Wencai Lu

List of Publications by Year
in descending order

60	629	623574 14	677027 22
papers	citations	h-index	g-index

60	60	60	739
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Study on superconducting Liâ€“Seâ€“H hydrides. Physical Chemistry Chemical Physics, 2022, 24, 8415-8421.	1.3	0
2	Energy decomposition analysis of cationic carbene analogues with group 13 and 16 elements as a central atom: a comparative study. Physical Chemistry Chemical Physics, 2022, 24, 8970-8978.	1.3	1
3	Integration of resonant band with asymmetry in ferroelectric tunnel junctions. Npj Computational Materials, 2022, 8, .	3.5	6
4	The Gutzwiller conjugate gradient minimization method for correlated electron systems. Journal of Physics Condensed Matter, 2022, 34, 243001.	0.7	4
5	Localized electronic and vibrational states in amorphous diamond. Physical Chemistry Chemical Physics, 2021, 23, 4835-4840.	1.3	2
6	Theoretical study on the Y-Ba-H hydrides at high pressure. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 390, 127109.	0.9	7
7	Superconductivity in alkaline earth metal doped boron hydrides. Physica B: Condensed Matter, 2021, 611, 412795.	1.3	6
8	Ultra-coarse-graining modeling of liquid water. Journal of Chemical Physics, 2021, 154, 224506.	1.2	3
9	Enhanced resistance switching in ultrathin Ag/SrTiO3/(La,Sr)MnO3 memristors and their long-term plasticity for neuromorphic computing. Applied Physics Letters, 2021, 119, .	1.5	11
10	Tracking Electron Dynamics of Single Molecules in Scanning Tunneling Microscopy Junctions with Laser Pulses. Journal of Physical Chemistry Letters, 2021, 12, 6398-6404.	2.1	3
11	3D Ordered Porous Hybrid of ZnSe/Nâ€doped Carbon with Anomalously High Na⁺ Mobility and Ultrathin Solid Electrolyte Interphase for Sodiumâ€ion Batteries. Advanced Functional Materials, 2021, 31, 2106194.	7.8	66
12	Superconductivity of K-Y-H hydrides under high pressure. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 420, 127750.	0.9	2
13	Pressure-induced superconductivity in the hydrogen-rich pseudobinary CaBâ‚‚Hn compounds. Physical Review B, 2021, 104, .	1.1	5
14	3D Ordered Porous Hybrid of ZnSe/Nâ€doped Carbon with Anomalously High Na⁺ Mobility and Ultrathin Solid Electrolyte Interphase for Sodiumâ€ion Batteries (Adv. Funct. Mater.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	7.8	2
15	Lithium Diffusion in Silicon Encapsulated with Graphene. Nanomaterials, 2021, 11, 3397.	1.9	3
16	Defect Interaction and Deformation in Graphene. Journal of Physical Chemistry C, 2020, 124, 2370-2378.	1.5	6
17	Stability and superconductivity of TiPHn (n = 1â‹’8) under high pressure. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126189.	0.9	11
18	A benchmark of Gutzwiller conjugate gradient minimization method in ground state energy calculations of dimers. Computational and Theoretical Chemistry, 2020, 1185, 112877.	1.1	4

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19	A three-point coarse-grained model of five-water cluster with permanent dipoles and quadrupoles. Physical Chemistry Chemical Physics, 2020, 22, 26289-26298.	1.3	2
20	Spin-Filtering Ferroelectric Tunnel Junctions as Multiferroic Synapses for Neuromorphic Computing. ACS Applied Materials & Interfaces, 2020, 12, 56300-56309.	4.0	37
21	Characterization of three phases of liquid carbon by tight-binding molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 14630-14636.	1.3	4
22	Atomic-level reconstruction of biomolecules by a rigid-fragment- and local-frame-based (RF-LF) strategy. Journal of Molecular Modeling, 2020, 26, 31.	0.8	3
23	Theoretical Study on Feâ€“Seâ€“H Hydrides under High Pressure. Journal of Physical Chemistry C, 2019, 123, 28008-28014.	1.5	5
24	Theoretical study on nanostructural modifications of the Si(111) surface. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950005.	1.8	0
25	Theoretical investigation of real-time charge dynamics in open systems coupled to bulk materials. Journal of Chemical Physics, 2019, 150, 174119.	1.2	4
26	Benchmark of correlation matrix renormalization method in molecule calculations. Journal of Physics Condensed Matter, 2019, 31, 195902.	0.7	2
27	Novel superconducting structures of BH₂ under high pressure. Physical Chemistry Chemical Physics, 2019, 21, 5466-5473.	1.3	16
28	Tunable Photoresponse by Gate Modulation in Bilayer Graphene Nanoribbon Devices. Journal of Physical Chemistry Letters, 2019, 10, 7719-7724.	2.1	13
29	Theoretical study on UH4, UH8 and UH10 at high pressure. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 774-780.	0.9	4
30	Ultrafast dynamics of solvated electrons at anatase TiO₂/H₂O interface. Journal of Physics Condensed Matter, 2019, 31, 114004.	0.7	5
31	Structures and Superconducting Properties of Ultraâ€Hydrogenâ€Rich Selenium Hydride H6Se. Physica Status Solidi (B): Basic Research, 2018, 255, 1800224.	0.7	3
32	Structure and Reactivity of Anatase TiO₂(001)-(1 Ã— 4) Surface. Journal of Physical Chemistry C, 2018, 122, 14528-14536.	1.5	16
33	Hybrid siliconâ€“carbon nanostructures for broadband optical absorption. RSC Advances, 2017, 7, 8070-8076.	1.7	5
34	High-pressure structures of yttrium hydrides. Journal of Physics Condensed Matter, 2017, 29, 325401.	0.7	17
35	Stability and superconducting properties of GaH 5 at high pressure. Physica B: Condensed Matter, 2017, 525, 36-40.	1.3	4
36	Theoretical Prediction of Si₂â€“Si₃₃ Absorption Spectra. Journal of Physical Chemistry A, 2017, 121, 6388-6397.	1.1	10

