Lizhong Sun

List of Publications by Year
in descending order

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127	3,001	172207	189595
papers	citations	29 h-index	50 g-index

128	128	128	4044
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Magnetic Properties of Single Transition-Metal Atom Absorbed Graphdiyne and Graphyne Sheet from DFT+U Calculations. Journal of Physical Chemistry C, 2012, 116, 26313-26321.	1.5	264
2	Raman scattering and high temperature ferromagnetism of Mn-doped ZnO nanoparticles. Applied Physics Letters, 2006, 88, 252502.	1.5	224
3	Nanoring structure and optical properties of Ga8As8. Chemical Physics Letters, 2003, 381, 397-403.	1.2	150
4	High temperature spin-polarized semiconductivity with zero magnetization in two-dimensional Janus MXenes. Journal of Materials Chemistry C, 2016, 4, 6500-6509.	2.7	127
5	Anisotropic interactions and strain-induced topological phase transition in Sb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<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>and Bi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	1.1	101
6	New superhard carbon phases between graphite and diamond. Solid State Communications, 2012, 152, 1560-1563.	0.9	89
7	First-principles study of native point defects in Bi2Se3. AIP Advances, 2013, 3, .	0.6	73
8	Z-BN: a novel superhard boron nitride phase. Physical Chemistry Chemical Physics, 2012, 14, 10967.	1.3	72
9	Nanoindentation models and Young's modulus of monolayer graphene: A molecular dynamics study. Applied Physics Letters, 2013, 102, .	1.5	72
10	Electronic band structure of Nb doped SrTiO3 from first principles calculation. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 317, 501-506.	0.9	70
11	Coexistence of open and closed type nodal line topological semimetals in two dimensional B₂C. Journal of Materials Chemistry C, 2018, 6, 1206-1214.	2.7	68
12	Four superhard carbon allotropes: a first-principles study. Physical Chemistry Chemical Physics, 2012, 14, 8410.	1.3	66
13	Magnetic Exchange Coupling and Anisotropy of 3d Transition Metal Nanowires on Graphyne. Scientific Reports, 2014, 4, 4014.	1.6	56
14	Strain control of the electronic structures, magnetic states, and magnetic anisotropy of Fe doped single-layer MoS2. Computational Materials Science, 2015, 110, 102-108.	1.4	51
15	First-principle study on bonding mechanism of ZnO by LDA+U method. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 368, 112-116.	0.9	49
16	Two viable three-dimensional carbon semiconductors with an entirely sp²configuration. Physical Chemistry Chemical Physics, 2013, 15, 680-684.	1.3	48
17	Stability of two-dimensional PN monolayer sheets and their electronic properties. Physical Chemistry Chemical Physics, 2015, 17, 32009-32015.	1.3	47
18	Phonon mean free path spectrum and thermal conductivity for Si1â˜'xGex nanowires. Applied Physics Letters, 2014, 104, .	1.5	46

