# Mingwen Zhao

List of Publications by Year
in descending order

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|---|---|---|---|
| 363 papers | 13,985 citations | 23500 58 h-index | 33814 99 g-index |
| 365 all docs | 365 docs citations | 365 times ranked | 13627 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Two-dimensional Dirac materials: Tight-binding lattice models and material candidates. ChemPhysMater, 2023, 2, 30-42. | 1.4 | 15 |
| 2 | Efficient anisotropic desalination by layer-stacked black phosphorus carbide (Î±-PC) membrane. Desalination, 2022, 522, 115422. | 4.0 | 9 |
| 3 | Ferromagnetic coupling in a two-dimensional Cairo pentagonal Ni2(TCNQ)2 lattice. Journal of Materiomics, 2022, 8, 627-632. | 2.8 | 1 |
| 4 | Ultrafine zirconium boride nanoparticles constructed bidirectional catalyst for ultrafast and long-lived lithium-sulfur batteries. Energy Storage Materials, 2022, 45, 130-141. | 9.5 | 34 |
| 5 | pH-switchable nanozyme cascade catalysis: a strategy for spatialâ€“temporal modulation of pathological wound microenvironment to rescue stalled healing in diabetic ulcer. Journal of Nanobiotechnology, 2022, 20, 12. | 4.2 | 50 |
| 6 | Nanophysical Antimicrobial Strategies: A Rational Deployment of Nanomaterials and Physical Stimulations in Combating Bacterial Infections. Advanced Science, 2022, 9, e2105252. | 5.6 | 56 |
| 7 | Structural and energetic features of the dimerization of the main proteinase of SARS-CoV-2 using molecular dynamic simulations. Physical Chemistry Chemical Physics, 2022, 24, 4324-4333. | 1.3 | 2 |
| 8 | Highly-anisotropic plasmons in two-dimensional hyperbolic copper borides. Optics Express, 2022, 30, 5596. | 1.7 | 6 |
| 9 | Manipulating Electrocatalytic Polysulfide Redox Kinetics by 1D Coreâ€“Shell Like Composite for Lithiumâ€“Sulfur Batteries. Advanced Energy Materials, 2022, 12, . | 10.2 | 47 |
| 10 | Screening of Transition-Metal Single-Atom Catalysts Anchored on Covalentâ€“Organic Frameworks for Efficient Nitrogen Fixation. ACS Applied Materials & Interfaces, 2022, 14, 1024-1033. | 4.0 | 32 |
| 11 | Sub-nanometer-sized carbon nanoparticle shows higher biocompatibility to DNA than nanometer-sized nanoparticles. Journal Physics D: Applied Physics, 2022, 55, 295401. | 1.3 | 1 |
| 12 | Strain-tunable self-passivated porous phosphorene for high-efficiency helium separation. Journal Physics D: Applied Physics, 2022, 55, 315501. | 1.3 | 1 |
| 13 | Photocatalytic hydrogen production and storage in carbon nanotubes: a first-principles study. RSC Advances, 2022, 12, 17029-17035. | 1.7 | 6 |
| 14 | Two-dimensional transition metal borides as highly efficient N2 fixation catalysts. Applied Surface Science, 2021, 536, 147742. | 3.1 | 58 |
| 15 | Anomalous plasmons in a two-dimensional Dirac nodal-line Lieb lattice. Nanoscale Advances, 2021, 3, 1127-1135. | 2.2 | 6 |
| 16 | Multi-functional photocatalytic activity of transition-metal tetraaza[14]annulene frameworks. Journal of Materials Chemistry A, 2021, 9, 4221-4229. | 5.2 | 12 |
| 17 | Photo-assisted high performance single atom electrocatalysis of the N<sub>2</sub> reduction reaction by a Mo-embedded covalent organic framework. Journal of Materials Chemistry A, 2021, 9, 19949-19957. | 5.2 | 27 |
| 18 | Key residues of the receptor binding domain in the spike protein of SARS-CoV-2 mediating the interactions with ACE2: a molecular dynamics study. Nanoscale, 2021, 13, 9364-9370. | 2.8 | 22 |

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|---|---|---|---|
| 19 | Interface-enhanced CO<sub>2</sub> capture via the synthetic effects of a nanomaterial-supported ionic liquid thin film. Nanoscale Advances, 2021, 3, 1397-1403. | 2.2 | 9 |
| 20 | Spontaneous DNA translocation through a van der Waals heterostructure nanopore for single-molecule detection. Nanoscale Advances, 2021, 3, 5941-5947. | 2.2 | 12 |
| 21 | Giant negative Poisson's ratio in two-dimensional V-shaped materials. Nanoscale Advances, 2021, 3, 4554-4560. | 2.2 | 15 |
| 22 | Defect effects and electronic structure regulation in low-dimensional materials. Chinese Science Bulletin, 2021, 66, 1998-2009. | 0.4 | 0 |
| 23 | Floquetâ€“Dirac fermions in monolayer graphene by Wannier functions. Journal of Physics Condensed Matter, 2021, 33, 145701. | 0.7 | 2 |
| 24 | Prediction of intrinsic topological superconductivity in Mn-doped GeTe monolayer from first-principles. Npj Computational Materials, 2021, 7, . | 3.5 | 15 |
| 25 | Defect-Induced Double-Stranded DNA Unwinding on Graphene. Journal of Physical Chemistry B, 2021, 125, 2833-2840. | 1.2 | 6 |
| 26 | Monolayer Fe<sub>3</sub>GeX<sub>2</sub> (X = S, Se, and Te) as Highly Efficient Electrocatalysts for Lithiumâ€“Sulfur Batteries. ACS Applied Materials & Interfaces, 2021, 13, 11845-11851. | 4.0 | 45 |
| 27 | Prediction of crossing nodal-lines and large intrinsic spin Hall conductivity in topological Dirac semimetal Ta3As family. Npj Computational Materials, 2021, 7, . | 3.5 | 14 |
| 28 | Direct Z-scheme photocatalytic CO2 conversion to solar fuels in a two-dimensional C2N/aza-CMP heterostructure. Applied Surface Science, 2021, 541, 148630. | 3.1 | 19 |
| 29 | Inâ€situ Nanoâ€Crystallization and Solvation Modulation to Promote Highly Stable Anode Involving Alloy/Deâ€alloy for Potassium Ion Batteries. Angewandte Chemie - International Edition, 2021, 60, 15381-15389. | 7.2 | 54 |
| 30 | Inâ€situ Nanoâ€Crystallization and Solvation Modulation to Promote Highly Stable Anode Involving Alloy/Deâ€alloy for Potassium Ion Batteries. Angewandte Chemie, 2021, 133, 15509-15517. | 1.6 | 7 |
| 31 | Efficient isotropic water desalination in anisotropic lamellar nano-channels formed by layered black phosphorus membrane. Desalination, 2021, 504, 114962. | 4.0 | 16 |
| 32 | Frontispiz: Inâ€situ Nanoâ€Crystallization and Solvation Modulation to Promote Highly Stable Anode Involving Alloy/Deâ€alloy for Potassium Ion Batteries. Angewandte Chemie, 2021, 133, . | 1.6 | 0 |
| 33 | Frontispiece: Inâ€situ Nanoâ€Crystallization and Solvation Modulation to Promote Highly Stable Anode Involving Alloy/Deâ€alloy for Potassium Ion Batteries. Angewandte Chemie - International Edition, 2021, 60, . | 7.2 | 1 |
| 34 | Construction and electrochemical mechanism investigation of hierarchical coreâ€”shell like composite as high performance anode for potassium ion batteries. Nano Research, 2021, 14, 3552-3561. | 5.8 | 21 |
| 35 | Stable multifunctional single-atom catalysts adsorbed on pyrazine-modified graphyne. Applied Surface Science, 2021, 553, 149464. | 3.1 | 32 |
| 36 | Highly Efficient Photocatalytic CO<sub>2</sub> Reduction in Two-Dimensional Ferroelectric CuInP<sub>2</sub>S<sub>6</sub> Bilayers. ACS Applied Materials & Interfaces, 2021, 13, 34486-34494. | 4.0 | 39 |

