

# Lizhong Sun

## List of Publications by Year in descending order

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127  
papers

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citations

172457

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h-index

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128  
docs citations

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times ranked

4044  
citing authors

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 1  | Intrinsic spin Hall conductivity plateau in topological semimetals with triply degenerate points. <i>Physica B: Condensed Matter</i> , 2022, 629, 413626.  | 2.7 | 0         |
| 2  | Slater-Koster parametrization for the phonons of monolayer $\text{MoX}_2$ ( $X = \text{S, Se or Te}$ ). <i>Journal of Physics Condensed Matter</i> , 2022, 34, 195702.   | 1.8 | 1         |
| 3  | Dirac Semimetals in Homogeneous Holey Carbon Nitride Monolayers. <i>Journal of Physical Chemistry C</i> , 2021, 125, 6082-6089.  | 3.1 | 17        |
| 4  | Dirac Semimetal Protected by Nonsymmorphic Mirror Symmetries in TP $\pi$ -Graphene. <i>Physica Status Solidi - Rapid Research Letters</i> , 2021, 15, 2100039.   | 2.4 | 7         |
| 5  | High temperature clarifier sulfate enhancing the infrared emission of Oxyfluorosilicate glass ceramics containing $\text{CaF}_2$ nanocrystals. <i>Journal of Non-Crystalline Solids</i> , 2021, 561, 120753.                       | 3.1 | 2         |
| 6  | Nontrivial topological states in new two-dimensional CdAs. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 365701.  | 1.8 | 2         |
| 7  | ZnS enhancing the infrared emission of $\text{Er}^{3+}$ doped oxyfluorosulfide glasses with low hydroxyl content. <i>Journal of Non-Crystalline Solids</i> , 2021, 566, 120906.  | 3.1 | 2         |
| 8  | 1T- $\text{CrO}_2$ monolayer: a high-temperature Dirac half-metal for high-speed spintronics. <i>Nanoscale Advances</i> , 2021, 3, 3093-3099.  | 4.6 | 15        |
| 9  | Enhanced $1.5\ \mu\text{m}$ near- and mid-infrared emission in $\text{Ho}^{3+}/\text{Yb}^{3+}$ codoped $\text{TeO}_2$ - $\text{ZnF}_2$ oxyfluorotellurite glasses. <i>Journal of Rare Earths</i> , 2020, 38, 1044-1052.            | 4.8 | 26        |
| 10 | Removal of hydroxyl groups to enhance the near- and mid-infrared emission of heavy-metal oxyfluoride glasses by chemical clarification : Nitrate ions. <i>Journal of Non-Crystalline Solids</i> , 2020, 544, 120165.               | 3.1 | 10        |
| 11 | Topological Phase Transition in 2D 1T $\pi$ -WTe $\pi$ . <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 2000010.  | 1.5 | 2         |
| 12 | Valley Polarization in Monolayer Ferromagnetic FeCl: A First-Principles Study. <i>Physica Status Solidi - Rapid Research Letters</i> , 2020, 14, 2000206.  | 2.4 | 2         |
| 13 | Topological nodal lines in three-dimensional single wall carbon nanotube network. <i>Computational Materials Science</i> , 2019, 169, 109123.  | 3.0 | 2         |
| 14 | Low-Energy GeP Monolayers with Natural Type-II Homojunctions for SunLight-Driven Water Splitting. <i>Physica Status Solidi - Rapid Research Letters</i> , 2019, 13, 1900470.   | 2.4 | 12        |
| 15 | Coexistence of Weyl and Type-II Triply Degenerate Fermions in a Ternary Topological Semimetal YPtP. <i>Physica Status Solidi - Rapid Research Letters</i> , 2019, 13, 1900421.   | 2.4 | 2         |
| 16 | Increasing $\text{ZnF}_2$ content enhancing the near- and mid-infrared emission in $\text{Er}^{3+}/\text{Yb}^{3+}$ codoped oxyfluorotellurite glasses with decreased hydroxyl. <i>Journal of Luminescence</i> , 2019, 216, 116683. | 3.1 | 11        |
| 17 | A constitutive model coupling irradiation with two-phase lithiation for lithium-ion battery electrodes. <i>Philosophical Magazine</i> , 2019, 99, 992-1013.  | 1.6 | 9         |
| 18 | First-principles study on the magnetic properties of $\text{Ti}_{68.75}\text{Nb}_{25}\text{X}_{6.25}$ ( $X=\text{Mo, Sn, Ta, Zr, Fe}$ ) alloys. <i>AIP Advances</i> , 2019, 9, 065102.   | 1.3 | 0         |