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37	Theoretical search for possible Au-Si crystal structures using a genetic algorithm. Physical Review B, 2017, 95, .	1.1	9
38	Structural and electronic characteristics of intercalated monopotassiumâ€“rubrene: Simulation on a commodity computing cluster. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650035.	1.8	1
39	Studies on optical properties of Si220 nanoclusters via time-dependent density functional theory calculations. Chemical Research in Chinese Universities, 2016, 32, 1028-1033.	1.3	1
40	Lattice distortion and electron charge redistribution induced by defects in graphene. Carbon, 2016, 110, 330-335.	5.4	28
41	Tight-binding calculation studies of vacancy and adatom defects in graphene. Journal of Physics Condensed Matter, 2016, 28, 115001.	0.7	17
42	Three-center tight-binding potential model for C and Si. Physical Review B, 2015, 92, .	1.1	17
43	Theoretical study on the structures and optical absorption of Si₁₇₂nanoclusters. Nanoscale, 2015, 7, 14444-14451.	2.8	15
44	Si₇₈ double cage structure and special optical properties. Physical Chemistry Chemical Physics, 2015, 17, 27734-27741.	1.3	9
45	Geometric and electronic structures of potassium-adsorbed rubrene complexes. Journal of Chemical Physics, 2015, 142, 244702.	1.2	3
46	Structures and stability of metal-doped GenM (n = 9, 10) clusters. AIP Advances, 2015, 5, .	0.6	14
47	Application of Koopmansâ€™ theorem for density functional theory to full valence-band photoemission spectroscopy modeling. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 149, 434-440.	2.0	10
48	Theoretical studies on complexes of calcium ion with amino acids. Chemical Research in Chinese Universities, 2014, 30, 125-129.	1.3	4
49	Comparison of Sn n (n=2â€“15) neutral and ionic structures. Chemical Research in Chinese Universities, 2013, 29, 579-583.	1.3	8
50	Growth morphology and thermal stability of metal islands on graphene. Physical Review B, 2012, 86, .	1.1	38
51	Double icosahedronâ€based motif of Ni_n (n = 20â”30). International Journal of Quantum Chemistry, 2012, 112, 1717-1724.	1.0	17
52	Geometries and stabilities of Ag n v (vÂ=ÂÂ±1, 0; nÂ=Â21â€“29) clusters. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	9
53	Fe-Fe adatom interaction and growth morphology on graphene. Physical Review B, 2011, 84, .	1.1	23
54	Appearance of bulk-like motifs in Si, Ge, and Al clusters. Physical Chemistry Chemical Physics, 2010, 12, 8551.	1.3	24

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55	Stabilities and fragmentation energies of Si_nclusters (n= 2â€“33). Journal of Physics Condensed Matter, 2009, 21, 455501.	0.7	40
56	Tight-binding Hamiltonian from first-principles calculations. Scientific Modeling and Simulation SMNS, 2008, 15, 81-95.	0.8	9
57	Comparison of the Growth Patterns of Si_n and Ge_n Clusters (n = 25â˜33). Journal of Physical Chemistry A, 2008, 112, 5815-5823.	1.1	28
58	Theoretical study on AlnO2 (n = 1â€“10) clusters and O2 adsorption on the Al(111) surface. International Journal of Quantum Chemistry, 2007, 107, 1915-1924.	1.0	9
59	Theoretical studies on the structures and isomerization of the LiSiF3 system. Science in China Series B: Chemistry, 1999, 42, 419-424.	0.8	3
60	Stable structures and superconducting properties of Ca â€“ La â€“ H compounds under pressure. Journal of Physics Condensed Matter, 0, , .	0.7	1