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|---|---|---|---|
| 37 | Undamped plasmon modes and enhanced superconductivity in metal diborides. New Journal of Physics, 2021, 23, 073036. | 1.2 | 3 |
| 38 | Multiple Dirac cones and Lifshitz transition in a two-dimensional Cairo lattice as a Hawking evaporation analogue. Journal of Physics Condensed Matter, 2021, 33, 365001. | 0.7 | 5 |
| 39 | Spin-Gapless States in Two-Dimensional Molecular Ferromagnet Fe<sub>2</sub>(TCNQ)<sub>2</sub>. Journal of Physical Chemistry Letters, 2021, 12, 7921-7927. | 2.1 | 4 |
| 40 | Laser-driven anisotropic and nonlinear Rashba spin splitting in GaAs monolayer. Physical Review B, 2021, 104, . | 1.1 | 1 |
| 41 | Bi-atom active sites embedded in a two-dimensional covalent organic framework for efficient nitrogen reduction reaction. Applied Surface Science, 2021, 563, 150352. | 3.1 | 25 |
| 42 | Regulating polysulfide intermediates by ultrathin Co-Bi nanosheet electrocatalyst in lithiumâ˜sulfur batteries. Nano Today, 2021, 40, 101246. | 6.2 | 34 |
| 43 | The role of sp-hybridized boron atoms in the highly efficient photocatalytic N<sub>2</sub> reduction activity of boron-doped triphenyleneâ€“graphdiyne. Journal of Materials Chemistry A, 2021, 9, 26077-26085. | 5.2 | 12 |
| 44 | Self-assembly of ultra-small-sized carbon nanoparticles in lipid membrane disrupts its integrity. Nanoscale Advances, 2021, 4, 163-172. | 2.2 | 6 |
| 45 | Corrugation effect, Dirac cone splitting, and plasmon properties of biased twisted bilayer graphene. Physical Review B, 2021, 104, . | 1.1 | 4 |
| 46 | OnionNet-2: A Convolutional Neural Network Model for Predicting Protein-Ligand Binding Affinity Based on Residue-Atom Contacting Shells. Frontiers in Chemistry, 2021, 9, 753002. | 1.8 | 39 |
| 47 | Floquet-engineered half-valley-metal state in two-dimensional gapped Dirac materials. Physical Review B, 2021, 104, . | 1.1 | 4 |
| 48 | New Spiral Form of Carbon Nitride with Ultrasoftness and Tunable Electronic Structures. ACS Omega, 2021, 6, 516-522. | 1.6 | 3 |
| 49 | Efficient Helium Separation with Two-Dimensional Metalâ€“Organic Framework Fe/Ni-PTC: A Theoretical Study. Membranes, 2021, 11, 927. | 1.4 | 1 |
| 50 | Robust broadband directional plasmons in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>MoO</mml:mi><mml:msub><mml:mi>Cl</mml:mi><mml monolayer. Physical Review B, 2021, 104, . | 1.1 | 9 |
| 51 | Two-dimensional XC<sub>6</sub>-enes (X = Ge, Sn, Pb) with moderate band gaps, biaxial negative Poisson's ratios, and high carrier mobility. Physical Chemistry Chemical Physics, 2021, 23, 26468-26475. | 1.3 | 2 |
| 52 | Prediction of topological superconductivity from type-IV, -III, -II, and -Iâ€² nodal points induced by Rashba spin-orbit coupling. Physical Review B, 2021, 104, . | 1.1 | 4 |
| 53 | Two-Dimensional Conductive Metalâ€“Organic Frameworks as Highly Efficient Electrocatalysts for Lithiumâ€“Sulfur Batteries. ACS Applied Materials & Interfaces, 2021, 13, 61205-61214. | 4.0 | 15 |
| 54 | Highly-efficient overall water splitting in 2D Janus group-III chalcogenide multilayers: the roles of intrinsic electric filed and vacancy defects. Science Bulletin, 2020, 65, 27-34. | 4.3 | 54 |

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|---|---|---|---|
| 55 | Metal-free highly efficient photocatalysts for overall water splitting: C<sub>3</sub>N<sub>5</sub> multilayers. Nanoscale, 2020, 12, 306-315. | 2.8 | 57 |
| 56 | Tunable ferroelectricity and antiferromagnetism via ferroelastic switching in an FeOOH monolayer. Journal of Materials Chemistry C, 2020, 8, 13982-13989. | 2.7 | 18 |
| 57 | Tunable valley splitting and anomalous valley Hall effect in VTe<sub>2</sub>/Ga<sub>2</sub>S<sub>3</sub> heterostructures. Journal of Materials Chemistry C, 2020, 8, 14895-14901. | 2.7 | 16 |
| 58 | Stable Multifunctional Single-Atom Catalysts Resulting from the Synergistic Effect of Anchored Transition-Metal Atoms and Host Covalentâ€“Organic Frameworks. Journal of Physical Chemistry C, 2020, 124, 17675-17683. | 1.5 | 46 |
| 59 | Serendipity for Topological Insulator as Multifunctional Electrocatalyst. ACS Applied Energy Materials, 2020, 3, 8929-8936. | 2.5 | 5 |
| 60 | Computational studies on triphenyldiyne as a two-dimensional visible-light-driven photocatalyst for overall water splitting. Physical Chemistry Chemical Physics, 2020, 22, 20061-20068. | 1.3 | 4 |
| 61 | Mild lipid extraction and anisotropic cell membrane penetration of Î±-phase phosphorene carbide nanoribbons by molecular dynamics simulation studies. Physical Chemistry Chemical Physics, 2020, 22, 23268-23275. | 1.3 | 7 |
| 62 | Tuning the binding behaviors of a protein YAP65WW domain on graphenic nano-sheets with boron or nitrogen atom doping. Nanoscale Advances, 2020, 2, 4539-4546. | 2.2 | 7 |
| 63 | Transition-metal monochalcogenide nanowires: highly efficient bi-functional catalysts for the oxygen evolution/reduction reactions. Nanoscale, 2020, 12, 12883-12890. | 2.8 | 8 |
| 64 | Ferroelectricity and multiferroicity in two-dimensional Sc<sub>2</sub>P<sub>2</sub>Se<sub>6</sub> and ScCrP<sub>2</sub>Se<sub>6</sub> monolayers. Physical Chemistry Chemical Physics, 2020, 22, 7489-7496. | 1.3 | 17 |
| 65 | Synergistic trifunctional electrocatalysis of pyridinic nitrogen and single transition-metal atoms anchored on pyrazine-modified graphdiyne. Science Bulletin, 2020, 65, 995-1002. | 4.3 | 34 |
| 66 | Tunable Valley Polarization in a Multiferroic CuCrP<sub>2</sub>Te<sub>6</sub> Monolayer. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000008. | 1.2 | 13 |
| 67 | Anisotropic protein diffusion on nanosurface. Nanoscale, 2020, 12, 5209-5216. | 2.8 | 15 |
| 68 | Multifunctional electrocatalytic activity of coronene-based two-dimensional metal-organic frameworks: TM-PTC. Applied Surface Science, 2020, 511, 145393. | 3.1 | 18 |
| 69 | Orientational DNA binding and directed transport on nanomaterial heterojunctions. Nanoscale, 2020, 12, 5217-5226. | 2.8 | 29 |
| 70 | High-efficiency helium separation through an inorganic graphenylene membrane: a theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 9789-9795. | 1.3 | 32 |
| 71 | Understanding CO2 capture kinetics and energetics by ionic liquids with molecular dynamics simulation. RSC Advances, 2020, 10, 13968-13974. | 1.7 | 7 |
| 72 | Prediction of a ternary two-dimensional pentagonal Zn2C2P2 monolayer for photocatalytic water splitting with high carriers mobility. Applied Surface Science, 2020, 518, 146197. | 3.1 | 13 |

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|---|---|---|---|
| 73 | Bifunctional HER/OER or OER/ORR Catalytic Activity of Two-Dimensional TM<sub>3</sub>(HITP)<sub>2</sub> with TM = Feâ€“Zn. Journal of Physical Chemistry C, 2020, 124, 9350-9359. | 1.5 | 67 |
| 74 | Inversion/Mirror Symmetry-Protected Dirac Cones in Distorted Ruby Lattices. Chinese Physics Letters, 2020, 37, 127102. | 1.3 | 2 |
| 75 | Low-loss hyperbolic dispersion and anisotropic plasmonic excitation in nodal-line semimetallic yttrium nitride. Optics Express, 2020, 28, 22076. | 1.7 | 8 |
| 76 | Strain-tunable CO<sub>2</sub> storage by black phosphorene and Î±-PC from combined first principles and molecular dynamics studies. Physical Chemistry Chemical Physics, 2019, 21, 20107-20117. | 1.3 | 11 |
| 77 | First-principles design of highly-efficient earth-abundant electrocatalysts for hydrogen evolution reaction: TiF3 and its analogs. Applied Surface Science, 2019, 495, 143623. | 3.1 | 13 |
| 78 | Spontaneous full photocatalytic water splitting on 2D MoSe<sub>2</sub>/SnSe<sub>2</sub> and WSe<sub>2</sub>/SnSe<sub>2</sub> vdW heterostructures. Nanoscale, 2019, 11, 14836-14843. | 2.8 | 156 |
| 79 | Enhancing superconductivity in bulk Î²â˜Bi2Pd by negative pressure induced by quantum electronic stress. Physical Review B, 2019, 100, . | 1.1 | 4 |
| 80 | Bifunctional Electrocatalytic Activity of Bis(iminothiolato)nickel Monolayer for Overall Water Splitting. Journal of Physical Chemistry C, 2019, 123, 25651-25656. | 1.5 | 17 |
| 81 | Dirac cones in a snub trihexagonal tiling lattice with reflective symmetry breaking. Journal of Physics Condensed Matter, 2019, 31, 155001. | 0.7 | 5 |
| 82 | Valley polarization and ferroelectricity in a two-dimensional GaAsC<sub>6</sub> monolayer. Physical Chemistry Chemical Physics, 2019, 21, 3954-3959. | 1.3 | 7 |
| 83 | Intrinsic multiferroicity in two-dimensional VOCl<sub>2</sub> monolayers. Nanoscale, 2019, 11, 1103-1110. | 2.8 | 62 |
| 84 | Porous-hollow nanorods constructed from alternate intercalation of carbon and MoS2 monolayers for lithium and sodium storage. Nano Research, 2019, 12, 1912-1920. | 5.8 | 39 |
| 85 | Tuning the electronic and magnetic properties of MoS2 nanotubes with vacancy defects. RSC Advances, 2019, 9, 17203-17210. | 1.7 | 12 |
| 86 | Tungsten boride: a 2D multiple Dirac semimetal for the hydrogen evolution reaction. Journal of Materials Chemistry C, 2019, 7, 8868-8873. | 2.7 | 52 |
| 87 | Hydrogen Confined in a Single Wall Carbon Nanotube Becomes a Metallic and Superconductive Nanowire under High Pressure. Nano Letters, 2019, 19, 2537-2542. | 4.5 | 9 |
| 88 | Two-dimensional graphyne-like carbon nitrides: Moderate band gaps, high carrier mobility, high flexibility and type-II band alignment. Carbon, 2019, 149, 234-241. | 5.4 | 38 |
| 89 | Li-III-VI bilayers for efficient photocatalytic overall water splitting: the role of intrinsic electric field. Journal of Materials Chemistry A, 2019, 7, 26123-26130. | 5.2 | 40 |
| 90 | Serendipity of a topological nontrivial band gap in the 2D borophene subunit lattice with broken mirror symmetry. Physical Chemistry Chemical Physics, 2019, 21, 22526-22530. | 1.3 | 1 |