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|----|---|-----|-----------|
| 19 | Strong anisotropic nodal lines in the TiBe family. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8402-8407.  | 2.8 | 10        |
| 20 | New type of hybrid nodal line semimetal in $\text{Be}_2\text{Si}$ . <i>New Journal of Physics</i> , 2019, 21, 033018.   | 2.9 | 20        |
| 21 | Topological dual double node-line semimetals $\text{NaAlSi}(\text{Ge})$ and their potential as cathode material for sodium ion batteries. <i>Journal of Materials Chemistry C</i> , 2019, 7, 15375-15381.                 | 5.5 | 34        |
| 22 | First-principles prediction of two atomic-thin phosphorene allotropes with potentials for sun-light-driven water splitting. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 075702.                                | 1.8 | 7         |
| 23 | Two dimensional topological insulators in bilayer BiB. <i>Computational Materials Science</i> , 2019, 160, 82-85.   | 3.0 | 1         |
| 24 | Lithiation-induced interfacial failure of electrode-collector: A first-principles study. <i>Materials Chemistry and Physics</i> , 2019, 222, 193-199.   | 4.0 | 9         |
| 25 | Domain Wall Motion in Perovskite Ferroelectrics Studied by the Nudged Elastic Band Method. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3091-3100.   | 3.1 | 31        |
| 26 | Coexistence of open and closed type nodal line topological semimetals in two dimensional $\text{B}_2\text{C}$ . <i>Journal of Materials Chemistry C</i> , 2018, 6, 1206-1214.   | 5.5 | 68        |
| 27 | Removal of hydroxyl routes enhancing $2.85\ \mu\text{m}$ mid-infrared luminescence in oxyfluorotellurite glass with high $\text{ZnF}_2$ content. <i>Journal of Non-Crystalline Solids</i> , 2018, 502, 97-105.            | 3.1 | 16        |
| 28 | Two-dimensional semiconductors $\text{XY}_2$ ( $\text{X}=\text{Ge, Sn}; \text{Y}=\text{S, Se}$ ) with promising piezoelectric properties. <i>Computational Condensed Matter</i> , 2017, 11, 33-39.                        | 2.1 | 10        |
| 29 | Ferrimagnetic half-metallic properties of Cr/Fe doped $\text{MoS}_2$ monolayer. <i>RSC Advances</i> , 2017, 7, 20116-20122.   | 3.6 | 12        |
| 30 | Prediction of two-dimensional BiSb with puckered structure. <i>Physica Status Solidi - Rapid Research Letters</i> , 2017, 11, 1700051.  | 2.4 | 11        |
| 31 | Large gap two dimensional topological insulators: the bilayer triangular lattice TIM ( $\text{M} = \text{N, P, As, Sb}$ ). <i>Journal of Materials Chemistry C</i> , 2017, 5, 4268-4274.                                  | 5.5 | 6         |
| 32 | Three-dimensional Dirac Semimetal $\text{PbO}_2$ . <i>Physica Status Solidi - Rapid Research Letters</i> , 2017, 11, 1700271.   | 2.4 | 9         |
| 33 | Response to "Comment on "Nanoindentation models and Young's modulus of monolayer graphene: A molecular dynamics study" [Appl. Phys. Lett. 110 (2017), 176101 (2017)]. <i>Applied Physics Letters</i> , 2017, 110, 176101. |     | 1         |
| 34 | Magnetic control of single transition metal doped $\text{MoS}_2$ through H/F chemical decoration. <i>Journal of Magnetism and Magnetic Materials</i> , 2017, 422, 243-248.  | 2.3 | 7         |
| 35 | Dead layer effect and its elimination in ferroelectric thin film with oxide electrodes. <i>Acta Materialia</i> , 2016, 112, 216-223.  | 7.9 | 30        |
| 36 | Two Dimensional Antiferromagnetic Chern Insulator: $\text{NiRuCl}_6$ . <i>Nano Letters</i> , 2016, 16, 6325-6330.   | 9.1 | 45        |

