Zhi Zeng

List of Publications by Year
in descending order

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83	2,171	279798	233421
papers	citations	23 h-index	45 g-index

83	83	83	3234
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Site and length dependent quantum interference and resonance in the electron transport of armchair carbon nanotube molecular junctions. Physical Chemistry Chemical Physics, 2022, 24, 8032-8040.	2.8	7
2	Giant Tunneling Electroresistance Induced by Interfacial Doping in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Pt</mml:mi><mml:mo>/</mml:mo><mml:mrow><mml:mi>Ba</mml:mi></mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mo>/</mml:mo> Ferroelectric Tunnel Junctions. Physical Review Applied, 2022, 17, .	4.6	11
3	Nonequilibrium electron and lattice dynamics of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sb</mml:mi><mml:mn>2</mml:mn></mml:msub> under pressure. Physical Review B, 2022, 105, .	3.2	3
4	Configuration stability and electronic properties of diamane with boron and nitrogen dopants. Physical Review B, 2022, 105, .	3.2	4
5	One-electron reduction induced spin transition in Fe(<scp>ii</scp>) spin crossover molecules and the effect of the ligand. Journal of Materials Chemistry C, 2021, 9, 4808-4814.	5.5	1
6	Two-dimensional centrosymmetrical antiferromagnets for spin photogalvanic devices. Npj Quantum Information, 2021, 7, .	6.7	18
7	Giant tunnel electroresistance in ferroelectric tunnel junctions with metal contacts to two-dimensional ferroelectric materials. Physical Review B, 2021, 103, .	3.2	26
8	Possibility of Doping <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Cu</mml:mi><mml:mi>Ga</mml:mi><mml:mi>Se</mml:mi></mml:mrow> n -Type by Hydrogen. Physical Review Applied, 2021, 15, .	4.6	2
9	Polymerization of Nitrogen in Nitrogenâ€“Fluorine Compounds under Pressure. Journal of Physical Chemistry Letters, 2021, 12, 5731-5737.	4.6	11
10	Entropic broadening of the spin-crossover pressure in ferropericlase. Physical Review B, 2021, 103, .	3.2	4
11	Prediction of the two-dimensional Janus ferrovalley material LaBrI. Physical Review B, 2021, 104, .	3.2	49
12	Structural, electronic and magnetic properties of TlFeSe2 under high pressure. Journal of Physics Condensed Matter, 2021, 33, 415702.	1.8	0
13	Domain-wall induced giant tunneling electroresistance effect in two-dimensional Graphene/In2Se3 ferroelectric tunnel junctions. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 133, 114783.	2.7	7
14	Identifying the Intermediate Free-Carrier Dynamics Across the Charge Separation in Monolayer MoS₂/ReSe₂ Heterostructures. ACS Nano, 2021, 15, 16760-16768.	14.6	17
15	Hydrostatic pressure effect of photocarrier dynamics in GaAs probed by time-resolved terahertz spectroscopy. , 2021, , .		0
16	Factors affecting the electronâ€“phonon coupling in FeSe under pressure. Physical Chemistry Chemical Physics, 2021, 23, 25107-25113.	2.8	3
17	Pressure effects on the lattice vibrations and ultrafast photocarrier dynamics in 2Hâ€“TaS2. Applied Physics Letters, 2020, 117, .	3.3	13
18	Pure spin current generation via photogalvanic effect with spatial inversion symmetry. Physical Review B, 2020, 102, .	3.2	43