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|---|---|---|---|
| 91 | Prediction of a flexible anode material for Li/Na ion batteries: Phosphorous carbide monolayer (Î±-PC). Carbon, 2019, 141, 444-450. | 5.4 | 70 |
| 92 | A Photoresponsive Rutile TiO<sub>2</sub> Heterojunction with Enhanced Electronâ€“Hole Separation for Highâ€Performance Hydrogen Evolution. Advanced Materials, 2019, 31, e1806596. | 11.1 | 240 |
| 93 | Promotion of Overall Water Splitting Activity Over a Wide pH Range by Interfacial Electrical Effects of Metallic NiCoâ€nitrides Nanoparticle/NiCo<sub>2</sub>O<sub>4</sub> Nanoflake/graphite Fibers. Advanced Science, 2019, 6, 1801829. | 5.6 | 122 |
| 94 | An unprecedented high-temperature-tolerance 2D laminar MXene membrane for ultrafast hydrogen sieving. Journal of Membrane Science, 2019, 569, 117-123. | 4.1 | 87 |
| 95 | Reversible out-of-plane spin texture in a two-dimensional ferroelectric material for persistent spin helix. Physical Review Materials, 2019, 3, . | 0.9 | 39 |
| 96 | Hyperbolic dispersion and negative refraction in a metal-organic framework Cu-BHT. Physical Review Materials, 2019, 3, . | 0.9 | 9 |
| 97 | Tunable broadband hyperbolic light dispersion in metal diborides. Optics Express, 2019, 27, 36911. | 1.7 | 12 |
| 98 | Strain-induced tunable negative differential resistance in triangle graphene spirals. Nanotechnology, 2018, 29, 205202. | 1.3 | 6 |
| 99 | Novel Conductive Metalâ€“Organic Framework for a High-Performance Lithiumâ€“Sulfur Battery Host: 2D Cu-Benzenehexathial (BHT). ACS Applied Materials & Interfaces, 2018, 10, 15012-15020. | 4.0 | 105 |
| 100 | Topological states in a two-dimensional metal alloy in Si surface: BiAg/Si(111)- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>4</mml:mn></mml surface. Physical Review B, 2018, 97, . | 1.1 | 10 |
| 101 | Kane Fermion in a Two-Dimensional Ï€-Conjugated Bis(iminothiolato)nickel Monolayer. Journal of Physical Chemistry Letters, 2018, 9, 614-619. | 2.1 | 25 |
| 102 | Promising half-metallicity in ductile NbF<sub>3</sub>: a first-principles prediction. Physical Chemistry Chemical Physics, 2018, 20, 4781-4786. | 1.3 | 10 |
| 103 | Zr<sub>2</sub>Si: an antiferromagnetic Dirac MXene. Physical Chemistry Chemical Physics, 2018, 20, 3946-3952. | 1.3 | 19 |
| 104 | Two-Dimensional Metalâ€“Organic Half-metallic Antiferromagnet: CoFePz. Journal of Physical Chemistry C, 2018, 122, 1846-1851. | 1.5 | 24 |
| 105 | Negative Poisson's ratio and high-mobility transport anisotropy in SiC<sub>6</sub>siligraphene. Nanoscale, 2018, 10, 2108-2114. | 2.8 | 51 |
| 106 | Silicene and germanene on InSe substrates: structures and tunable electronic properties. Physical Chemistry Chemical Physics, 2018, 20, 11369-11377. | 1.3 | 44 |
| 107 | PNTCDA: a promising versatile organic electrode material for alkali-metal ion batteries. Journal of Materials Chemistry A, 2018, 6, 24869-24876. | 5.2 | 11 |
| 108 | Theoretical Design of an InSe/GaTe vdW Heterobilayer: A Potential Visible-Light Photocatalyst for Water Splitting. Journal of Physical Chemistry C, 2018, 122, 27803-27810. | 1.5 | 55 |

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|---|---|---|---|
| 109 | Conductive and Polar Titanium Boride as a Sulfur Host for Advanced Lithiumâ€“Sulfur Batteries. Chemistry of Materials, 2018, 30, 6969-6977. | 3.2 | 101 |
| 110 | Electronic properties of a Ï€-conjugated Cairo pentagonal lattice: Direct band gap, ultrahigh carrier mobility, and slanted Dirac cones. Physical Review B, 2018, 98, . | 1.1 | 22 |
| 111 | Anchoring effects of S-terminated Ti2C MXene for lithium-sulfur batteries: A first-principles study. Applied Surface Science, 2018, 455, 522-526. | 3.1 | 134 |
| 112 | Irradiation resistance study of binderless nanopore-isotropic graphite for use in molten salt nuclear reactors. Nuclear Engineering and Design, 2018, 335, 231-240. | 0.8 | 7 |
| 113 | Direct Z-scheme photocatalytic overall water splitting on 2D CdS/InSe heterostructures. Journal Physics D: Applied Physics, 2018, 51, 395501. | 1.3 | 51 |
| 114 | Valley-selective circular dichroism and high carrier mobility of graphene-like BC<sub>6</sub>N. Nanoscale, 2018, 10, 13179-13186. | 2.8 | 37 |
| 115 | Predicting a graphene-like WB4 nanosheet with a double Dirac cone, an ultra-high Fermi velocity and significant gap opening by spinâ€“orbit coupling. Physical Chemistry Chemical Physics, 2017, 19, 5449-5453. | 1.3 | 40 |
| 116 | Ultrabroadband MoS<sub>2</sub> Photodetector with Spectral Response from 445 to 2717 nm. Advanced Materials, 2017, 29, 1605972. | 11.1 | 256 |
| 117 | Strain-Modulated Electronic Structure and Infrared Light Adsorption in Palladium Diselenide Monolayer. Scientific Reports, 2017, 7, 39995. | 1.6 | 39 |
| 118 | Gallium bismuth halide GaBi-X2 (X = I, Br, Cl) monolayers with distorted hexagonal framework: Novel room-temperature quantum spin Hall insulators. Nano Research, 2017, 10, 2168-2180. | 5.8 | 18 |
| 119 | Tuning of Interlayer Coupling in Large-Area Graphene/WSe<sub>2</sub> van der Waals Heterostructure via Ion Irradiation: Optical Evidences and Photonic Applications. ACS Photonics, 2017, 4, 1531-1538. | 3.2 | 75 |
| 120 | Efficient hydrogen isotopologues separation through a tunable potential barrier: The case of a C2N membrane. Scientific Reports, 2017, 7, 1483. | 1.6 | 21 |
| 121 | Dirac node lines in two-dimensional Lieb lattices. Nanoscale, 2017, 9, 8740-8746. | 2.8 | 46 |
| 122 | Cu<sub>3</sub>N and its analogs: a new class of electrodes for lithium ion batteries. Journal of Materials Chemistry A, 2017, 5, 8762-8768. | 5.2 | 29 |
| 123 | A niobium and tantalum co-doped perovskite cathode for solid oxide fuel cells operating below 500â€‰Â°C. Nature Communications, 2017, 8, 13990. | 5.8 | 180 |
| 124 | Low-energy transmission electron diffraction and imaging of large-area graphene. Science Advances, 2017, 3, e1603231. | 4.7 | 35 |
| 125 | Half-metallic TiF<sub>3</sub>: a potential anode material for Li-ion spin batteries. Journal of Materials Chemistry A, 2017, 5, 21486-21490. | 5.2 | 16 |
| 126 | Theoretical Discovery of a Superconducting Two-Dimensional Metalâ€“Organic Framework. Nano Letters, 2017, 17, 6166-6170. | 4.5 | 86 |