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|----|---|------|-----------|
| 37 | 3d Transition Metal Adsorption Induced the valley-polarized Anomalous Hall Effect in Germanene. <i>Scientific Reports</i> , 2016, 6, 27830.   | 3.3  | 10        |
| 38 | High temperature spin-polarized semiconductivity with zero magnetization in two-dimensional Janus MXenes. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6500-6509.   | 5.5  | 127       |
| 39 | High-temperature behavior of monolayer graphyne and graphdiyne. <i>Carbon</i> , 2016, 99, 547-555.  | 10.3 | 27        |
| 40 | Two-dimensional tricycle arsenene with a direct band gap. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8723-8729.   | 2.8  | 27        |
| 41 | Hydroxylated graphyne and graphdiyne: First-principles study. <i>Applied Surface Science</i> , 2016, 361, 206-212.  | 6.1  | 22        |
| 42 | Prediction of two planar carbon allotropes with large meshes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1172-1177.   | 2.8  | 12        |
| 43 | Anisotropic optical properties of graphene/graphane superlattices. <i>Solid State Sciences</i> , 2015, 40, 71-76.   | 3.2  | 6         |
| 44 | A first-principles study of oxygen vacancy induced changes in structural, electronic and magnetic properties of La <sub>2</sub> /3Sr <sub>1</sub> /3MnO <sub>3</sub> . <i>Journal of Alloys and Compounds</i> , 2015, 649, 973-980. | 5.5  | 13        |
| 45 | Electronic and transmission properties of magnetotunnel junctions of cobalt/iron intercalated bilayer two dimensional sheets. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015, 379, 2661-2666.    | 2.1  | 1         |
| 46 | Prediction of half-semiconductor antiferromagnets with vanishing net magnetization. <i>RSC Advances</i> , 2015, 5, 46640-46647.   | 3.6  | 21        |
| 47 | Stability of two-dimensional PN monolayer sheets and their electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 32009-32015.   | 2.8  | 47        |
| 48 | Strain control of the electronic structures, magnetic states, and magnetic anisotropy of Fe doped single-layer MoS <sub>2</sub> . <i>Computational Materials Science</i> , 2015, 110, 102-108.                                      | 3.0  | 51        |
| 49 | Reduction mechanism of hydroxyl group from graphene oxide with and without "NH <sub>2</sub> agent. <i>Physica B: Condensed Matter</i> , 2015, 477, 70-74.   | 2.7  | 16        |
| 50 | Phonon mean free path spectrum and thermal conductivity for Si <sub>1-x</sub> Gex nanowires. <i>Applied Physics Letters</i> , 2014, 104, .  | 3.3  | 46        |
| 51 | Transport properties of graphene/metal planar junction. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014, 378, 1321-1325.  | 2.1  | 14        |
| 52 | Effective Fermi level tuning of Bi <sub>2</sub> Se <sub>3</sub> by introducing CdBi/CaBi dopant. <i>RSC Advances</i> , 2014, 4, 10499.  | 3.6  | 1         |
| 53 | Spin Switch of the Transition-Metal-Doped Boron Nitride Sheet through H/F Chemical Decoration. <i>Journal of Physical Chemistry C</i> , 2014, 118, 8899-8906.   | 3.1  | 27        |
| 54 | Stable configurations and electronic structures of hydrogenated graphyne. <i>Computational Materials Science</i> , 2014, 91, 274-278.   | 3.0  | 7         |

