silicon clusters at shape-transition sizes. Journal of Chemical Physics, 2011, 134, 234505.	3.0	17
93	A quantitative analysis of intramolecular charge transfer contribution to polarizability responses in donor-Ï€-acceptor molecules. Chemical Physics Letters, 2011, 511, 12-15.	2.6	4
94	Physisorption of cisâ€•and transâ€decalin on Pt₄ clusters from density functional theory calculations. Physica Status Solidi (A) Applications and Materials Science, 2011, 208, 2380-2383.	1.8	1
95	First-principles study of electronic structures of hexa- and dodecanuclear silver clusters coordinated with organic ligands. Computational and Theoretical Chemistry, 2011, 965, 206-210.	2.5	4
96	First-principles absorption spectra of Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mi>n</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math>(<mml:math) Tj ETQq0 0 0 rgBT /Overlock	3.2	45
97	Competition between monomer and dimer fragmentation pathways of cationic Cu_Nclusters ofN= 2â€“20. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 205103.	1.5	16
98	Interplay between geometrical and electronic stability of neutral and anionic Cu13 clusters: a first-principles study. European Physical Journal D, 2010, 58, 125-129.	1.3	20
99	A G3(MP2B3) investigation on the structures and properties of silaprismanes. Computational and Theoretical Chemistry, 2010, 955, 123-129.	1.5	8
100	Ab initio study of structure and magnetism of bimetallic oxide clusters TiVOm, VMnOm, and MnCoOm, m=3,4. Computational and Theoretical Chemistry, 2010, 953, 55-60.	1.5	4
101	Preparation of high purity helical carbon nanofibers by the catalytic decomposition of acetylene and their growth mechanism. Carbon, 2010, 48, 4535-4541.	10.3	40
102	Identifying Tm@C82isomers with density functional theory calculations. Journal of Physics Condensed Matter, 2010, 22, 235301.	1.8	2
103	A first-principles study of methylcyclohexane adsorption on Pt₄clusters. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 185101.	1.5	4
104	Geometrical and electronic properties of AuC<inf>60</inf> complexes. , 2010, , .		0
105	A theoretical characterization of the interaction of cis- and trans-decalin with Pt<inf>4</inf> clusters. , 2010, , .		0
106	Effect of hydrogen bonds on polarizability of a water molecule in (H2O)N (N = 6, 10, 20) isomers. Physical Chemistry Chemical Physics, 2010, 12, 9239.	2.8	36
107	Ab initio study of the structure and magnetism of atomic oxygen adsorbed Scn (n = 2â€“14) clusters. Physical Chemistry Chemical Physics, 2009, 11, 5980.	2.8	18
108	Dipole polarizabilities of noble gas endohedral fullerenes. Chemical Physics Letters, 2008, 456, 223-226.	2.6	50

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109	Density functional theory study of cationic group VI transition metalâ€“benzene clusters. Computational and Theoretical Chemistry, 2008, 869, 37-40.	1.5	10
110	HPLC COUPLED WITH ION TRAP MS/MS FOR ANALYSIS OF TERTIARY BUTYLHYDROQUINONE IN EDIBLE OIL SAMPLES. Journal of Food Lipids, 2008, 15, 1-12.	1.0	14
111	First-principles study of static polarizability, first and second hyperpolarizabilities of small-sized ZnO clusters. Physical Chemistry Chemical Physics, 2008, 10, 6829.	2.8	28
112	Size- and Shape-Dependent Polarizabilities of Sandwich and Rice-Ball ConBzm Clusters from Density Functional Theory. Journal of Physical Chemistry A, 2008, 112, 8226-8230.	2.5	16
113	Density functional study of CO adsorption on Scnâ€ˆ(n=2â€“13) clusters. Journal of Chemical Physics, 2008, 128, 224315.	3.0	20
114	Optical absorption spectra of intermediate-size silver clusters from first principles. Physical Review B, 2008, 78, .	3.2	67
115	Site-Specific Analysis of Dielectric Properties of Finite Systems. Journal of Physical Chemistry C, 2007, 111, 17952-17960.	3.1	45
116	Structure and shape variations in intermediate-size copper clusters. Journal of Chemical Physics, 2006, 124, 024308.	3.0	100
117	First-principles absorption spectra ofSin(n=20â€“28)clusters: Time-dependent local-density approximation versus predictions from Mie theory. Physical Review B, 2006, 74, .	3.2	22
118	CHARGE DISTRIBUTION AND POLARISABILITIES OF WATER CLUSTERS. , 2006, , 657-679.		3
119	Dipole polarizabilities of medium-sized gold clusters. Physical Review A, 2006, 74, .	2.5	41
120	Relation between the Fukui function and the Coulomb hole. Journal of Chemical Sciences, 2005, 117, 411-418.	1.5	20
121	DFT study of polarizabilities and dipole moments of water clusters. International Journal of Quantum Chemistry, 2005, 101, 535-542.	2.0	70
122	First-principles investigations of the polarizability of small-sized and intermediate-sized copper clusters. Journal of Chemical Physics, 2005, 122, 184317.	3.0	32
123	Dipole polarizabilities of germanium clusters. Chemical Physics Letters, 2003, 367, 448-454.	2.6	39
124	Large Off-Diagonal Contribution to the Second-Order Optical Nonlinearities of Î›-Shaped Molecules. Journal of Physical Chemistry A, 2003, 107, 3942-3951.	2.5	105
125	Intramolecular charge transfer and first-order hyperpolarizability of planar and twisted sesquifulvalenes. Physical Chemistry Chemical Physics, 2002, 4, 5566-5571.	2.8	28
126	An MP2 study of linear polarizabilities and second-order hyperpolarizabilities for centrosymmetric squaraines. Chemical Physics Letters, 2002, 354, 316-323.	2.6	22

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127	A theoretical study of second hyperpolarizabilities for donorâ€“acceptorâ€“donor molecules. Physical Chemistry Chemical Physics, 2001, 3, 167-171.	2.8	20
128	Molecular design for squaraines with large positive or negative third-order optical nonlinearity. Physical Chemistry Chemical Physics, 2001, 3, 4213-4217.	2.8	28
129	Structureâ€“property correlation in static electronic second-order hyperpolarizabilities of centrosymmetric squaraines. Chemical Physics, 2001, 274, 121-130.	1.9	18
130	Mechanism of the interaction of color reagent 1, 3-N, Nâ€™-bis-4-(4â€™-nitro benzenediazo) phenyl squaraine with oxoacid anions. Science in China Series B: Chemistry, 1999, 42, 70-76.	0.8	0