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|---|---|---|---|
| 127 | Efficient <sup>3</sup>He/<sup>4</sup>He separation in a nanoporous graphenylene membrane. Physical Chemistry Chemical Physics, 2017, 19, 21522-21526. | 1.3 | 9 |
| 128 | Theoretical Design of Highly Efficient CO<sub>2</sub>/N<sub>2</sub> Separation Membranes Based on Electric Quadrupole Distinction. Journal of Physical Chemistry C, 2017, 121, 17925-17931. | 1.5 | 15 |
| 129 | Metal-free Ternary BCN Nanosheets with Synergetic Effect of Band Gap Engineering and Magnetic Properties. Scientific Reports, 2017, 7, 6617. | 1.6 | 41 |
| 130 | Chern Insulator and Chern Half-Metal States in the Two-Dimensional Spin-Gapless Semiconductor Mn<sub>2</sub>C<sub>6</sub>S<sub>12</sub>. Journal of Physical Chemistry Letters, 2017, 8, 3770-3775. | 2.1 | 30 |
| 131 | A promising alkali-metal ion battery anode material: 2D metallic phosphorus carbide (Î²0-PC). Electrochimica Acta, 2017, 258, 582-590. | 2.6 | 40 |
| 132 | Tunable Dirac cones in two-dimensional covalent organic materials: C2N6S3 and its analogs. RSC Advances, 2017, 7, 52065-52070. | 1.7 | 9 |
| 133 | Dirac cones and highly anisotropic electronic structure of super-graphyne. Carbon, 2017, 113, 40-45. | 5.4 | 34 |
| 134 | Energetics of carbon and nitrogen impurities and their interactions with vacancy in vanadium. Chinese Physics B, 2016, 25, 036104. | 0.7 | 8 |
| 135 | Tunable C2N Membrane for High Efficient Water Desalination. Scientific Reports, 2016, 6, 29218. | 1.6 | 67 |
| 136 | Intrinsic currentâ€“voltage characteristics of metal-carbon nanotube networks: A first-principles study. Organic Electronics, 2016, 31, 278-286. | 1.4 | 5 |
| 137 | Prediction of an ultrasoft graphene allotrope with Dirac cones. Carbon, 2016, 105, 323-329. | 5.4 | 62 |
| 138 | Germanium sulfide nanosheet: a universal anode material for alkali metal ion batteries. Journal of Materials Chemistry A, 2016, 4, 8905-8912. | 5.2 | 188 |
| 139 | Band inversion and topological aspects in a TiNI monolayer. Physical Chemistry Chemical Physics, 2016, 18, 22154-22159. | 1.3 | 26 |
| 140 | Tunable topological states in electron-doped HTT-Pt. Physical Review B, 2016, 93, . | 1.1 | 38 |
| 141 | Electron spin-polarization and spin-gapless states in an oxidized carbon nitride monolayer. RSC Advances, 2016, 6, 108280-108285. | 1.7 | 0 |
| 142 | Highly Efficient Quantum Sieving in Porous Graphene-like Carbon Nitride for Light Isotopes Separation. Scientific Reports, 2016, 6, 19952. | 1.6 | 45 |
| 143 | Spin-polarized Dirac cones and topological nontriviality in a metalâ€“organic framework Ni<sub>2</sub>C<sub>24</sub>S<sub>6</sub>H<sub>12</sub>. Physical Chemistry Chemical Physics, 2016, 18, 8059-8064. | 1.3 | 48 |
| 144 | Gas Adsorption Effects on the Electronic Properties of Two-Dimensional Nickel Bis(dithiolene) Complex. Journal of Physical Chemistry C, 2016, 120, 3846-3852. | 1.5 | 31 |

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|---|---|---|---|
| 145 | Unusual electronic and mechanical properties of sodium chlorides at high pressures. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 1556-1561. | 0.9 | 2 |
| 146 | Strain-driven band inversion and topological aspects in Antimonene. Scientific Reports, 2015, 5, 16108. | 1.6 | 203 |
| 147 | Robust half-metallicity and topological aspects in two-dimensional Cu-TPyB. Scientific Reports, 2015, 5, 14098. | 1.6 | 29 |
| 148 | â€œChemical Weatheringâ€•Exfoliation of Atomâ€Thick Transition Metal Dichalcogenides and Their Ultrafast Saturable Absorption Properties. Advanced Functional Materials, 2015, 25, 5292-5299. | 7.8 | 69 |
| 149 | High hydrogen storage capacity in calciumâ€decorated silicene nanostructures. Physica Status Solidi (B): Basic Research, 2015, 252, 2072-2078. | 0.7 | 12 |
| 150 | Dumbbell stanane: a large-gap quantum spin hall insulator. Physical Chemistry Chemical Physics, 2015, 17, 16624-16629. | 1.3 | 25 |
| 151 | Intrinsic half-metallicity in fractal carbon nitride honeycomb lattices. Physical Chemistry Chemical Physics, 2015, 17, 21837-21844. | 1.3 | 14 |
| 152 | Role of edge dehydrogenation in magnetization and spin transport of zigzag graphene nanoribbons with line defects. Organic Electronics, 2015, 27, 212-220. | 1.4 | 5 |
| 153 | A comparative study of SrCo<sub>0.8</sub>Nb<sub>0.2</sub>O<sub>3â^Î´</sub>and SrCo<sub>0.8</sub>Ta<sub>0.2</sub>O<sub>3â^Î´</sub>as low-temperature solid oxide fuel cell cathodes: effect of non-geometry factors on the oxygen reduction reaction. Journal of Materials Chemistry A, 2015, 3, 24064-24070. | 5.2 | 52 |
| 154 | Tensile strain induced half-metallicity in graphene-like carbon nitride. Physical Chemistry Chemical Physics, 2015, 17, 6028-6035. | 1.3 | 45 |
| 155 | Giant Topological Nontrivial Band Gaps in Chloridized Gallium Bismuthide. Nano Letters, 2015, 15, 1296-1301. | 4.5 | 92 |
| 156 | Kinetics of Nonlinear Optical Response at Insulatorâ€“Metal Transition in Vanadium Dioxide. Advanced Optical Materials, 2015, 3, 64-70. | 3.6 | 9 |
| 157 | High activity and durability of novel perovskite electrocatalysts for water oxidation. Materials Horizons, 2015, 2, 495-501. | 6.4 | 128 |
| 158 | Stacking dependent electronic properties of the nanofilms composing of super-aligned single-walled carbon nanotubes. Journal Physics D: Applied Physics, 2015, 48, 215307. | 1.3 | 0 |
| 159 | Sulfur and nitrogen self-doped carbon nanosheets derived from peanut root nodules as high-efficiency non-metal electrocatalyst for hydrogen evolution reaction. Nano Energy, 2015, 16, 357-366. | 8.2 | 162 |
| 160 | Prediction of quantum anomalous Hall effect on graphene nanomesh. RSC Advances, 2015, 5, 9875-9880. | 1.7 | 26 |
| 161 | Driving a GaAs film to a large-gap topological insulator by tensile strain. Scientific Reports, 2015, 5, 8441. | 1.6 | 55 |
| 162 | Electron spin-polarization and band gap engineering in carbon-modified graphitic carbon nitrides. Journal of Materials Chemistry C, 2015, 3, 10886-10891. | 2.7 | 13 |