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19	A review of surface damage/microstructures and their effects on hydrogen/helium retention in tungsten. Tungsten, 2020, 2, 34-71.	4.8	32
20	Giant tunneling electroresistance in two-dimensional ferroelectric tunnel junctions with out-of-plane ferroelectric polarization. Physical Review B, 2020, 101, .	3.2	52
21	Bias induced spin state transition mediated by electron excitations. Journal of Chemical Physics, 2020, 152, 134301.	3.0	3
22	Ferroelectric control of electron half-metallicity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>A</mml:mi></mml:math> -type antiferromagnets and its application to nonvolatile memory devices. Physical Review B, 2020, 102, .	3.2	23
23	Realizing giant tunneling electroresistance in two-dimensional graphene/BiP ferroelectric tunnel junction. Nanoscale, 2019, 11, 16837-16843.	5.6	35
24	Highâ€pressure Raman spectroscopy of CeOCl: Observation of the isostructural phase transition. Journal of Raman Spectroscopy, 2019, 50, 1962-1968.	2.5	5
25	Superconductivity of boron-doped graphane under high pressure. RSC Advances, 2019, 9, 7680-7686.	3.6	4
26	High-Pressure Synthesis of CeOCl Crystals and Investigation of Their Photoluminescence and Compressibility Properties. Crystal Growth and Design, 2018, 18, 1843-1847.	3.0	5
27	The polymerization of nitrogen in Li2N2 at high pressures. Scientific Reports, 2018, 8, 13144.	3.3	4
28	Pressure-induced structural, magnetic and transport transitions in Sr2FeO3from first-principles. AIP Advances, 2017, 7, 055703.	1.3	0
29	Bias induced spin transitions of spin crossover molecules: the role of charging effect. Physical Chemistry Chemical Physics, 2017, 19, 7652-7658.	2.8	6
30	The role of Sb in solar cell material Cu₂ZnSnS₄. Journal of Materials Chemistry A, 2017, 5, 6606-6612.	10.3	36
31	Adsorption of carbon dots onto Al2O3 in aqueous: Experimental and theoretical studies. Environmental Pollution, 2017, 227, 31-38.	7.5	20
32	An investigation of Na-related defects in Cu₂ZnSnSe₄. Physical Chemistry Chemical Physics, 2017, 19, 17799-17804.	2.8	21
33	Thermal spin current in zigzag silicene nanoribbons with sp2â€“sp3 edges. RSC Advances, 2017, 7, 28124-28129.	3.6	9
34	Defect physics in intermediate-band materials: Insights from an optimized hybrid functional. Physical Review B, 2017, 96, .	3.2	13
35	Schottky defects induced effects on the behaviors of high velocity shock compression of MgO. RSC Advances, 2017, 7, 45304-45310.	3.6	1
36	First-principles study on the electronic, optical and thermodynamic properties of ABO₃ (AÂ= La,Sr, B = Fe,Co) perovskites. RSC Advances, 2017, 7, 38798-38804.	3.6	51

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37	Robust and Pristine Topological Dirac Semimetal Phase in Pressured Two-Dimensional Black Phosphorus. Journal of Physical Chemistry C, 2017, 121, 20931-20936.	3.1	18
38	Realizing bias-induced spin transition with high-spin Mn^{II} complexes at room temperature. Journal of Materials Chemistry C, 2017, 5, 11598-11604.	5.5	1
39	Investigations of the mechanical properties of the Zr₈Ti₈ random alloy. International Journal of Modern Physics C, 2016, 27, 1650076.	1.7	2
40	Spin density waves predicted in zigzag puckered phosphorene, arsenene and antimonene nanoribbons. AIP Advances, 2016, 6, .	1.3	20
41	Origin of low thermal conductivity in SnSe. Physical Review B, 2016, 94, .	3.2	287
42	Hydrostatic pressure induced three-dimensional Dirac semimetal in black phosphorus. Physical Review B, 2016, 93, .	3.2	49
43	Î±-K2AgF4: Ferromagnetism induced by the weak superexchange of different eg orbitals from the nearest neighbor Ag ions. AIP Advances, 2016, 6, .	1.3	3
44	Hydrogen influence on generalized stacking fault energies of Zr {0001} basal plane: a first-principles study. RSC Advances, 2016, 6, 54371-54376.	3.6	4
45	Structural and electronic properties of solid naphthalene under pressure: density functional calculations. European Physical Journal B, 2016, 89, 1.	1.5	5
46	Chemical substitution assisted ion sensing with organic molecules: a case study of naphthalene. RSC Advances, 2016, 6, 6191-6195.	3.6	1
47	Theoretical study on structural and electronic properties of solid anthracene under high pressure by density functional theory. Molecular Physics, 2016, 114, 283-289.	1.7	7
48	IM3D: A parallel Monte Carlo code for efficient simulations of primary radiation displacements and damage in 3D geometry. Scientific Reports, 2015, 5, 18130.	3.3	43
49	Enhanced thermoelectric performance of Î²-Zn4Sb3 based nanocomposites through combined effects of density of states resonance and carrier energy filtering. Scientific Reports, 2015, 5, 17803.	3.3	58
50	From 1D chain to 3D network: A theoretical study on TiO2 low dimensional structures. Journal of Chemical Physics, 2015, 142, 224305.	3.0	1
51	Roles of Mass, Structure, and Bond Strength in the Phonon Properties and Lattice Anharmonicity of Single-Layer Mo and W Dichalcogenides. Journal of Physical Chemistry C, 2015, 119, 18779-18789.	3.1	67
52	Room temperature memory device using single-molecule magnets. RSC Advances, 2015, 5, 54667-54671.	3.6	15
53	Absence of phase transformation of dense anthracene from Raman scattering. High Pressure Research, 2015, 35, 379-387.	1.2	0
54	Phonon properties, thermal expansion, and thermomechanics of silicene and germanene. Physical Review B, 2015, 91, .	3.2	96

