

Jinlan Wang

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

300
papers

15,181
citations

62
h-index

112
g-index

317
ext. papers

18,653
ext. citations

9.1
avg, IF

7.06
L-index

| # | Paper | IF | Citations |
|-----|--|------|-----------|
| 300 | Strong photoluminescence enhancement of MoS ₂ through defect engineering and oxygen bonding. <i>ACS Nano</i> , 2014 , 8, 5738-45 | 16.7 | 774 |
| 299 | Hopping transport through defect-induced localized states in molybdenum disulphide. <i>Nature Communications</i> , 2013 , 4, 2642 | 17.4 | 740 |
| 298 | An organic-inorganic perovskite ferroelectric with large piezoelectric response. <i>Science</i> , 2017 , 357, 306-309 | 39.3 | 506 |
| 297 | Metal-Free Single Atom Catalyst for N Fixation Driven by Visible Light. <i>Journal of the American Chemical Society</i> , 2018 , 140, 14161-14168 | 16.4 | 460 |
| 296 | Towards intrinsic charge transport in monolayer molybdenum disulfide by defect and interface engineering. <i>Nature Communications</i> , 2014 , 5, 5290 | 17.4 | 448 |
| 295 | Density-functional study of Au _n (n=200) clusters: Lowest-energy structures and electronic properties. <i>Physical Review B</i> , 2002 , 66, | 3.3 | 393 |
| 294 | Light-Induced Ambient Degradation of Few-Layer Black Phosphorus: Mechanism and Protection. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 11437-41 | 16.4 | 387 |
| 293 | Chemically activating MoS ₂ via spontaneous atomic palladium interfacial doping towards efficient hydrogen evolution. <i>Nature Communications</i> , 2018 , 9, 2120 | 17.4 | 300 |
| 292 | Activating Inert Basal Planes of MoS ₂ for Hydrogen Evolution Reaction through the Formation of Different Intrinsic Defects. <i>Chemistry of Materials</i> , 2016 , 28, 4390-4396 | 9.6 | 277 |
| 291 | Two-dimensional quasi-freestanding molecular crystals for high-performance organic field-effect transistors. <i>Nature Communications</i> , 2014 , 5, 5162 | 17.4 | 270 |
| 290 | Accelerated discovery of stable lead-free hybrid organic-inorganic perovskites via machine learning. <i>Nature Communications</i> , 2018 , 9, 3405 | 17.4 | 263 |
| 289 | Nanosheet Supported Single-Metal Atom Bifunctional Catalyst for Overall Water Splitting. <i>Nano Letters</i> , 2017 , 17, 5133-5139 | 11.5 | 253 |
| 288 | Transition Metal-Promoted VCO (MXenes): A New and Highly Active Catalyst for Hydrogen Evolution Reaction. <i>Advanced Science</i> , 2016 , 3, 1600180 | 13.6 | 204 |
| 287 | Te-Doped Black Phosphorus Field-Effect Transistors. <i>Advanced Materials</i> , 2016 , 28, 9408-9415 | 24 | 195 |
| 286 | High-Temperature Ferroelectricity and Photoluminescence in a Hybrid Organic-Inorganic Compound: (3-Pyrrolinium)MnCl ₃ . <i>Journal of the American Chemical Society</i> , 2015 , 137, 13148-54 | 16.4 | 191 |
| 285 | Recent progress and challenges in graphene nanoribbon synthesis. <i>ChemPhysChem</i> , 2013 , 14, 47-54 | 3.2 | 180 |
| 284 | A General Two-Step Strategy Based High-Throughput Screening of Single Atom Catalysts for Nitrogen Fixation. <i>Small Methods</i> , 2019 , 3, 1800376 | 12.8 | 175 |