| # | Article | IF | Citations |
|---|---|---|---|
| 163 | Prediction of a large-gap quantum-spin-Hall insulator: Diamond-like GaBi bilayer. Nano Research, 2015, 8, 3823-3829. | 5.8 | 11 |
| 164 | Hydrogenation-induced large-gap quantum-spin-Hall insulator states in a germaniumâ€“tin dumbbell structure. RSC Advances, 2015, 5, 72462-72468. | 1.7 | 12 |
| 165 | Phagraphene: A Low-Energy Graphene Allotrope Composed of 5â€“6â€“7 Carbon Rings with Distorted Dirac Cones. Nano Letters, 2015, 15, 6182-6186. | 4.5 | 482 |
| 166 | Efficient helium separation of graphitic carbon nitride membrane. Carbon, 2015, 95, 51-57. | 5.4 | 115 |
| 167 | Large-Scale Synthesis of Few-Layer F-BN Nanocages with Zigzag-Edge Triangular Antidot Defects and Investigation of the Advanced Ferromagnetism. Nano Letters, 2015, 15, 8122-8128. | 4.5 | 30 |
| 168 | Spin-gapless semiconducting graphitic carbon nitrides: A theoretical design from first principles. Carbon, 2015, 84, 1-8. | 5.4 | 72 |
| 169 | Strain-induced phase transition and electron spin-polarization in graphene spirals. Scientific Reports, 2015, 4, 5699. | 1.6 | 17 |
| 170 | From UV to Nearâ€Infrared, WS<sub>2</sub> Nanosheet: A Novel Photocatalyst for Full Solar Light Spectrum Photodegradation. Advanced Materials, 2015, 27, 363-369. | 11.1 | 494 |
| 171 | Self-Organized Micro-Columns and Nano-Spheres Generated by Pulsed Laser Ablation of Ti/Al Alloy in Water. Chinese Physics Letters, 2014, 31, 015202. | 1.3 | 1 |
| 172 | Stoichiometry determined exchange interactions in amorphous ternary transition metal oxides: Theory and experiment. Journal of Applied Physics, 2014, 116, 043711. | 1.1 | 3 |
| 173 | Lattice match and lattice mismatch models of graphene on hexagonal boron nitride from first principles. Journal of Physics Condensed Matter, 2014, 26, 095002. | 0.7 | 24 |
| 174 | Manifold electronic structure transition of hybrid silicaneâ€“silicene nanoribbons. Chemical Physics Letters, 2014, 595-596, 20-24. | 1.2 | 9 |
| 175 | Direct characterization of ion implanted pyrolytic carbon coatings deposited from natural gas. Carbon, 2014, 68, 95-103. | 5.4 | 16 |
| 176 | Oneâ€Step Exfoliation and Fluorination of Boron Nitride Nanosheets and a Study of Their Magnetic Properties. Angewandte Chemie - International Edition, 2014, 53, 3645-3649. | 7.2 | 127 |
| 177 | Broadband Fewâ€Layer MoS<sub>2</sub> Saturable Absorbers. Advanced Materials, 2014, 26, 3538-3544. | 11.1 | 645 |
| 178 | The stability and electronic structure of Fe atoms embedded in zigzag graphene nanoribbons. Physica B: Condensed Matter, 2014, 441, 28-32. | 1.3 | 15 |
| 179 | A metallic carbon allotrope with superhardness: a first-principles prediction. Journal of Materials Chemistry C, 2014, 2, 2751-2757. | 2.7 | 40 |
| 180 | Theoretical characterization of layered silica nanostructures from first-principles prediction. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 3348-3353. | 0.9 | 8 |

| # | Article | IF | Citations |
|---|---|---|---|
| 181 | Electron spin-polarization and spin lattices in the boron- and nitrogen-doped organic framework COF-5. Physical Chemistry Chemical Physics, 2014, 16, 23286-23291. | 1.3 | 17 |
| 182 | Structures, Energetics, and Electronic Properties of Multifarious Stacking Patterns for High-Buckled and Low-Buckled Silicene on the MoS<sub>2</sub> Substrate. Journal of Physical Chemistry C, 2014, 118, 19129-19138. | 1.5 | 76 |
| 183 | Two-dimensional topological insulators with binary honeycomb lattices:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Si</mml:mi><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>siligraphene and its analogs. Physical Review B, 2014, 89, . | 1.1 | 83 |
| 184 | Effect of the alloying element titanium on the stability and trapping of hydrogen in pure vanadium: A first-principles study. International Journal of Modern Physics B, 2014, 28, 1450207. | 1.0 | 16 |
| 185 | Topological insulator states in a honeycomb lattice of s-triazines. Nanoscale, 2014, 6, 11157-11162. | 2.8 | 79 |
| 186 | SiC coating: An alternative for the protection of nuclear graphite from liquid fluoride salt. Journal of Nuclear Materials, 2014, 448, 1-3. | 1.3 | 53 |
| 187 | Half-metallicity of C/BN hybrid nanoribbons containing a topological defective interface. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 60, 224-228. | 1.3 | 1 |
| 188 | Graphyne-based carbon allotropes with tunable properties: From Dirac fermion to semiconductor. Diamond and Related Materials, 2014, 41, 65-72. | 1.8 | 32 |
| 189 | Gold atom and dimer adsorbed on perfect and defective graphene and boron nitride monolayer: A first-principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 59, 235-242. | 1.3 | 9 |
| 190 | A comparative first-principles study of the electronic, mechanical, defect and acoustic properties of Ti<sub>2</sub>AlC and Ti<sub>3</sub>AlC. Journal Physics D: Applied Physics, 2014, 47, 215301. | 1.3 | 27 |
| 191 | Characterization of the effects of 3-MeV proton irradiation on fine-grained isotropic nuclear graphite. Carbon, 2014, 77, 311-318. | 5.4 | 30 |
| 192 | Spin memristive magnetic tunnel junctions with CoO-ZnO nano composite barrier. Scientific Reports, 2014, 4, 3835. | 1.6 | 21 |
| 193 | First-principles prediction of the transition from graphdiyne to a superlattice of carbon nanotubes and graphene nanoribbons. Carbon, 2013, 65, 341-348. | 5.4 | 52 |
| 194 | Protection of nuclear graphite toward liquid fluoride salt by isotropic pyrolytic carbon coating. Journal of Nuclear Materials, 2013, 442, 306-308. | 1.3 | 26 |
| 195 | Stable ferromagnetism and half-metallicity in two-dimensional polyporphyrin frameworks. RSC Advances, 2013, 3, 7016. | 1.7 | 43 |
| 196 | First-principles prediction of a new Dirac-fermion material: silicon germanide monolayer. Journal of Physics Condensed Matter, 2013, 25, 395501. | 0.7 | 35 |
| 197 | First-principles identifications of superstructures of germanene on Ag(111) surface and h-BN substrate. Physical Chemistry Chemical Physics, 2013, 15, 16853. | 1.3 | 56 |
| 198 | Three-dimensional diffusion of molecular hydrogen in graphdiyne: a first-principles study. Journal Physics D: Applied Physics, 2013, 46, 495307. | 1.3 | 21 |

| # | Article | IF | Citations |
|---|---|---|---|
| 199 | Irradiation-induced magnetic ordering in SiC: Experimental results and a density functional study. Applied Physics Letters, 2013, 103, 262409. | 1.5 | 13 |
| 200 | Tuning the electronic and magnetic properties of triangular boron nitride quantum dots via carbon doping. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 49, 52-60. | 1.3 | 17 |
| 201 | Spin-polarization and ferromagnetism of graphitic carbon nitride materials. Journal of Materials Chemistry C, 2013, 1, 6265. | 2.7 | 82 |
| 202 | Half-metallicity of a kagome spin lattice: the case of a manganese bis-dithiolene monolayer. Nanoscale, 2013, 5, 10404. | 2.8 | 84 |
| 203 | A Highly Active Perovskite Electrode for the Oxygen Reduction Reaction Below 600â€‰Â°C. Angewandte Chemie - International Edition, 2013, 52, 14036-14040. | 7.2 | 138 |
| 204 | Two-dimensional carbon topological insulators superior to graphene. Scientific Reports, 2013, 3, 3532. | 1.6 | 140 |
| 205 | Role of acetylenic bonds in the mechanical, electronic and optical properties of yne-diamonds. Diamond and Related Materials, 2013, 37, 55-63. | 1.8 | 9 |
| 206 | Spin-polarized zero-energy states in BN/C coreâ€“shell quantum dots. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 1102-1108. | 0.9 | 9 |
| 207 | Exfoliation of Hexagonal Boron Nitride by Molten Hydroxides. Advanced Materials, 2013, 25, 2200-2204. | 11.1 | 275 |
| 208 | Magnetic and optical properties of Cu-doped ZnO nanosheet: First-principles calculations. Physica E: Low-Dimensional Systems and Nanostructures, 2013, 53, 101-105. | 1.3 | 40 |
| 209 | Can cation vacancy defects induce room temperature ferromagnetism in GaN?. Applied Physics Letters, 2013, 102, 062411. | 1.5 | 28 |
| 210 | MoirÃ© superstructures of silicene on hexagonal boron nitride: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 2628-2632. | 0.9 | 51 |
| 211 | Graphdiyne: A promising anode material for lithium ion batteries with high capacity and rate capability. Journal of Applied Physics, 2013, 113, . | 1.1 | 131 |
| 212 | Formation and annealing behaviors of qubit centers in 4H-SiC from first principles. Journal of Applied Physics, 2013, 114, . | 1.1 | 18 |
| 213 | The mechanism of effect of lens-to-sample distance on laser-induced plasma. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 025203. | 0.2 | 7 |
| 214 | Adsorption and diffusion of gold adatoms on boron nitride nanoribbons: A first-principles study. Journal of Applied Physics, 2012, 112, . | 1.1 | 5 |
| 215 | Spin-polarization of VGaON center in GaN and its application in spin qubit. Applied Physics Letters, 2012, 100, 192401. | 1.5 | 25 |
| 216 | Is yne-diamond a super-hard material?. Europhysics Letters, 2012, 100, 56003. | 0.7 | 19 |