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|----|---|-----|-----------|
| 55 | Magnetic Exchange Coupling and Anisotropy of 3d Transition Metal Nanowires on Graphyne. Scientific Reports, 2014, 4, 4014.  | 3.3 | 56        |
| 56 | Carbon nanotube oscillators encapsulating a platinum nanocluster: A molecular dynamics study. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 54, 237-241.   | 2.7 | 4         |
| 57 | First-principles study of native point defects in Bi <sub>2</sub> Se <sub>3</sub> . AIP Advances, 2013, 3, .  | 1.3 | 73        |
| 58 | Tunable differential conductance of single wall C/BN nanotube heterostructure. Journal of Molecular Modeling, 2013, 19, 2965-2969.  | 1.8 | 9         |
| 59 | Electronic properties of graphene on the C-decorated Si(111) surface: An ab initio study. Current Applied Physics, 2013, 13, 1512-1519.   | 2.4 | 2         |
| 60 | Two viable three-dimensional carbon semiconductors with an entirely sp <sup>2</sup> configuration. Physical Chemistry Chemical Physics, 2013, 15, 680-684.  | 2.8 | 48        |
| 61 | Hydrogen-Te antisite complex impurity (H <sup>+</sup> Te <sup>-</sup> Hg) in Hg <sub>0.75</sub> Cd <sub>0.25</sub> Te: First-principles study. Journal of Physics and Chemistry of Solids, 2013, 74, 1086-1092. | 4.0 | 4         |
| 62 | A molecular dynamics study of the Si-nanowire@carbon-nanotube nanocomposite with sp <sup>3</sup> interfacial bonding. Computational Materials Science, 2013, 79, 650-655.                                       | 3.0 | 6         |
| 63 | Nanoindentation models and Young's modulus of monolayer graphene: A molecular dynamics study. Applied Physics Letters, 2013, 102, .   | 3.3 | 72        |
| 64 | 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.                                      | 2.1 | 7         |
| 65 | Stability, electronic structures and transport properties of armchair (10, 10) BN/C nanotubes. Journal of Solid State Chemistry, 2013, 200, 294-298.  | 2.9 | 10        |
| 66 | Low energy three-dimensional hydrocarbon crystal from cold compression of benzene. Journal of Physics Condensed Matter, 2013, 25, 205403.   | 1.8 | 10        |
| 67 | Electric and Magnetic Manipulation in Graphene Absorption by the Electric Field. Journal of Computational and Theoretical Nanoscience, 2013, 10, 515-520.   | 0.4 | 2         |
| 68 | Work Functions of Boron Nitride Nanoribbons: First-Principles Study. Journal of Computational and Theoretical Nanoscience, 2012, 9, 16-22.  | 0.4 | 21        |
| 69 | Modulation effect of hydrogen and fluorine decoration on the surface work function of BN sheets. AIP Advances, 2012, 2, .   | 1.3 | 18        |
| 70 | 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.                                    | 3.1 | 264       |
| 71 | Effects of contact oxidization on the transport properties of Au/ZGNR junctions. Physica Status Solidi - Rapid Research Letters, 2012, 6, 457-459.  | 2.4 | 4         |
| 72 | Size effect of half-metallic properties of BN/C hybrid nanoribbons. Physica B: Condensed Matter, 2012, 407, 4770-4772.  | 2.7 | 11        |

