Zhigang Wu

List of Publications by Year
in descending order

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55 papers	4,900 citations	218592 26 h-index	161767 54 g-index
58 all docs	58 docs citations	58 times ranked	5878 citing authors

#	Article	IF	Citations
1	More accurate generalized gradient approximation for solids. Physical Review B, 2006, 73, .	1.1	1,785
2	Origin of morphotropic phase boundaries in ferroelectrics. Nature, 2008, 451, 545-548.	13.7	759
3	Pressure-Induced Anomalous Phase Transitions and Colossal Enhancement of Piezoelectricity inPbTiO3. Physical Review Letters, 2005, 95, 037601.	2.9	284
4	Hard superconducting nitrides. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 3198-3201.	3.3	256
5	Trends in elasticity and electronic structure of transition-metal nitrides and carbides from first principles. Physical Review B, 2005, 71, .	1.1	186
6	Bandgap Opening by Patterning Graphene. Scientific Reports, 2013, 3, 2289.	1.6	176
7	Comparing the weighted density approximation with the LDA and GGA for ground-state properties of ferroelectric perovskites. Physical Review B, 2004, 70, .	1.1	139
8	Origin of the Variation of Exciton Binding Energy in Semiconductors. Physical Review Letters, 2013, 110, 016402.	2.9	132
9	Charge Separation via Strain in Silicon Nanowires. Nano Letters, 2009, 9, 2418-2422.	4.5	131
10	Energy gaps in graphene nanomeshes. Physical Review B, 2012, 85, .	1.1	72
11	Quantum Confinement and Electronic Properties of Tapered Silicon Nanowires. Physical Review Letters, 2008, 100, 246804.	2.9	71
12	First-principles calculations of piezoelectricity and polarization rotation inPb(Zr0.5Ti0.5)O3. Physical Review B, 2003, 68, .	1.1	70
13	Role of the plasmon-pole model in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>approximation. Physical Review B, 2013, 88, .	1.1	65
14	Quantum Monte Carlo Simulation of Nanoscale MgH2 Cluster Thermodynamics. Journal of the American Chemical Society, 2009, 131, 13918-13919.	6.6	57
15	Improving the optical absorption of BiFeO3 for photovoltaic applications via uniaxial compression or biaxial tension. Applied Physics Letters, 2013, 102, .	1.5	54
16	Ab initiolinear response and frozen phonons for the relaxorPbMg1â^•3Nb2â^•3O3. Physical Review B, 2005, 71, .	1.1	44
17	Quantum Monte Carlo computations of phase stability, equations of state, and elasticity of high-pressure silica. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9519-9524.	3.3	43
18	Atomistic Model Potential for PbTiO3and PMN by Fitting First Principles Results. Ferroelectrics, 2004, 301, 55-59.	0.3	42

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19	Intrinsic magnetism and spontaneous band gap opening in bilayer silicene and germanene. Physical Chemistry Chemical Physics, 2017, 19, 2148-2152.	1.3	39
20	Charge separation in nanoscale photovoltaic materials: recent insights from first-principles electronic structure theory. Journal of Materials Chemistry, 2010, 20, 1053-1061.	6.7	38
21	First-principles investigations of ferroelectricity and piezoelectricity in BaTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>/PbTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math> superlattices. Physical Review B, 2012, 85, .	1.1	35
22	Electronic structure of calcium hexaboride within the weighted density approximation. Physical Review B, 2004, 69, .	1.1	31
23	Dangling Bond Defects: The Critical Roadblock to Efficient Photoconversion in Hybrid Quantum Dot Solar Cells. Journal of Physical Chemistry C, 2014, 118, 46-53.	1.5	31
24	Electronic stiffness of a superconducting niobium nitride single crystal under pressure. Physical Review B, 2005, 72, .	1.1	29
25	Unified picture of the oxygen isotope effect in cuprate superconductors. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 3732-3735.	3.3	27
26	Reply to â€œComment on â€˜More accurate generalized gradient approximation for solidsâ€™â€• Physical Review B, 2008, 78, .	1.1	27
27	Weighted-density-approximation description of rare-earth trihydrides. Physical Review B, 2004, 69, .	1.1	25
28	Advances in First-Principles Studies of Transducer Materials. Ferroelectrics, 2006, 333, 69-78.	0.3	22
29	Dirac point movement and topological phase transition in patterned graphene. Nanoscale, 2015, 7, 3645-3650.	2.8	18
30	Reduction of heat capacity and phonon group velocity in silicon nanowires. Journal of Applied Physics, 2015, 117, .	1.1	18
31	Phonon-mediated superconducting transitions in layered cuprate superconductors. Physical Review B, 2007, 75, .	1.1	17
32	Pressure effect on structural and vibrational properties of Sm-substituted BiFeO3. Journal of Applied Physics, 2013, 114, 154110.	1.1	15
33	Geometrically induced transitions between semimetal and semiconductor in graphene. Physical Review B, 2014, 90, .	1.1	15
34	Charge-transfer electrostatic model of compositional order in perovskite alloys. Physical Review B, 2001, 63, .	1.1	14
35	Quantum Monte Carlo calculations of the energy-level alignment at hybrid interfaces: Role of many-body effects. Physical Review B, 2009, 79, .	1.1	12
36	Tailoring the optical gap of silicon quantum dots without changing their size. Physical Chemistry Chemical Physics, 2014, 16, 19275-19281.	1.3	12