| # | Article | IF | Citations |
|---|---|---|---|
| 217 | Role of lens to sample distance during laser-induced damage in zinc targets. Laser Physics Letters, 2012, 9, 730-733. | 0.6 | 14 |
| 218 | Silicon Carbide Nanocages and Nanotubes: Analogs of Carbon Fullerenes and Nanotubes or Not?. Journal of Computational and Theoretical Nanoscience, 2012, 9, 1999-2007. | 0.4 | 5 |
| 219 | Tunable Hydrogen Separation in spâ€“sp<sup>2</sup> Hybridized Carbon Membranes: A First-Principles Prediction. Journal of Physical Chemistry C, 2012, 116, 16634-16638. | 1.5 | 135 |
| 220 | Isoelectronic Doping of Graphdiyne with Boron and Nitrogen: Stable Configurations and Band Gap Modification. Journal of Physical Chemistry A, 2012, 116, 3934-3939. | 1.1 | 142 |
| 221 | First-principles study of hydrogenated graphyne and its family: Stable configurations and electronic structures. Diamond and Related Materials, 2012, 29, 42-47. | 1.8 | 71 |
| 222 | Zinc oxide micro-spheres with faceted surfaces produced by laser ablation of zinc targets. Journal of Applied Physics, 2012, 111, 103108. | 1.1 | 10 |
| 223 | Hybrid density functional study of band alignment in ZnOâ€“GaN and ZnOâ€“(Ga1â^'xZnx)(N1â^'xOx)â€“GaN heterostructures. Physical Chemistry Chemical Physics, 2012, 14, 15693. | 1.3 | 46 |
| 224 | Ultra-high hydrogen storage capacity of Li-decorated graphyne: A first-principles prediction. Journal of Applied Physics, 2012, 112, . | 1.1 | 64 |
| 225 | First-principles study of electronic structure and magnetic properties of Cu-doped CeO2. Journal of Applied Physics, 2012, 112, . | 1.1 | 6 |
| 226 | Special structures and properties of hydrogen nanowire confined in a single walled carbon nanotube at extreme high pressure. AIP Advances, 2012, 2, 022161. | 0.6 | 2 |
| 227 | Effects of substrate temperature upon optical properties of ZnTe epilayers grown on (100) GaAs substrates by MOVPE. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 2041-2044. | 0.8 | 1 |
| 228 | The roles of Ï€ electrons in the electronic structures and optical properties of graphyne. Science Bulletin, 2012, 57, 3080-3085. | 1.7 | 15 |
| 229 | Characterization of regular periodic surface structure by multi-pulse laser irradiation of a Zinc target. Chinese Optics Letters, 2012, 10, 051402-51404. | 1.3 | 6 |
| 230 | Honeycomb-Patterned Quantum Dots beyond Graphene. Journal of Physical Chemistry C, 2011, 115, 17743-17749. | 1.5 | 25 |
| 231 | First-principles characterization of an AlSiVC center in cubic silicon carbide. Journal of Applied Physics, 2011, 110, 033711. | 1.1 | 9 |
| 232 | Tunable electronic structures of graphene/boron nitride heterobilayers. Applied Physics Letters, 2011, 98, . | 1.5 | 211 |
| 233 | Localized defects closely related with the magnetism of graphite induced by 12C+ ion implantation. Journal of Applied Physics, 2011, 109, 083933. | 1.1 | 4 |
| 234 | Investigating the ferromagnetic exchange interaction in Co-doped ZnO magnetic semiconductors. Scripta Materialia, 2011, 64, 864-867. | 2.6 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 235 | High Mobility and High Storage Capacity of Lithium in spâ€“sp<sup>2</sup> Hybridized Carbon Network: The Case of Graphyne. Journal of Physical Chemistry C, 2011, 115, 8845-8850. | 1.5 | 228 |
| 236 | An ab initio study on gas sensing properties of graphene and Si-doped graphene. European Physical Journal B, 2011, 81, 475-479. | 0.6 | 143 |
| 237 | Effect of native defects and Co doping on ferromagnetism in HfO<sub>2</sub>: Firstâ€principles calculations. Journal of Computational Chemistry, 2011, 32, 1298-1302. | 1.5 | 7 |
| 238 | Enhancing the ferromagnetization of graphite by successive 12C+ ion implantation steps. Carbon, 2011, 49, 1931-1938. | 5.4 | 19 |
| 239 | Structural and electronic properties of ZnS/ZnO heteronanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1522-1527. | 1.3 | 7 |
| 240 | Possible origin of ferromagnetism in un-doped ZnO: First-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 638-641. | 0.9 | 13 |
| 241 | Theoretical insights into the built-in electric field and band offsets of BN/C heterostructured zigzag nanotubes. Journal Physics D: Applied Physics, 2011, 44, 095405. | 1.3 | 19 |
| 242 | Manifold electronic structure transition of BNC biribbons. Journal of Applied Physics, 2011, 110, . | 1.1 | 30 |
| 243 | Proton inelastic mean free path in a group of bioorganic compounds and water in 0.05â€“10 MeV range â€“ Including higher-order corrections. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 2337-2342. | 0.6 | 9 |
| 244 | Neutral vacancy-defect-induced magnetism in SiC monolayer. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 2451-2454. | 1.3 | 26 |
| 245 | Tight-binding model for the electronic structures of SiC and BN nanoribbons. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 43, 440-445. | 1.3 | 59 |
| 246 | Atomic-scale characterization of silicon diffusion on carbon nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 43, 610-613. | 1.3 | 3 |
| 247 | Concentration dependent magnetism induced by hydrogen adsorption on graphene and single walled carbon nanotubes. Journal of Magnetism and Magnetic Materials, 2010, 322, 838-843. | 1.0 | 16 |
| 248 | Proton inelastic mean free path in amino acids and protein over the energy range of 0.05â€“10 MeV. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 2606-2610. | 0.6 | 3 |
| 249 | Size-dependent structural and electronic properties of ZnS nanofilms: An ab initio study. Journal of Applied Physics, 2010, 108, 064317. | 1.1 | 13 |
| 250 | Tuning Bandgap of Si-C Heterofullerene-Based Aanotubes by H Adsorption. Chinese Physics Letters, 2010, 27, 097101. | 1.3 | 0 |
| 251 | Energetic Evolution of Single-Crystalline ZnO Nanowires and Nanotubes. Chinese Physics Letters, 2010, 27, 086105. | 1.3 | 3 |
| 252 | Proton Inelastic Mean Free Path in a Group of Organic Materials in 0.05â€“10 MeV Range. Chinese Physics Letters, 2010, 27, 113403. | 1.3 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 253 | Tunable rectification and giant positive magnetoresistance in Ge1â^'xMnx/Ge epitaxial heterojunction diodes. Journal of Applied Physics, 2010, 107, . | 1.1 | 8 |
| 254 | Ferromagnetic ordering of silicon vacancies in N-doped silicon carbide. Applied Physics Letters, 2010, 96, . | 1.5 | 44 |
| 255 | Long-ranged and high temperature ferromagnetism in (Mn,C)-codoped ZnO studied by first-principles calculations. Journal of Applied Physics, 2010, 107, 033903. | 1.1 | 20 |
| 256 | Vacancy-defectâ€"derived magnetism in titanium oxide nanosheet: A first-principles study. Europhysics Letters, 2010, 90, 66005. | 0.7 | 4 |
| 257 | Orientation-selective unzipping of carbon nanotubes. Physical Chemistry Chemical Physics, 2010, 12, 13674. | 1.3 | 18 |
| 258 | Natural charge spatial separation and quantum confinement of ZnO/GaN-core/shell nanowires. Journal of Applied Physics, 2010, 108, 123707. | 1.1 | 12 |
| 259 | First-Principles Study of Titania Nanoribbons: Formation, Energetics, and Electronic Properties. Journal of Physical Chemistry C, 2010, 114, 9234-9238. | 1.5 | 17 |
| 260 | Controllable spin-polarized electrical transport in wide-band-gap oxide ferromagnetic semiconductors. Journal of Applied Physics, 2010, 107, . | 1.1 | 10 |
| 261 | First-principles prediction of the negatively-charged nitrogen-silicon-vacancy center in cubic silicon carbide. Journal of Applied Physics, 2010, 108, . | 1.1 | 15 |
| 262 | Diffusion and coalescence of vacancies and interstitials in graphite: A first-principles study. Diamond and Related Materials, 2010, 19, 1240-1244. | 1.8 | 66 |
| 263 | Rhodium atoms confined in boron nitride nanotubes: Density functional calculations. Europhysics Letters, 2010, 90, 47003. | 0.7 | 2 |
| 264 | Electronic properties of BN/C nanotube heterostructures. Journal of Applied Physics, 2010, 107, . | 1.1 | 34 |
| 265 | Hydrogen saturation stabilizes vacancy-induced ferromagnetic ordering in graphene. Physical Chemistry Chemical Physics, 2010, 12, 13699. | 1.3 | 31 |
| 266 | Temporal and spatial evolution of Si atoms in plasmas produced by a nanosecond laser ablating silicon carbide crystals. Physical Review E, 2009, 80, 016405. | 0.8 | 15 |
| 267 | First-principles identification of two- and four-membered-ring hybrid structures of silica nanorings. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 4376-4380. | 0.9 | 1 |
| 268 | First-principles study of cobalt silicide nanosheet and nanotubes: Stability and electronic properties. Physica E: Low-Dimensional Systems and Nanostructures, 2009, 41, 1795-1799. | 1.3 | 5 |
| 269 | A new calculation on the stopping power and mean free path for low energy electrons in toluene over energy range of 20â€"10 000 eV. Applied Radiation and Isotopes, 2009, 67, 625-629. | 0.7 | 12 |
| 270 | Correlation between the vacancy defects and ferromagnetism in graphite. Carbon, 2009, 47, 1399-1406. | 5.4 | 94 |