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19	Asymmetric transport in asymmetric T-shaped graphene nanoribbons. Applied Physics Letters, 2008, 93, 092104.	1.5	45
20	Transport Properties of Hybrid Zigzag Graphene and Boron Nitride Nanoribbons. Journal of Physical Chemistry C, 2011, 115, 10836-10841.	1.5	45
21	Two Dimensional Antiferromagnetic Chern Insulator: NiRuCl₆. Nano Letters, 2016, 16, 6325-6330.	4.5	45
22	Structure, stability and electronic properties of tricycle type graphane. Physica Status Solidi - Rapid Research Letters, 2012, 6, 427-429.	1.2	43
23	Structural, electronic and magnetic properties of single transition-metal adsorbed BN sheet: A density functional study. Chemical Physics Letters, 2012, 532, 40-46.	1.2	42
24	Tunneling Magnetoresistance of Bilayer Hexagonal Boron Nitride and Its Linear Response to External Uniaxial Strain. Journal of Physical Chemistry C, 2011, 115, 8260-8264.	1.5	38
25	Topological dual double node-line semimetals NaAlSi(Ge) and their potential as cathode material for sodium ion batteries. Journal of Materials Chemistry C, 2019, 7, 15375-15381.	2.7	34
26	Molecular dynamics study of ripples in graphene nanoribbons on 6H-SiC(0001): Temperature and size effects. Journal of Applied Physics, 2008, 104, 113536.	1.1	33
27	Transport properties of corrugated graphene nanoribbons. Applied Physics Letters, 2010, 96, .	1.5	33
28	Domain Wall Motion in Perovskite Ferroelectrics Studied by the Nudged Elastic Band Method. Journal of Physical Chemistry C, 2018, 122, 3091-3100.	1.5	31
29	Dead layer effect and its elimination in ferroelectric thin film with oxide electrodes. Acta Materialia, 2016, 112, 216-223.	3.8	30
30	Improved ferroelectric properties of bismuth titanate films by Nd and Mn cosubstitution. Applied Physics Letters, 2007, 90, 012906.	1.5	29
31	Spin Switch of the Transition-Metal-Doped Boron Nitride Sheet through H/F Chemical Decoration. Journal of Physical Chemistry C, 2014, 118, 8899-8906.	1.5	27
32	High-temperature behavior of monolayer graphyne and graphdiyne. Carbon, 2016, 99, 547-555.	5.4	27
33	Two-dimensional tricycle arsenene with a direct band gap. Physical Chemistry Chemical Physics, 2016, 18, 8723-8729.	1.3	27
34	Enhanced 1â€“5ÂÎ¼m near- and mid-infrared emission in Ho3+/Yb3+ codoped TeO2-ZnF2 oxyfluorotellurite glasses. Journal of Rare Earths, 2020, 38, 1044-1052.	2.5	26
35	Hydroxylated graphyne and graphdiyne: First-principles study. Applied Surface Science, 2016, 361, 206-212.	3.1	22
36	Work Functions of Boron Nitride Nanoribbons: First-Principles Study. Journal of Computational and Theoretical Nanoscience, 2012, 9, 16-22.	0.4	21

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37	Prediction of half-semiconductor antiferromagnets with vanishing net magnetization. RSC Advances, 2015, 5, 46640-46647.	1.7	21
38	Structural and electronic properties of thein situimpurityAsHginHg0.5Cd0.5Te: First-principles study. Physical Review B, 2005, 71, .	1.1	20
39	Effects of carrier degeneracy and conduction band non-parabolicity on the simulation of HgCdTe photovoltaic devices. Infrared Physics and Technology, 2007, 50, 1-8.	1.3	20
40	New type of hybrid nodal line semimetal in Be₂Si. New Journal of Physics, 2019, 21, 033018.	1.2	20
41	Relaxations and bonding mechanism inHg1âˆ'xCdxTewith mercury vacancy defect: First-principles study. Physical Review B, 2006, 73, .	1.1	18
42	Modulation effect of hydrogen and fluorine decoration on the surface work function of BN sheets. AIP Advances, 2012, 2, .	0.6	18
43	Prediction of superhard carbon allotropes from the segment combination method. Journal of Superhard Materials, 2012, 34, 386-399.	0.5	17
44	Dirac Semimetals in Homogeneous Holey Carbon Nitride Monolayers. Journal of Physical Chemistry C, 2021, 125, 6082-6089.	1.5	17
45	Composition dependent electronic properties, optical transitions, and anionic relaxations of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Cd</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>âˆ'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:mi mathvariant="normal">Zn</mml:mi><mml:msub><mml:mi>x</mml:mi></mml:msub><mml:mi mathvariant="normal">Te</mml:mi></mml:mrow></mml:math> alloys from first principles. Physical Re	1.1	16
46	Reduction mechanism of hydroxyl group from graphene oxide with and without â€“NH2 agent. Physica B: Condensed Matter, 2015, 477, 70-74.	1.3	16
47	Removal of hydroxyl routes enhancing 2.85â€Î¼m mid-infrared luminescence in oxyfluorotellurite glass with high ZnF2 content. Journal of Non-Crystalline Solids, 2018, 502, 97-105.	1.5	16
48	Electronic properties and chemical trends of the arsenicin situimpurities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Hg</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>âˆ'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">Cd</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi mathvariant="normal">Te</mml:mi></mml:mrow></mml:math>: First-principles study. Physical Review B, 2007, 76, .	1.1	15
49	Transport properties of zigzag graphene nanoribbons with oxygen edge decoration. Organic Electronics, 2012, 13, 2494-2501.	1.4	15
50	1T-CrO₂monolayer: a high-temperature Dirac half-metal for high-speed spintronics. Nanoscale Advances, 2021, 3, 3093-3099.	2.2	15
51	Electronic structures and optical properties of hexagonal boron nitride under hydrostatic pressures. Journal of Applied Physics, 2011, 109, 073708.	1.1	14
52	A DFT-LDA study of electronic and optical properties of hexagonal boron nitride under uniaxial strain. Computational Materials Science, 2012, 54, 165-169.	1.4	14
53	Transport properties of graphene/metal planar junction. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 1321-1325.	0.9	14
54	Ferroelectric and dielectric properties of Nd3+â•Zr4+ cosubstituted Bi4Ti3O12 thin films. Applied Physics Letters, 2007, 90, 102906.	1.5	13

