Zhigang Wu

List of Publications by Year
in descending order

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	Predicting copper gallium diselenide and band structure engineering through order-disordered transition. Physical Review Materials, 2019, 3, .	0.9	5
2	Ferroelectricity and Elasticity of Rhombohedral BiFeO₃ Under Uniaxial Stress. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1700431.	1.2	3
3	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
4	Structural impact on the eigenenergy renormalization for carbon and silicon allotropes and boron nitride polymorphs. Physical Review B, 2018, 97, .	1.1	9
5	Is sodium a superconductor under high pressure?. Journal of Chemical Physics, 2017, 146, 014705.	1.2	3
6	Intrinsic magnetism and spontaneous band gap opening in bilayer silicene and germanene. Physical Chemistry Chemical Physics, 2017, 19, 2148-2152.	1.3	39
7	Intermediate bands in type-II silicon clathrate with Cu and Ag guest atoms. Physical Review B, 2017, 95, .	1.1	0
8	Formation of spherical ice-shells inside carbon fullerenes. Physical Chemistry Chemical Physics, 2017, 19, 30726-30733.	1.3	2
9	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
10	Tunable many-body interactions in semiconducting graphene: Giant excitonic effect and strong optical absorption. Physical Review B, 2015, 92, .	1.1	3
11	Dirac point movement and topological phase transition in patterned graphene. Nanoscale, 2015, 7, 3645-3650.	2.8	18
12	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
13	Reduction of heat capacity and phonon group velocity in silicon nanowires. Journal of Applied Physics, 2015, 117, .	1.1	18
14	Charge separation at nanoscale interfaces: Energy-level alignment including two-quasiparticle interactions. Journal of Chemical Physics, 2014, 141, 154701.	1.2	0
15	Double superexchange in quantum dot mesomaterials. Energy and Environmental Science, 2014, 7, 1023.	15.6	6
16	Geometrically induced transitions between semimetal and semiconductor in graphene. Physical Review B, 2014, 90, .	1.1	15
17	Tailoring the optical gap of silicon quantum dots without changing their size. Physical Chemistry Chemical Physics, 2014, 16, 19275-19281.	1.3	12
18	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

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19	Quasiparticle energies and excitonic effects in dense solid hydrogen near metallization. Physical Review B, 2014, 90, .	1.1	8
20	Pressure effect on structural and vibrational properties of Y-substituted BiFeO3. Journal of Physics Condensed Matter, 2013, 25, 365401.	0.7	5
21	Bandgap Opening by Patterning Graphene. Scientific Reports, 2013, 3, 2289.	1.6	176
22	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
23	Origin of the Variation of Exciton Binding Energy in Semiconductors. Physical Review Letters, 2013, 110, 016402.	2.9	132
24	Improving the optical absorption of BiFeO3 for photovoltaic applications via uniaxial compression or biaxial tension. Applied Physics Letters, 2013, 102, .	1.5	54
25	Pressure effect on structural and vibrational properties of Sm-substituted BiFeO3. Journal of Applied Physics, 2013, 114, 154110.	1.1	15
26	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
27	Optimal Size Regime for Oxidation-Resistant Silicon Quantum Dots. ACS Nano, 2012, 6, 9690-9699.	7.3	10
28	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
29	Energy gaps in graphene nanomeshes. Physical Review B, 2012, 85, .	1.1	72
30	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
31	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
32	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
33	Quantum Monte Carlo Simulation of Nanoscale MgH2 Cluster Thermodynamics. Journal of the American Chemical Society, 2009, 131, 13918-13919.	6.6	57
34	Charge Separation via Strain in Silicon Nanowires. Nano Letters, 2009, 9, 2418-2422.	4.5	131
35	Origin of morphotropic phase boundaries in ferroelectrics. Nature, 2008, 451, 545-548.	13.7	759
36	Reply to â€œComment on â€˜More accurate generalized gradient approximation for solidsâ€™â€• Physical Review B, 2008, 78, .	1.1	27

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37	Prediction of Ultra-High Aspect Ratio Nanowires from Self-Assembly. Nano Letters, 2008, 8, 2697-2705.	4.5	8
38	Quantum Confinement and Electronic Properties of Tapered Silicon Nanowires. Physical Review Letters, 2008, 100, 246804.	2.9	71
39	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
40	Phonon-mediated superconducting transitions in layered cuprate superconductors. Physical Review B, 2007, 75, .	1.1	17
41	Oxygen isotope effect inBi2Sr2Canâ^'1CunO2n+4+Î´(n=1,2,3)single crystals. Physical Review B, 2007, 76, .	1.1	10
42	Structural 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 ETQq0 0 0 rgBT /Overlock 10 Tf 50 5	1.1	11
43	mathvariant="normal">O</mml:mi><mml:mn>3</mml:. Physical Review B, 2007, 76, . More accurate generalized gradient approximation for solids. Physical Review B, 2006, 73, .	1.1	1,785
44	Advances in First-Principles Studies of Transducer Materials. Ferroelectrics, 2006, 333, 69-78.	0.3	22
45	Trends in elasticity and electronic structure of transition-metal nitrides and carbides from first principles. Physical Review B, 2005, 71, .	1.1	186
46	Ab initiolinear response and frozen phonons for the relaxorPbMg1âˆ•3Nb2âˆ•3O3. Physical Review B, 2005, 71, .	1.1	44
47	Electronic stiffness of a superconducting niobium nitride single crystal under pressure. Physical Review B, 2005, 72, .	1.1	29
48	Hard superconducting nitrides. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 3198-3201.	3.3	256
49	Pressure-Induced Anomalous Phase Transitions and Colossal Enhancement of Piezoelectricity inPbTiO3. Physical Review Letters, 2005, 95, 037601.	2.9	284
50	Weighted-density-approximation description of rare-earth trihydrides. Physical Review B, 2004, 69, .	1.1	25
51	Electronic structure of calcium hexaboride within the weighted density approximation. Physical Review B, 2004, 69, .	1.1	31
52	Atomistic Model Potential for PbTiO3and PMN by Fitting First Principles Results. Ferroelectrics, 2004, 301, 55-59.	0.3	42
53	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
54	First-principles calculations of piezoelectricity and polarization rotation inPb(Zr0.5Ti0.5)O3. Physical Review B, 2003, 68, .	1.1	70

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55	Charge-transfer electrostatic model of compositional order in perovskite alloys. Physical Review B, 2001, 63, .	1.1	14