| # | Article | IF | Citations |
|---|---|---|---|
| 271 | Orientation-Dependent Stability and Quantum-Confinement Effects of Silicon Carbide Nanowires. Journal of Physical Chemistry C, 2009, 113, 12731-12735. | 1.5 | 27 |
| 272 | Early-stage evolution of the plasma over KTiOPO_4 samples generated by high-intensity laser radiations. Optics Letters, 2009, 34, 2682. | 1.7 | 10 |
| 273 | Energetic Minimum Structures of Imogolite Nanotubes: A First-Principles Prediction. Journal of Physical Chemistry C, 2009, 113, 14834-14837. | 1.5 | 28 |
| 274 | Layered Titanium Oxide Nanosheet and Ultrathin Nanotubes: A First-Principles Prediction. Journal of Physical Chemistry C, 2009, 113, 13610-13615. | 1.5 | 41 |
| 275 | Covalent-adsorption induced magnetism in graphene. Journal of Materials Chemistry, 2009, 19, 9274. | 6.7 | 58 |
| 276 | First-Principles Study of Faceted Single-Crystalline Silicon Carbide Nanowires and Nanotubes. Journal of Physical Chemistry C, 2009, 113, 856-861. | 1.5 | 17 |
| 277 | Tunable Magnetism in Carbonâ€ionâ€Implanted Highly Oriented Pyrolytic Graphite. Advanced Materials, 2008, 20, 4679-4683. | 11.1 | 103 |
| 278 | The dimension of the core and the tail of the plasma produced by laser ablating SiC targets. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 5891-5895. | 0.9 | 8 |
| 279 | Theoretical models of ZnS nanoclusters and nanotubes: First-principles calculations. Solid State Communications, 2008, 147, 165-168. | 0.9 | 20 |
| 280 | Electronic stopping power for proton in amino acids and protein in 0.05â€“10 MeV range. Nuclear Instruments & Methods in Physics Research B, 2008, 266, 1938-1942. | 0.6 | 11 |
| 281 | First-principles study of ZnS nanostructures: nanotubes, nanowires and nanosheets. Nanotechnology, 2008, 19, 305708. | 1.3 | 36 |
| 282 | Theoretical Insight into Faceted ZnS Nanowires and Nanotubes from Interatomic Potential and First-Principles Calculations. Journal of Physical Chemistry C, 2008, 112, 3509-3514. | 1.5 | 37 |
| 283 | From pure C60 to silicon carbon fullerene-based nanotube: An ab initio study. Journal of Chemical Physics, 2008, 128, 154719. | 1.2 | 10 |
| 284 | Ab Initio Calculations on the Magnetic Properties of Hydrogenated Boron Nitride Nanotubes. Journal of Physical Chemistry C, 2008, 112, 16231-16235. | 1.5 | 23 |
| 285 | The electronic structure evolution of DNA during its conformation transition process. Physical Chemistry Chemical Physics, 2008, 10, 5077. | 1.3 | 2 |
| 286 | Theoretical Models of Silica Nanorings: First-Principles Calculations. Journal of Physical Chemistry C, 2008, 112, 17071-17075. | 1.5 | 3 |
| 287 | First-principles study of Co-doped single-walled silicon nanotubes. Nanotechnology, 2008, 19, 205707. | 1.3 | 12 |
| 288 | The electronic structure of a single-walled aluminosilicate nanotube. Nanotechnology, 2008, 19, 175702. | 1.3 | 17 |

| # | Article | IF | Citations |
|---|---|---|---|
| 289 | Fluorination-induced magnetism in boron nitride nanotubes from ab initio calculations. Applied Physics Letters, 2008, 92, 102515. | 1.5 | 52 |
| 290 | Analysis of plasma profile over KTiOAsO4 surface produced by 532 and 1064 nm laser radiations. Journal of Applied Physics, 2008, 104, . | 1.1 | 3 |
| 291 | Theoretical prediction for the (AlN)<sub>12</sub>fullerene-like cage-based nanomaterials. Journal of Physics Condensed Matter, 2007, 19, 346228. | 0.7 | 17 |
| 292 | Surface structures and electronic states of silicon nanotubes stabilized by oxygen atoms. Journal of Applied Physics, 2007, 102, . | 1.1 | 7 |
| 293 | Faceted Silicon Nanotubes:â€‰ Structure, Energetic, and Passivation Effects. Journal of Physical Chemistry C, 2007, 111, 1234-1238. | 1.5 | 32 |
| 294 | Stabilizing Zigzag Single-Walled Silicon Nanotubes and Tailoring the Electronic Structures by Oxygen Atoms:â€‰ First-Principles Studies. Journal of Physical Chemistry C, 2007, 111, 2942-2946. | 1.5 | 8 |
| 295 | Geometric and Electronic Structures of Hydrogen-Stabilized Silicon Nitride Nanosheets and Nanotubes. Journal of Physical Chemistry C, 2007, 111, 16840-16845. | 1.5 | 10 |
| 296 | First-Principles Design of Well-Ordered Silica Nanotubes from Silica Monolayers and Nanorings. Journal of Physical Chemistry C, 2007, 111, 9652-9657. | 1.5 | 10 |
| 297 | From a fullerene-like cage (SiC)12 to novel silicon carbide nanowires: An ab initio study. Chemical Physics Letters, 2007, 442, 384-389. | 1.2 | 12 |
| 298 | Design and energetic characterization of ZnO clusters from first-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 372, 39-43. | 0.9 | 54 |
| 299 | Theoretical study of the Â· H reaction with cytosine. International Journal of Quantum Chemistry, 2007, 107, 240-246. | 1.0 | 3 |
| 300 | Structural characterization of fully coordinated ultrathin silica nanotubes by first-principles calculations. Physical Review B, 2006, 73, . | 1.1 | 21 |
| 301 | First-Principles Calculations of AlN Nanowires and Nanotubes:Â Atomic Structures, Energetics, and Surface States. Journal of Physical Chemistry B, 2006, 110, 8764-8768. | 1.2 | 72 |
| 302 | Theoretical study of hydrogen atom adsorbed on carbon-doped BN nanotubes. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 357, 369-373. | 0.9 | 56 |
| 303 | Functionalization of silicon-doped single walled carbon nanotubes at the doping site: An ab initio study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 358, 166-170. | 0.9 | 12 |
| 304 | Proton stopping power in a group of bioorganic compounds over the energy range of 0.05â€“10MeV. Nuclear Instruments & Methods in Physics Research B, 2006, 248, 1-6. | 0.6 | 31 |
| 305 | Electron stopping power and inelastic mean free path in amino acids and protein over the energy range of 20â€“20,000ÂeV. Radiation and Environmental Biophysics, 2006, 45, 135-143. | 0.6 | 28 |
| 306 | The effect of salt concentration on DNA conformation transition: a molecular-dynamics study. Journal of Molecular Modeling, 2006, 12, 249-254. | 0.8 | 11 |