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55	Thermal decomposition behaviour of RDX by first-principles molecular dynamics simulation. Molecular Simulation, 2008, 34, 961-965.	0.9	13
56	A first-principles study of oxygen vacancy induced changes in structural, electronic and magnetic properties of La2/3Sr1/3MnO3. Journal of Alloys and Compounds, 2015, 649, 973-980.	2.8	13
57	Local structural distortions and Mn random distributions in (Ga,Mn)As: A first-principles study. Physical Review B, 2004, 69, .	1.1	12
58	The effect of corner form on electron transport of L-shaped graphene nanoribbons. Physica B: Condensed Matter, 2009, 404, 1771-1775.	1.3	12
59	Direct or indirect semiconductor: The role of stacking fault in h-BN. Physica B: Condensed Matter, 2011, 406, 2293-2297.	1.3	12
60	Effects of oxygen-containing defect complex on the electronic structures and transport properties of single-walled carbon nanotubes. Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 1686-1691.	0.9	12
61	Prediction of two planar carbon allotropes with large meshes. Physical Chemistry Chemical Physics, 2016, 18, 1172-1177.	1.3	12
62	Ferrimagnetic half-metallic properties of Cr/Fe Î´ doped MoS₂ monolayer. RSC Advances, 2017, 7, 20116-20122.	1.7	12
63	Lowâ€Energy GeP Monolayers with Natural Typeâ€Ⅱ Homojunctions for SunLightâ€Driven Water Splitting. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1900470.	1.2	12
64	Size effect of half-metallic properties of BN/C hybrid nanoribbons. Physica B: Condensed Matter, 2012, 407, 4770-4772.	1.3	11
65	Prediction of twoâ€dimensional BiSb with puckered structure. Physica Status Solidi - Rapid Research Letters, 2017, 11, 1700051.	1.2	11
66	Increasing ZnF2 content enhancing the near- and mid-infrared emission in Er3+/Yb3+ codoped oxyfluorotellurite glasses with decreased hydroxyl. Journal of Luminescence, 2019, 216, 116683.	1.5	11
67	Transport properties of hybrid graphene/graphane nanoribbons. Applied Physics Letters, 2012, 100, 103109.	1.5	10
68	Stability, electronic structures and transport properties of armchair (10, 10) BN/C nanotubes. Journal of Solid State Chemistry, 2013, 200, 294-298.	1.4	10
69	Low energy three-dimensional hydrocarbon crystal from cold compression of benzene. Journal of Physics Condensed Matter, 2013, 25, 205403.	0.7	10
70	3d Transition Metal Adsorption Induced the valley-polarized Anomalous Hall Effect in Germanene. Scientific Reports, 2016, 6, 27830.	1.6	10
71	Two-dimensional semiconductors XY 2 (XÂ=ÂGe,Sn;YÂ=ÂS,Se) with promising piezoelectric properties. Computational Condensed Matter, 2017, 11, 33-39.	0.9	10
72	Strong anisotropic nodal lines in the TiBe family. Physical Chemistry Chemical Physics, 2019, 21, 8402-8407.	1.3	10