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|----|---|-----|-----------|
| 73 | Structures, stability and electronic properties of two- or four-segment BN/C nanotubes. , 2012, , .   |     | 0         |
| 74 | New superhard carbon phases between graphite and diamond. Solid State Communications, 2012, 152, 1560-1563.   | 1.9 | 89        |
| 75 | A DFT-LDA study of electronic and optical properties of hexagonal boron nitride under uniaxial strain. Computational Materials Science, 2012, 54, 165-169.  | 3.0 | 14        |
| 76 | Structure, stability and electronic properties of tricycle type graphane. Physica Status Solidi - Rapid Research Letters, 2012, 6, 427-429.   | 2.4 | 43        |
| 77 | Four superhard carbon allotropes: a first-principles study. Physical Chemistry Chemical Physics, 2012, 14, 8410.  | 2.8 | 66        |
| 78 | Prediction of superhard carbon allotropes from the segment combination method. Journal of Superhard Materials, 2012, 34, 386-399.   | 1.2 | 17        |
| 79 | Transport properties of zigzag graphene nanoribbons with oxygen edge decoration. Organic Electronics, 2012, 13, 2494-2501.  | 2.6 | 15        |
| 80 | Z-BN: a novel superhard boron nitride phase. Physical Chemistry Chemical Physics, 2012, 14, 10967.  | 2.8 | 72        |
| 81 | Transport properties of hybrid graphene/graphane nanoribbons. Applied Physics Letters, 2012, 100, 103109.   | 3.3 | 10        |
| 82 | Hydrogenated graphene: Structures and surface work function. , 2012, , .  |     | 2         |
| 83 | Structural, electronic and magnetic properties of single transition-metal adsorbed BN sheet: A density functional study. Chemical Physics Letters, 2012, 532, 40-46.  | 2.6 | 42        |
| 84 | Zigzag graphene nanoribbons: Flexible and robust transparent conductors. Solid State Sciences, 2012, 14, 711-714.   | 3.2 | 6         |
| 85 | 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.   | 2.1 | 12        |
| 86 | Transport Properties of Zigzag Graphene Nanoribbons Decorated by Carboxyl Group Chains. Journal of Physical Chemistry C, 2011, 115, 21893-21898.  | 3.1 | 8         |
| 87 | Tunneling Magnetoresistance of Bilayer Hexagonal Boron Nitride and Its Linear Response to External Uniaxial Strain. Journal of Physical Chemistry C, 2011, 115, 8260-8264.  | 3.1 | 38        |
| 88 | Hydrogen passivation and multiple hydrogenâ€“Hg vacancy complex impurities ( $nH\hat{=}V\langle i\rangle Hg\langle /i\rangle$ , $n\hat{=}\%0=\hat{=}\%01,2,3,4$ ) in $Hg_{0.75}Cd_{0.25}Te$ . Journal of Applied Physics, 2011, 110, .  |     | 5         |
| 89 | Antiferromagnetic interactions and spin-induced topological phase transition in $Sb_{2-x}Se_x$ $xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math /><mml:mn>3</mml:mn></mml:msub></mml:math>$ and $Bi_{1-x}Sb_x$ $xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>$ | 3.2 | 101       |
| 90 | Transport Properties of Hybrid Zigzag Graphene and Boron Nitride Nanoribbons. Journal of Physical Chemistry C, 2011, 115, 10836-10841.  | 3.1 | 45        |

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|-----|--|-----|-----------|
| 91  | Configuration and electronic properties of graphene nanoribbons on Si(211) surface. Applied Surface Science, 2011, 257, 2474-2480.   | 6.1 | 2         |
| 92  | Direct or indirect semiconductor: The role of stacking fault in h-BN. Physica B: Condensed Matter, 2011, 406, 2293-2297.   | 2.7 | 12        |
| 93  | Electronic structures and optical properties of hexagonal boron nitride under hydrostatic pressures. Journal of Applied Physics, 2011, 109, 073708.  | 2.5 | 14        |
| 94  | 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         |
| 95  | Nucleation effect of Si on SiC(001) surface: First-principles study. Physica B: Condensed Matter, 2010, 405, 3576-3580.  | 2.7 | 5         |
| 96  | Resonant transmission in three-terminal triangle graphene nanojunctions with zigzag edges. Solid State Communications, 2010, 150, 675-679.   | 1.9 | 5         |
| 97  | Transport properties of corrugated graphene nanoribbons. Applied Physics Letters, 2010, 96, .  | 3.3 | 33        |
| 98  | Novel transport properties of gold-single wall carbon nanotubes composite contacts. Journal of Applied Physics, 2010, 108, 064318.   | 2.5 | 2         |
| 99  | Electronic properties of the Au impurity in Si: First-principles study. Physica B: Condensed Matter, 2009, 404, 131-137.   | 2.7 | 6         |
| 100 | The effect of corner form on electron transport of L-shaped graphene nanoribbons. Physica B: Condensed Matter, 2009, 404, 1771-1775.   | 2.7 | 12        |
| 101 | Binding energy of hydrogen-Cd vacancy complex in CdTe. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 791-794.  | 2.1 | 5         |
| 102 | Bonding mechanism and relaxation energy of H in Si: First-principles study. Journal of Physics and Chemistry of Solids, 2009, 70, 707-712.   | 4.0 | 8         |
| 103 | Evolution of the bonding mechanism of ZnO under isotropic compression: A first-principles study. Physica B: Condensed Matter, 2008, 403, 2832-2837.  | 2.7 | 9         |
| 104 | Thermal decomposition behaviour of RDX by first-principles molecular dynamics simulation. Molecular Simulation, 2008, 34, 961-965.   | 2.0 | 13        |
| 105 | Molecular dynamics study of ripples in graphene nanoribbons on 6H-SiC(0001): Temperature and size effects. Journal of Applied Physics, 2008, 104, 113536.  | 2.5 | 33        |
| 106 | Asymmetric transport in asymmetric T-shaped graphene nanoribbons. Applied Physics Letters, 2008, 93, 092104.   | 3.3 | 45        |
| 107 | Effects of lattice strain and ion displacement on the bonding mechanism of the ferroelectric perovskite material BaTiO <sub>3</sub> : first-principles study. Journal of Physics Condensed Matter, 2007, 19, 276213. | 1.8 | 4         |
| 108 | Improved ferroelectric properties of bismuth titanate films by Nd and Mn cosubstitution. Applied Physics Letters, 2007, 90, 012906.  | 3.3 | 29        |