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| 283 | Searching for Highly Active Catalysts for Hydrogen Evolution Reaction Based on O-Terminated MXenes through a Simple Descriptor. <i>Chemistry of Materials</i> , 2016 , 28, 9026-9032 | 9.6 | 165 |
| 282 | Single Molybdenum Atom Anchored on N-Doped Carbon as a Promising Electrocatalyst for Nitrogen Reduction into Ammonia at Ambient Conditions. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 16842-16847 | 3.8 | 163 |
| 281 | Robust room-temperature ferromagnetism with giant anisotropy in Nd-doped ZnO nanowire arrays. <i>Nano Letters</i> , 2012 , 12, 3994-4000 | 11.5 | 146 |
| 280 | Static polarizabilities and optical absorption spectra of gold clusters (Aun, n=20 and 20) from first principles. <i>Physical Review B</i> , 2007 , 76, | 3.3 | 145 |
| 279 | Structure and electronic properties of Gen (n=205) clusters from density-functional theory. <i>Physical Review B</i> , 2001 , 64, | 3.3 | 138 |
| 278 | Structure and magnetism of VnBz(n+1) sandwich clusters. <i>Journal of the American Chemical Society</i> , 2005 , 127, 2812-3 | 16.4 | 135 |
| 277 | Endohedral silicon fullerenes sinN (27 Journal of the American Chemical Society, 2004 , 126, 13845-9 | 16.4 | 125 |
| 276 | Convincing Synthesis of Atomically Thin, Single-Crystalline InVO Sheets toward Promoting Highly Selective and Efficient Solar Conversion of CO into CO. <i>Journal of the American Chemical Society</i> , 2019 , 141, 4209-4213 | 16.4 | 124 |
| 275 | Structures and electronic properties of Cu20, Ag20, and Au20 clusters with density functional method. <i>Chemical Physics Letters</i> , 2003 , 380, 716-720 | 2.5 | 121 |
| 274 | Bimetallic Nickel Cobalt Sulfide as Efficient Electrocatalyst for Zn-Air Battery and Water Splitting. <i>Nano-Micro Letters</i> , 2019 , 11, 2 | 19.5 | 119 |
| 273 | Water-Catalyzed Oxidation of Few-Layer Black Phosphorous in a Dark Environment. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 9131-9135 | 16.4 | 115 |
| 272 | Switchable dielectric, piezoelectric, and second-harmonic generation bistability in a new improper ferroelectric above room temperature. <i>Advanced Materials</i> , 2014 , 26, 4515-20 | 24 | 111 |
| 271 | Hydrogen Storage on Metal-Coated B80 Buckyballs with Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 7052-7057 | 3.8 | 110 |
| 270 | Passivation of Black Phosphorus via Self-Assembled Organic Monolayers by van der Waals Epitaxy. <i>Advanced Materials</i> , 2017 , 29, 1603990 | 24 | 101 |
| 269 | Recent advances in oxidation and degradation mechanisms of ultrathin 2D materials under ambient conditions and their passivation strategies. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 4291-4312 | 13 | 100 |
| 268 | Hollow cages versus space-filling structures for medium-sized gold clusters: the spherical aromaticity of the Au50 cage. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 9265-9 | 2.8 | 95 |
| 267 | Melting behavior in ultrathin metallic nanowires. <i>Physical Review B</i> , 2002 , 66, | 3.3 | 95 |
| 266 | Electronic and Optical Properties of Edge-Functionalized Graphene Quantum Dots and the Underlying Mechanism. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 24950-24957 | 3.8 | 94 |