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55	First-principles calculations on spin-polarized transport properties of Mn4O4 cluster. Rare Metals, 2015, 34, 45-50.	7.1	0
56	Rare case of magnetic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi mathvariant="normal">Ag</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:mat Double perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Cs</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math><mml:math xmlns:	3.2	7
57	Curvature and ionization-induced reversible hydrogen storage in metalized hexagonal B36. Journal of Chemical Physics, 2014, 141, 194306.	3.0	47
58	Quantum-size effect on the electronic and optical properties of hybrid TiO2/Au clusters. Journal of Chemical Physics, 2014, 141, 054301.	3.0	1
59	Carbon Nanotubeâ€Encapsulated Noble Metal Nanoparticle Hybrid as a Cathode Material for Liâ€Oxygen Batteries. Advanced Functional Materials, 2014, 24, 6516-6523.	14.9	157
60	Dimensionality-induced insulator-metal crossover in layered nickelates Lan+1NinO2n+2 (n = 2, 3, and â^ž). AIP Advances, 2014, 4, .	1.3	15
61	Correlation between structure, phonon spectra, thermal expansion, and thermomechanics of single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	3.2	138
62	Ferromagnetic sandwich-like wires constructed with transition metals and anthracene. Applied Physics Letters, 2013, 103, 032404.	3.3	4
63	Lattice dynamics and disorder-induced contraction in functionalized graphene. Journal of Applied Physics, 2013, 113, .	2.5	49
64	Understanding the stability and dynamical process of hydrogen trimers on graphene. Journal of Applied Physics, 2013, 113, 173707.	2.5	5
65	Spin-flip effect on transport properties of a Mn3 molecule. Journal of Applied Physics, 2012, 111, 07B303.	2.5	3
66	Tuning the adatom-surface and interadatom interactions in hydrogenated graphene by charge doping. Physical Review B, 2012, 86, .	3.2	20
67	Patterning graphene nanostripes in substrate-supported functionalized graphene: A promising route to integrated, robust, and superior transistors. Frontiers of Physics, 2012, 7, 324-327.	5.0	13
68	Li-doped B2C graphene as potential hydrogen storage medium. Applied Physics Letters, 2011, 98, .	3.3	53
69	Ab initiostudy of the giant ferroelectric distortion and pressure-induced spin-state transition in BiCoO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2011, 83, .	3.2	30
70	Magnetic frustration in Î±-NaMnO2 and CuMnO2. Journal of Applied Physics, 2011, 109, .	2.5	12
71	Spin states of Co ions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>La</mml:mtext></mml:mrow><mml:mrow><mml:mn>3 first principles. Physical Review B, 2010, 82, .	3.2	1.5</mml
72	Ab Initio Simulations of the Kinetic Properties of the Hydrogen Monomer on Graphene. Journal of Physical Chemistry C, 2010, 114, 22636-22643.	3.1	46

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73	FIRST-PRINCIPLES STUDY OF THE STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF MgSiO3 AT HIGH PRESSURE. International Journal of Modern Physics C, 2009, 20, 1093-1101.	1.7	5
74	Oxygen vacancy configuration of Î´â€Bi₂O₃: an ab initio study. Physica Status Solidi (B): Basic Research, 2009, 246, 97-101.	1.5	19
75	First-principles study on the enhancement of lithium storage capacity in boron doped graphene. Applied Physics Letters, 2009, 95, .	3.3	116
76	The doping effects in Î´â€Bi₂O₃ oxide ionic conductor. Physica Status Solidi (B): Basic Research, 2008, 245, 2737-2742.	1.5	19
77	Density-functional investigation of metal-silicon cage clusters<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>M</mml:mi><mml:msub><mml:mi		