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73	Removal of hydroxyl groups to enhance the near- and mid-infrared emission of heavy-metal oxyfluoride glasses by chemical clarification : Nitrate ions. Journal of Non-Crystalline Solids, 2020, 544, 120165.	1.5	10
74	Evolution of the bonding mechanism of ZnO under isotropic compression: A first-principles study. Physica B: Condensed Matter, 2008, 403, 2832-2837.	1.3	9
75	Tunable differential conductance of single wall C/BN nanotube heterostructure. Journal of Molecular Modeling, 2013, 19, 2965-2969.	0.8	9
76	ThreeâEDimensional Dirac Semimetal Î²â€PbO₂. Physica Status Solidi - Rapid Research Letters, 2017, 11, 1700271.	1.2	9
77	A constitutive model coupling irradiation with two-phase lithiation for lithium-ion battery electrodes. Philosophical Magazine, 2019, 99, 992-1013.	0.7	9
78	Lithiation-induced interfacial failure of electrode-collector: A first-principles study. Materials Chemistry and Physics, 2019, 222, 193-199.	2.0	9
79	Ferromagnetism of 3d-impurities substituted in Ge. Journal of Magnetism and Magnetic Materials, 2004, 284, 253-259.	1.0	8
80	Bonding mechanism and relaxation energy of (): First-principles study. Journal of Physics and Chemistry of Solids, 2009, 70, 707-712.	1.9	8
81	Transport Properties of Zigzag Graphene Nanoribbons Decorated by Carboxyl Group Chains. Journal of Physical Chemistry C, 2011, 115, 21893-21898.	1.5	8
82	Surface work function of chemically derived graphene: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 1760-1765.	0.9	7
83	Stable configurations and electronic structures of hydrogenated graphyne. Computational Materials Science, 2014, 91, 274-278.	1.4	7
84	Magnetic control of single transition metal doped MoS2 through H/F chemical decoration. Journal of Magnetism and Magnetic Materials, 2017, 422, 243-248.	1.0	7
85	First-principles prediction of two atomic-thin phosphorene allotropes with potentials for sun-light-driven water splitting. Journal of Physics Condensed Matter, 2019, 31, 075702.	0.7	7
86	Dirac Semimetal Protected by Nonsymmorphic Mirror Symmetries in TPHâ€Graphene. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100039.	1.2	7
87	The influence of the additional confining potentials on ferromagnetism in IIIâ€“V digital ferromagnetic heterostructures. Journal of Applied Physics, 2006, 99, 113903.	1.1	6
88	Electronic properties of the Au impurity in : First-principles study. Physica B: Condensed Matter, 2009, 404, 131-137.	1.3	6
89	Zigzag graphene nanoribbons: Flexible and robust transparent conductors. Solid State Sciences, 2012, 14, 711-714.	1.5	6
90	A molecular dynamics study of the Si-nanowire@carbon-nanotube nanocomposite with sp3 interfacial bonding. Computational Materials Science, 2013, 79, 650-655.	1.4	6

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91	Anisotropic optical properties of graphene/graphane superlattices. Solid State Sciences, 2015, 40, 71-76.	1.5	6
92	Large gap two dimensional topological insulators: the bilayer triangular lattice TlM (M = N, P, As, Sb). Journal of Materials Chemistry C, 2017, 5, 4268-4274.	2.7	6
93	First principle study on the bonding mechanism of nanoring structure Ga8As8. European Physical Journal D, 2005, 34, 47-50.	0.6	5
94	Binding energy of hydrogenâ€“Cd vacancy complex in CdTe. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 791-794.	0.9	5
95	Nucleation effect of Sia of 6Hâ€“SiC-(0 0 0 1)â€“(âˆš3Ã—âˆš3)R30Â° surface: First-principles study. Physica B: Condensed Matter, 2010, 405, 3576-3580.	1.3	5
96	Resonant transmission in three-terminal triangle graphene nanojunctions with zigzag edges. Solid State Communications, 2010, 150, 675-679.	0.9	5
97	Hydrogen passivation and multiple hydrogenâ€“Hg vacancy complex impurities (nHâ€“VHg, nâ€‰=â€‰1,2,3,4) in Hg0.75Cd0.25Te. Journal of Applied Physics, 2011, 110, .	1.1	5
98	Effects of lattice strain and ion displacement on the bonding mechanism of the ferroelectric perovskite material BaTiO3: first-principles study. Journal of Physics Condensed Matter, 2007, 19, 276213.	0.7	4
99	Effects of contact oxidization on the transport properties of Au/ZGNR junctions. Physica Status Solidi - Rapid Research Letters, 2012, 6, 457-459.	1.2	4
100	Carbon nanotube oscillators encapsulating a platinum nanocluster: A molecular dynamics study. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 54, 237-241.	1.3	4
101	Hydrogenâ€“Te antisite complex impurity (Hâ€“TeHg) in Hg0.75Cd0.25Te: First-principles study. Journal of Physics and Chemistry of Solids, 2013, 74, 1086-1092.	1.9	4
102	First-Principles Study of the Initial Growth Stages of Carbon Chain on Ni(111) Surface. Journal of Computational and Theoretical Nanoscience, 2010, 7, 2063-2067.	0.4	3
103	Novel transport properties of gold-single wall carbon nanotubes composite contacts. Journal of Applied Physics, 2010, 108, 064318.	1.1	2
104	Configuration and electronic properties of graphene nanoribbons on Si(211) surface. Applied Surface Science, 2011, 257, 2474-2480.	3.1	2
105	Hydrogenated graphene: Structures and surface work function. , 2012, , .		2
106	Electronic properties of graphene on the C-decorated Si(111) surface: An ab initio study. Current Applied Physics, 2013, 13, 1512-1519.	1.1	2
107	Electric and Magnetic Manipulation in Graphene Absorption by the Electric Field. Journal of Computational and Theoretical Nanoscience, 2013, 10, 515-520.	0.4	2
108	Topological nodal lines in three-dimensional single wall carbon nanotube network. Computational Materials Science, 2019, 169, 109123.	1.4	2