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|-----|---|------|----|
| 265 | Surface Vacancy-Induced Switchable Electric Polarization and Enhanced Ferromagnetism in Monolayer Metal Trihalides. <i>Nano Letters</i> , 2018 , 18, 2943-2949 | 11.5 | 94 |
| 264 | New Mechanism for N Reduction: The Essential Role of Surface Hydrogenation. <i>Journal of the American Chemical Society</i> , 2019 , 141, 18264-18270 | 16.4 | 94 |
| 263 | Electronic Structure of Twisted Bilayers of Graphene/MoS ₂ and MoS ₂ /MoS ₂ . <i>Journal of Physical Chemistry C</i> , 2015 , 119, 4752-4758 | 3.8 | 94 |
| 262 | Molecular Dynamics Simulation of Chemical Vapor Deposition Graphene Growth on Ni (111) Surface. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 6097-6102 | 3.8 | 93 |
| 261 | Defect Engineering for Modulating the Trap States in 2D Photoconductors. <i>Advanced Materials</i> , 2018 , 30, e1804332 | 24 | 90 |
| 260 | Ethylene Selectivity in Electrocatalytic CO Reduction on Cu Nanomaterials: A Crystal Phase-Dependent Study. <i>Journal of the American Chemical Society</i> , 2020 , 142, 12760-12766 | 16.4 | 89 |
| 259 | Foam-like Co ₉ S ₈ /Ni ₃ S ₂ heterostructure nanowire arrays for efficient bifunctional overall water splitting. <i>Applied Catalysis B: Environmental</i> , 2019 , 253, 246-252 | 21.8 | 88 |
| 258 | Transition-Metal Dihydride Monolayers: A New Family of Two-Dimensional Ferromagnetic Materials with Intrinsic Room-Temperature Half-Metallicity. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 4260-4266 | 6.4 | 87 |
| 257 | Breaking scaling relations for efficient CO electrochemical reduction through dual-atom catalysts. <i>Chemical Science</i> , 2020 , 11, 1807-1813 | 9.4 | 86 |
| 256 | Tailoring band gap in GaN sheet by chemical modification and electric field: Ab initio calculations. <i>Applied Physics Letters</i> , 2011 , 98, 053102 | 3.4 | 82 |
| 255 | High intrinsic catalytic activity of two-dimensional boron monolayers for the hydrogen evolution reaction. <i>Nanoscale</i> , 2017 , 9, 533-537 | 7.7 | 81 |
| 254 | Precise, Self-Limited Epitaxy of Ultrathin Organic Semiconductors and Heterojunctions Tailored by van der Waals Interactions. <i>Nano Letters</i> , 2016 , 16, 3754-9 | 11.5 | 81 |
| 253 | MnX (X = P, As) monolayers: a new type of two-dimensional intrinsic room temperature ferromagnetic half-metallic material with large magnetic anisotropy. <i>Nanoscale</i> , 2019 , 11, 4204-4209 | 7.7 | 81 |
| 252 | Metal-free electrocatalyst for reducing nitrogen to ammonia using a Lewis acid pair. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 4865-4871 | 13 | 78 |
| 251 | Anomalous Size Dependence of Optical Properties in Black Phosphorus Quantum Dots. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 370-5 | 6.4 | 78 |
| 250 | Aqueous acid-based synthesis of lead-free tin halide perovskites with near-unity photoluminescence quantum efficiency. <i>Chemical Science</i> , 2019 , 10, 4573-4579 | 9.4 | 77 |
| 249 | Epitaxial growth of wafer-scale molybdenum disulfide semiconductor single crystals on sapphire. <i>Nature Nanotechnology</i> , 2021 , 16, 1201-1207 | 28.7 | 75 |
| 248 | Light-Induced Ambient Degradation of Few-Layer Black Phosphorus: Mechanism and Protection. <i>Angewandte Chemie</i> , 2016 , 128, 11609-11613 | 3.6 | 70 |