| # | Article | IF | Citations |
|---|---|---|---|
| 307 | Silver-filled single-walled carbon nanotubes: Atomic and electronic structures from first-principles calculations. Physical Review B, 2006, 74, . | 1.1 | 14 |
| 308 | First-principlesLDA+Ucalculations of the Co-dopedZnOmagnetic semiconductor. Physical Review B, 2006, 73, . | 1.1 | 81 |
| 309 | Tuning the electronic structures of semiconducting SiC nanotubes by N and NHx (x=1,2) groups. Journal of Chemical Physics, 2006, 125, 194710. | 1.2 | 30 |
| 310 | Monte-Carlo simulation of low-energy electron scattering in PMMA â€“ using stopping powers from dielectric formalism. Microelectronic Engineering, 2005, 77, 285-291. | 1.1 | 22 |
| 311 | Curvature-induced condensation of lithium confined inside single-walled carbon nanotubes: First-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2005, 340, 434-439. | 0.9 | 42 |
| 312 | Theoretical study of the OH reaction with cytosine. Computational and Theoretical Chemistry, 2005, 723, 123-129. | 1.5 | 30 |
| 313 | Ab initio study of base-functionalized single walled carbon nanotubes. Chemical Physics Letters, 2005, 415, 183-187. | 1.2 | 24 |
| 314 | Monte Carlo simulation of interactions between energetic electron and cellulose film. Applied Surface Science, 2005, 246, 117-125. | 3.1 | 1 |
| 315 | An investigation of distribution parameters for fluorine ion implantation in indium-tin-oxide films. Applied Physics A: Materials Science and Processing, 2005, 81, 635-638. | 1.1 | 1 |
| 316 | Reactions of Â·OH with thymine studied using density functional theory. International Journal of Quantum Chemistry, 2005, 101, 211-218. | 1.0 | 26 |
| 317 | Self-assembly of base-functionalized carbon nanotubes. Physical Review B, 2005, 72, . | 1.1 | 9 |
| 318 | Manipulating the electronic structures of silicon carbide nanotubes by selected hydrogenation. Journal of Chemical Physics, 2005, 122, 214707. | 1.2 | 72 |
| 319 | Diffusion and condensation of lithium atoms in single-walled carbon nanotubes. Physical Review B, 2005, 71, . | 1.1 | 70 |
| 320 | Distribution patterns and controllable transport of water inside and outside charged single-walled carbon nanotubes. Journal of Chemical Physics, 2005, 122, 084708. | 1.2 | 46 |
| 321 | Strain energy and electronic structures of silicon carbide nanotubes: Density functional calculations. Physical Review B, 2005, 71, . | 1.1 | 239 |
| 322 | Enhancement of hydrogen physisorption on single-walled carbon nanotubes resulting from defects created by carbon bombardment. Physical Review B, 2005, 71, . | 1.1 | 19 |
| 323 | Density-functional theory calculations of XH3-decorated SiC nanotubes (X={C,Si}): Structures, energetics, and electronic structures. Journal of Applied Physics, 2005, 97, 104311. | 1.1 | 35 |
| 324 | Electron stopping power and mean free path in organic compounds over the energy range of 20â€“10,000 eV. Nuclear Instruments & Methods in Physics Research B, 2004, 222, 27-43. | 0.6 | 71 |

| # | Article | IF | Citations |
|---|---|---|---|
| 325 | Cross sections of electron inelastic interactions in DNA. Radiation and Environmental Biophysics, 2004, 43, 173-182. | 0.6 | 28 |
| 326 | A scheme for the economical use of numerical basis sets in calculations with SIESTA. Theoretical Chemistry Accounts, 2004, 112, 158. | 0.5 | 33 |
| 327 | Ambient gas effects on high-power Nd:YAG laser ablation of SnO2:Sb transparent conducting thin film. Optics and Lasers in Engineering, 2004, 41, 537-544. | 2.0 | 7 |
| 328 | Electronic stopping powers for fluorine ions in -implanted potassium titanyl arsenate. Applied Surface Science, 2004, 228, 77-83. | 3.1 | 1 |
| 329 | Strain energy and thermal stability of single-walled aluminum nitride nanotubes from first-principles calculations. Chemical Physics Letters, 2004, 389, 160-164. | 1.2 | 63 |
| 330 | Stable and extendable cage containing nanosize silica clusters based on three-membered rings. Physical Review B, 2004, 69, . | 1.1 | 28 |
| 331 | Chemical Reactivity of Single-Walled Carbon Nanotubes to Amidogen from Density Functional Calculations. Journal of Physical Chemistry B, 2004, 108, 9599-9603. | 1.2 | 35 |
| 332 | Recombination and Exchange Reactions of Hydrogen and Dihydrogen Molecular Condensation in Single-Walled Carbon Nanotubes. Journal of Physical Chemistry B, 2004, 108, 4711-4715. | 1.2 | 5 |
| 333 | Stable tetrahedral structure of the silica cluster(SiO2)10. Physical Review B, 2004, 70, . | 1.1 | 15 |
| 334 | Two- and Three-Membered-Ring Hybrid Structures of Silica Nanoclusters. Journal of Physical Chemistry B, 2004, 108, 18451-18454. | 1.2 | 23 |
| 335 | Selectable functionalization of single-walled carbon nanotubes resulting fromCHn(n=1â€“3)adsorption. Physical Review B, 2004, 69, . | 1.1 | 23 |
| 336 | Silicon Monoxide Clusters: The Favorable Precursors for Forming Silicon Nanostructures. Physical Review Letters, 2004, 93, 095503. | 2.9 | 55 |
| 337 | Emission properties of laser ablation of SnO2: Sb transparent conducting film and KTiOPO4 crystal. Optics and Laser Technology, 2003, 35, 475-480. | 2.2 | 2 |
| 338 | Investigation of intermixing induced by sputtering and annealing in multiple quantum well. Applied Surface Science, 2003, 205, 182-187. | 3.1 | 0 |
| 339 | Study of the plasma produced from laser ablation of a KTP crystal. Applied Surface Science, 2003, 207, 227-235. | 3.1 | 27 |
| 340 | Influence of annealing condition on photoluminescence characteristics of AlGaAs/GaAs multiple quantum well. Materials Letters, 2003, 57, 2932-2935. | 1.3 | 9 |
| 341 | Stability and electronic structure of AlN nanotubes. Physical Review B, 2003, 68, . | 1.1 | 148 |
| 342 | Plasma properties of a laser-ablated aluminum target in air. Laser and Particle Beams, 2003, 21, 97-101. | 0.4 | 33 |

| # | Article | IF | Citations |
|---|---|---|---|
| 343 | Condensation and phase transition of hydrogen molecules confined in single-walled carbon nanotubes. Physical Review B, 2003, 67, . | 1.1 | 20 |
| 344 | First-principles calculations for nitrogen-containing single-walled carbon nanotubes. Journal of Applied Physics, 2003, 94, 2398-2402. | 1.1 | 93 |
| 345 | Exohedral and endohedral adsorption of nitrogen on the sidewall of single-walled carbon nanotubes. Physical Review B, 2002, 66, . | 1.1 | 45 |
| 346 | Hydrogen storage capacity in single-walled carbon nanotubes. Physical Review B, 2002, 65, . | 1.1 | 31 |
| 347 | Tensile strength of single-walled carbon nanotubes with defects under hydrostatic pressure. Physical Review B, 2002, 65, . | 1.1 | 45 |
| 348 | Electronic stopping powers for fluorine ions in 19F+-implanted tin-oxide films prepared by APCVD. Nuclear Instruments & Methods in Physics Research B, 2002, 187, 431-436. | 0.6 | 3 |
| 349 | Electronic stopping powers of molybdenum metal for 19F ions at low velocity. Nuclear Instruments & Methods in Physics Research B, 2002, 197, 17-21. | 0.6 | 0 |
| 350 | An investigation of range distribution parameters for bismuth ion-implantation in silver gallium disulphur. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2002, 96, 65-68. | 1.7 | 0 |
| 351 | DFT calculation on the energy thresholds of DNA damages under irradiation conditions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2002, 300, 421-426. | 0.9 | 6 |
| 352 | Structures of hydrogen molecules in single-walled carbon nanotubes. Chemical Physics Letters, 2002, 357, 97-102. | 1.2 | 24 |
| 353 | The importance of electronic exchange-correlation in non-self-consistent frozen density approximation. Chemical Physics Letters, 2002, 360, 436-442. | 1.2 | 2 |
| 354 | Effective hydrogen storage in single-wall carbon nanotubes. Physical Review B, 2001, 63, . | 1.1 | 101 |
| 355 | Chemical adsorption of C60 on diamond (100)(2Ã—1) surfaces. Applied Physics A: Materials Science and Processing, 2001, 73, 365-369. | 1.1 | 1 |
| 356 | Depth profiles and electronic stopping powers for fluorine ions in -implanted KTN. Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 280, 58-64. | 0.9 | 3 |
| 357 | Collisions of deuterium and tritium atoms with single-wall carbon nanotube: adsorption, encapsulation, and healing. Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 288, 207-213. | 0.9 | 11 |
| 358 | Range distribution and electronic stopping powers for fluorine ions in -implanted potassium titanyl phosphate and LiNbO3. Nuclear Instruments & Methods in Physics Research B, 2001, 174, 1-8. | 0.6 | 7 |
| 359 | Collision of hydrogen atom with single-walled carbon nanotube: Adsorption, insertion, and healing. Journal of Chemical Physics, 2001, 115, 8152-8156. | 1.2 | 30 |
| 360 | Low-energy interaction and adsorption of C60 on diamond surfaces. Nuclear Instruments & Methods in Physics Research B, 2000, 168, 169-180. | 0.6 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 361 | Efficient Helium and Helium Isotopes Separation by Phosphorus Carbide P 2 C 3 Membrane. Advanced Theory and Simulations, 0, , 2100327. | 1.3 | 2 |
| 362 | Tunable topological electronic states in the Honeycomb-kagome lattices of nitrogen/oxygen-doped graphene nanomeshes. Nanoscale Advances, 0, , . | 2.2 | 1 |
| 363 | Two-Dimensional Multiferroic Î´-PbO Monolayer with a Large In-Plane Negative Poissonâ€™s Ratio. ACS Applied Electronic Materials, 0, , . | 2.0 | 3 |