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37	Vibrational dependence of electric field gradients in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Pb</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.1	11
38	mathvariant="normal">O</mml:mi><mml:mn>3</mml:. Physical Review B, 2007, 76, . Oxygen isotope effect inBi2Sr2Canâ^'1CunO2n+4+Î´(n=1,2,3)single crystals. Physical Review B, 2007, 76, .	1.1	10
39	Optimal Size Regime for Oxidation-Resistant Silicon Quantum Dots. ACS Nano, 2012, 6, 9690-9699.	7.3	10
40	Structural impact on the eigenenergy renormalization for carbon and silicon allotropes and boron nitride polymorphs. Physical Review B, 2018, 97, .	1.1	9
41	Prediction of Ultra-High Aspect Ratio Nanowires from Self-Assembly. Nano Letters, 2008, 8, 2697-2705.	4.5	8
42	Quasiparticle energies and excitonic effects in dense solid hydrogen near metallization. Physical Review B, 2014, 90, .	1.1	8
43	First principles analysis of the initial oxidation of Si(001) and Si(111) surfaces terminated with H and CH3. Journal of Chemical Physics, 2012, 136, 064507.	1.2	7
44	Double superexchange in quantum dot mesomaterials. Energy and Environmental Science, 2014, 7, 1023.	15.6	6
45	Hybrid functionals with fixed mixing parameter perform no better than PBE for fundamental band gaps of nanoscale materials. Physical Review B, 2016, 94, .	1.1	6
46	Pressure effect on structural and vibrational properties of Y-substituted BiFeO3. Journal of Physics Condensed Matter, 2013, 25, 365401.	0.7	5
47	Comment on â€œ<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>d</mml:mi><mml:mo>+</mml:mo><mml:mi>i</mml:mi><mml:msup><mml:mrow><mml:mi>d< Superconductivity in Bilayer Siliceneâ€• Physical Review Letters, 2015, 114, 099701.	2.9	5
48	Predicting copper gallium diselenide and band structure engineering through order-disordered transition. Physical Review Materials, 2019, 3, .	0.9	5
49	Tunable many-body interactions in semiconducting graphene: Giant excitonic effect and strong optical absorption. Physical Review B, 2015, 92, .	1.1	3
50	Is sodium a superconductor under high pressure?. Journal of Chemical Physics, 2017, 146, 014705.	1.2	3
51	Ferroelectricity and Elasticity of Rhombohedral BiFeO₃ Under Uniaxial Stress. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1700431.	1.2	3
52	Formation of spherical ice-shells inside carbon fullerenes. Physical Chemistry Chemical Physics, 2017, 19, 30726-30733.	1.3	2
53	Charge separation at nanoscale interfaces: Energy-level alignment including two-quasiparticle interactions. Journal of Chemical Physics, 2014, 141, 154701.	1.2	0
54	Intermediate bands in type-II silicon clathrate with Cu and Ag guest atoms. Physical Review B, 2017, 95, .	1.1	0

#	Article	IF	Citations
55	Large Band Gap in a Quantum Spin Hall Insulator with Weak Spinâ€“Orbit Coupling. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1800141.	1.2	0