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|-----|--|------|----|
| 247 | Structural evolution of anionic silicon clusters SiN (20 . <i>Journal of Physical Chemistry A</i> , 2006 , 110, 908-122.8 | | 69 |
| 246 | Recent Progress on Two-Dimensional Materials. <i>Wuli Huaxue Xuebao/Acta Physico - Chimica Sinica</i> , 2021 , 2108017-0 | 3.8 | 69 |
| 245 | Rational Design and Characterization of Direct Z-Scheme Photocatalyst for Overall Water Splitting from Excited State Dynamics Simulations. <i>ACS Catalysis</i> , 2020 , 10, 1976-1983 | 13.1 | 68 |
| 244 | A new Dirac cone material: a graphene-like BeC monolayer. <i>Nanoscale</i> , 2017 , 9, 5577-5582 | 7.7 | 66 |
| 243 | Electronic and Optical Properties of Graphene Quantum Dots: The Role of Many-Body Effects. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 4983-4989 | 3.8 | 65 |
| 242 | Mechanically robust tri-wing graphene nanoribbons with tunable electronic and magnetic properties. <i>Nano Letters</i> , 2010 , 10, 494-8 | 11.5 | 65 |
| 241 | Janus MoSSe/WSeTe heterostructures: a direct Z-scheme photocatalyst for hydrogen evolution. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 21835-21842 | 13 | 64 |
| 240 | Covalent Functionalization of Black Phosphorus from First-Principles. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 4540-4546 | 6.4 | 63 |
| 239 | Towards a Comprehensive Understanding of the Reaction Mechanisms Between Defective MoS and Thiol Molecules. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 10501-10505 | 16.4 | 62 |
| 238 | Template-Grown MoS ₂ Nanowires Catalyze the Hydrogen Evolution Reaction: Ultralow Kinetic Barriers with High Active Site Density. <i>ACS Catalysis</i> , 2017 , 7, 5097-5102 | 13.1 | 61 |
| 237 | Photo-oxidative degradation of methylammonium lead iodide perovskite: mechanism and protection. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 2275-2282 | 13 | 60 |
| 236 | Prediction of a two-dimensional high-TC f-electron ferromagnetic semiconductor. <i>Materials Horizons</i> , 2020 , 7, 1623-1630 | 14.4 | 59 |
| 235 | Formation and electronic properties of hydrogenated few layer graphene. <i>Nanotechnology</i> , 2011 , 22, 185202 | 3.4 | 59 |
| 234 | Geometric and electronic properties of titanium clusters studied by ultrasoft pseudopotential. <i>Solid State Communications</i> , 2001 , 118, 157-161 | 1.6 | 59 |
| 233 | Ab initio study of structural and magnetic properties of TM(n)(ferrocene)(n+1) (TM = Sc, Ti, V, Mn) sandwich clusters and nanowires (n = infinity). <i>ACS Nano</i> , 2009 , 3, 537-45 | 16.7 | 58 |
| 232 | Chromium sulfide halide monolayers: intrinsic ferromagnetic semiconductors with large spin polarization and high carrier mobility. <i>Nanoscale</i> , 2018 , 10, 18036-18042 | 7.7 | 58 |
| 231 | Efficient Carrier Separation in Graphitic Zinc Oxide and Blue Phosphorus van der Waals Heterostructure. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 3648-3653 | 3.8 | 55 |
| 230 | Nonmetal-metal transition in Z _n (n=20) clusters. <i>Physical Review A</i> , 2003 , 68, | 2.6 | 55 |