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109	Coexistence of Weyl and Typeâ€Ⅱ Triply Degenerate Fermions in a Ternary Topological Semimetal YPtP. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1900421.	1.2	2
110	Topological Phase Transition in 2D 1Tâ€²â€WSTe. Physica Status Solidi (B): Basic Research, 2020, 257, 2000010.	0.7	2
111	Valley Polarization in Monolayer Ferromagnetic FeCl: A Firstâ€Principles Study. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000206.	1.2	2
112	High temperature clarifier sulfate enhancing the infrared emission of Oxyfluorosilicate glass ceramics containing CaF2 nanocrystals. Journal of Non-Crystalline Solids, 2021, 561, 120753.	1.5	2
113	Nontrivial topological states in new two-dimensional CdAs. Journal of Physics Condensed Matter, 2021, 33, 365701.	0.7	2
114	ZnS enhancing the infrared emission of Er3+ doped oxyfluorosulfide glasses with low hydroxyl content. Journal of Non-Crystalline Solids, 2021, 566, 120906.	1.5	2
115	Structural and magnetic properties of ultrathin bcc Fe films on Ge(001). Journal Physics D: Applied Physics, 2005, 38, 1055-1060.	1.3	1
116	Relaxations and bonding mechanism of arsenic in-situ impurities in MCT: first-principles study. Transactions of Nonferrous Metals Society of China, 2006, 16, 907-911.	1.7	1
117	Effective Fermi level tuning of Bi2Se3 by introducing CdBi/CaBi dopant. RSC Advances, 2014, 4, 10499.	1.7	1
118	Electronic and transmission properties of magnetotunnel junctions of cobalt/iron intercalated bilayer two dimensional sheets. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 2661-2666.	0.9	1
119	Response to â€œComment on â€˜Nanoindentation models and Young's modulus of monolayer graphene: A molecular dynamics studyâ€™â€•[Appl. Phys. Lett. 110, 176101 (2017)]. Applied Physics Letters, 2017, 110, .	1.5	1
120	Two dimensional topological insulators in bilayer BiB. Computational Materials Science, 2019, 160, 82-85.	1.4	1
121	Slaterâ€“Koster parametrization for the phonons of monolayer MoX₂ (X = S, Se or Te). Journal of Physics Condensed Matter, 2022, 34, 195702.	0.7	1
122	FERROMAGNETISM IN Co-DOPED TiO2 ANATASE DUE TO THE COBALT CLUSTERING. International Journal of Modern Physics B, 2005, 19, 2520-2525.	1.0	0
123	Formation Energy of Arsenic Impurities in MCT: First-Principles Study. , 2006, , .		0
124	Structures, stability and electronic properties of two- or four-segment BN/C nanotubes. , 2012, , .		0
125	First-principles study on the magnetic properties of Î²-Ti68.75Nb25X6.25 (X=Mo, Sn, Ta, Zr, Fe) alloys. AIP Advances, 2019, 9, 065102.	0.6	0
126	Intrinsic spin Hall conductivity plateau in topological semimetals with triply degenerate points. Physica B: Condensed Matter, 2022, 629, 413626.	1.3	0

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127	Computational discovery of spin-polarized semimetals in spinel materials. Materials Advances, 0, , .	2.6	0