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|-----|--|-----|-----------|
| 109 | Electronic properties and chemical trends of the arsenic in-situ impurities in CdZnTe. Physical Review B, 2007, 76, .  | 3.2 | 15        |
| 110 | Electronic properties and chemical trends of the arsenic in-situ impurities in CdZnTe. Physical Review B, 2007, 76, .  | 3.2 | 15        |
| 111 | Ferroelectric and dielectric properties of Nd <sup>3+</sup> -Zr <sup>4+</sup> cosubstituted Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> thin films. Applied Physics Letters, 2007, 90, 102906. | 3.3 | 13        |
| 112 | Effects of carrier degeneracy and conduction band non-parabolicity on the simulation of HgCdTe photovoltaic devices. Infrared Physics and Technology, 2007, 50, 1-8.                               | 2.9 | 20        |
| 113 | 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.  | 2.1 | 49        |
| 114 | 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.                             | 4.2 | 1         |
| 115 | Raman scattering and high temperature ferromagnetism of Mn-doped ZnO nanoparticles. Applied Physics Letters, 2006, 88, 252502.   | 3.3 | 224       |
| 116 | The influence of the additional confining potentials on ferromagnetism in III-V digital ferromagnetic heterostructures. Journal of Applied Physics, 2006, 99, 113903.                              | 2.5 | 6         |
| 117 | Relaxations and bonding mechanism in Hg <sub>1-x</sub> Cd <sub>x</sub> Te with mercury vacancy defect: First-principles study. Physical Review B, 2006, 73, .                                      | 3.2 | 18        |
| 118 | Formation Energy of Arsenic Impurities in MCT: First-Principles Study. , 2006, , .   |     | 0         |
| 119 | First principle study on the bonding mechanism of nanoring structure Ga <sub>8</sub> As <sub>8</sub> . European Physical Journal D, 2005, 34, 47-50.   | 1.3 | 5         |
| 120 | Structural and magnetic properties of ultrathin bcc Fe films on Ge(001). Journal Physics D: Applied Physics, 2005, 38, 1055-1060.  | 2.8 | 1         |
| 121 | FERROMAGNETISM IN Co-DOPED TiO <sub>2</sub> ANATASE DUE TO THE COBALT CLUSTERING. International Journal of Modern Physics B, 2005, 19, 2520-2525.  | 2.0 | 0         |
| 122 | Structural and electronic properties of their situ impurity As <sub>1-x</sub> Hg <sub>x</sub> in Hg <sub>0.5</sub> Cd <sub>0.5</sub> Te: First-principles study. Physical Review B, 2005, 71, .    | 3.2 | 20        |
| 123 | Ferromagnetism of 3d-impurities substituted in Ge. Journal of Magnetism and Magnetic Materials, 2004, 284, 253-259.  | 2.3 | 8         |
| 124 | Local structural distortions and Mn random distributions in (Ga,Mn)As: A first-principles study. Physical Review B, 2004, 69, .  | 3.2 | 12        |
| 125 | Electronic band structure of Nb doped SrTiO <sub>3</sub> from first principles calculation. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 317, 501-506.               | 2.1 | 70        |
| 126 | Nanoring structure and optical properties of Ga <sub>8</sub> As <sub>8</sub> . Chemical Physics Letters, 2003, 381, 397-403.   | 2.6 | 150       |



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|-----|--|-----|-----------|
| 127 | Computational discovery of spin-polarized semimetals in spinel materials. Materials Advances, 0, , . | 5.4 | 0         |