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| 229 | Boron and Nitrogen Doping Induced Half-Metallicity in Zigzag Triwing Graphene Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 6195-6199 | 3.8 | 54 |
| 228 | Transition-metal-catalyzed unzipping of single-walled carbon nanotubes into narrow graphene nanoribbons at low temperature. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 8041-5 | 16.4 | 54 |
| 227 | Gold-coated transition-metal anion [Mn ₁₃ @Au ₂₀]- with ultrahigh magnetic moment. <i>Journal of the American Chemical Society</i> , 2007 , 129, 4110-1 | 16.4 | 54 |
| 226 | Strain-induced orientation-selective cutting of graphene into graphene nanoribbons on oxidation. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 1161-4 | 16.4 | 53 |
| 225 | Computation-Aided Design of Single-Atom Catalysts for One-Pot CO Capture, Activation, and Conversion. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 36866-36872 | 9.5 | 53 |
| 224 | Nanoconfined Iron Oxychloride Material as a High-Performance Cathode for Rechargeable Chloride Ion Batteries. <i>ACS Energy Letters</i> , 2017 , 2, 2341-2348 | 20.1 | 51 |
| 223 | Structure and magnetic properties of Co-Cu bimetallic clusters. <i>Physical Review B</i> , 2002 , 66, | 3.3 | 51 |
| 222 | Topological transport and atomic tunnelling-clustering dynamics for aged Cu-doped Bi ₂ Te ₃ crystals. <i>Nature Communications</i> , 2014 , 5, 5022 | 17.4 | 50 |
| 221 | Band structure engineering of monolayer MoS ₂ by surface ligand functionalization for enhanced photoelectrochemical hydrogen production activity. <i>Nanoscale</i> , 2014 , 6, 13565-71 | 7.7 | 50 |
| 220 | Oxidation Mechanism and Protection Strategy of Ultrathin Indium Selenide: Insight from Theory. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 4368-4373 | 6.4 | 50 |
| 219 | Revealing the underlying absorption and emission mechanism of nitrogen doped graphene quantum dots. <i>Nanoscale</i> , 2016 , 8, 19376-19382 | 7.7 | 49 |
| 218 | High Curie-temperature intrinsic ferromagnetism and hole doping-induced half-metallicity in two-dimensional scandium chlorine monolayers. <i>Nanoscale Horizons</i> , 2018 , 3, 551-555 | 10.8 | 49 |
| 217 | Uniformly wetting deposition of Co atoms on MoS ₂ monolayer: a promising two-dimensional robust half-metallic ferromagnet. <i>ACS Applied Materials & Interfaces</i> , 2014 , 6, 16835-40 | 9.5 | 49 |
| 216 | Highly Efficient Photo-/Electrocatalytic Reduction of Nitrogen into Ammonia by Dual-Metal Sites. <i>ACS Central Science</i> , 2020 , 6, 1762-1771 | 16.8 | 49 |
| 215 | Half-metallicity and enhanced ferromagnetism in Li-adsorbed ultrathin chromium triiodide. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 5716-5720 | 7.1 | 46 |
| 214 | Structural transition of Si clusters and their thermodynamics. <i>Chemical Physics Letters</i> , 2001 , 341, 529-534 | 4.5 | 45 |
| 213 | Theoretical studies on structural, magnetic, and spintronic characteristics of sandwiched Eu(n)COT(n+1) (n = 1-4) clusters. <i>ACS Nano</i> , 2009 , 3, 2515-22 | 16.7 | 44 |
| 212 | Structural, electronic, and magnetic properties of Sc _n (n=2-8) clusters from density functional calculations. <i>Physical Review B</i> , 2007 , 75, | 3.3 | 44 |

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| 211 | Quasiparticle Energies and Optical Excitations in Chevron-Type Graphene Nanoribbon. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 10193-10197 | 3.8 | 43 |
| 210 | Rapid Discovery of Ferroelectric Photovoltaic Perovskites and Material Descriptors via Machine Learning. <i>Small Methods</i> , 2019 , 3, 1900360 | 12.8 | 42 |
| 209 | High Curie temperature and intrinsic ferromagnetic half-metallicity in two-dimensional Cr ₃ X ₄ (X = S, Se, Te) nanosheets. <i>Nanoscale Horizons</i> , 2019 , 4, 859-866 | 10.8 | 42 |
| 208 | Topological insulators based on 2D shape-persistent organic ligand complexes. <i>Nanoscale</i> , 2015 , 7, 727-357 | 3.7 | 42 |
| 207 | Infrared spectra of V(n)Bz(n+1) sandwich clusters: a theoretical study of size evolution. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 10180-2 | 2.8 | 42 |
| 206 | Hybrid Cu and Cu as Atomic Interfaces Promote High-Selectivity Conversion of CO to C H OH at Low Potential. <i>Small</i> , 2020 , 16, e1901981 | 11 | 42 |
| 205 | Heterophase fcc-2H-fcc gold nanorods. <i>Nature Communications</i> , 2020 , 11, 3293 | 17.4 | 41 |
| 204 | Ultrathin Semiconducting BiTeS and BiTeSe with High Electron Mobilities. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 487-490 | 6.4 | 41 |
| 203 | Ab Initio Study of Structural, Electronic, and Magnetic Properties of Transition Metal Borazine Molecular Wires. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 8767-8771 | 3.8 | 41 |
| 202 | Greatly Enhanced Optical Absorption of a Defective MoS ₂ Monolayer through Oxygen Passivation. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 13150-6 | 9.5 | 41 |
| 201 | Highly efficient photogenerated electron transfer at a black phosphorus/indium selenide heterostructure interface from ultrafast dynamics. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 1864-1870 | 7.1 | 39 |
| 200 | Scaling dopant states in a semiconducting nanostructure by chemically resolved electron energy-loss spectroscopy: a case study on Co-doped ZnO. <i>Journal of the American Chemical Society</i> , 2010 , 132, 6492-7 | 16.4 | 39 |
| 199 | Highly Fluorescent and Stable Black Phosphorus Quantum Dots in Water. <i>Small</i> , 2018 , 14, e1803132 | 11 | 39 |
| 198 | Inch-Scale Grain Boundary Free Organic Crystals Developed by Nucleation Seed-Controlled Shearing Method. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 35395-35403 | 9.5 | 37 |
| 197 | Coupling a Crystal Graph Multilayer Descriptor to Active Learning for Rapid Discovery of 2D Ferromagnetic Semiconductors/Half-Metals/Metals. <i>Advanced Materials</i> , 2020 , 32, e2002658 | 24 | 36 |
| 196 | The stacking dependent electronic structure and optical properties of bilayer black phosphorus. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 6085-91 | 3.6 | 36 |
| 195 | Edge-passivation induced half-metallicity of zigzag zinc oxide nanoribbons. <i>Applied Physics Letters</i> , 2009 , 95, 133116 | 3.4 | 36 |
| 194 | Structural, Electronic, and Optical Properties of Noble Metal Clusters from First Principles. <i>Journal of Cluster Science</i> , 2006 , 17, 609-626 | 3 | 36 |

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| 193 | Cobalt phosphosulfide in the tetragonal phase: a highly active and durable catalyst for the hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 12353-12360 | 13 | 36 |
| 192 | Molecular self-assembly on two-dimensional atomic crystals: insights from molecular dynamics simulations. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4518-24 | 6.4 | 35 |
| 191 | Molybdenum sulfide clusters immobilized on defective graphene: a stable catalyst for the hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 2289-2294 | 13 | 35 |
| 190 | Abnormal Near-Infrared Absorption in 2D Black Phosphorus Induced by Ag Nanoclusters Surface Functionalization. <i>Advanced Materials</i> , 2018 , 30, e1801931 | 24 | 35 |
| 189 | Photo-oxidative Degradation and Protection Mechanism of Black Phosphorus: Insights from Ultrafast Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 5034-5039 | 6.4 | 35 |
| 188 | Dipole polarizabilities of medium-sized gold clusters. <i>Physical Review A</i> , 2006 , 74, | 2.6 | 35 |
| 187 | Magnetic two-dimensional layered crystals meet with ferromagnetic semiconductors. <i>Information Materials</i> , 2020 , 2, 639-655 | 23.1 | 34 |
| 186 | Tuning the vertical location of helical surface states in topological insulator heterostructures via dual-proximity effects. <i>Scientific Reports</i> , 2013 , 3, 1233 | 4.9 | 34 |
| 185 | Dipole polarizabilities of germanium clusters. <i>Chemical Physics Letters</i> , 2003 , 367, 448-454 | 2.5 | 34 |
| 184 | Density functional study of beryllium clusters, with gradient correction. <i>Journal of Physics Condensed Matter</i> , 2001 , 13, L753-L758 | 1.8 | 34 |
| 183 | Oxygen Intercalation of Graphene on Transition Metal Substrate: An Edge-Limited Mechanism. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4099-105 | 6.4 | 33 |
| 182 | Structural, electronic, and magnetic properties of Con(benzene) _m complexes. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 296-304 | 2.8 | 33 |
| 181 | Metal single-atom coordinated graphitic carbon nitride as an efficient catalyst for CO oxidation. <i>Nanoscale</i> , 2020 , 12, 364-371 | 7.7 | 33 |
| 180 | Copper(i) sulfide: a two-dimensional semiconductor with superior oxidation resistance and high carrier mobility. <i>Nanoscale Horizons</i> , 2019 , 4, 223-230 | 10.8 | 32 |
| 179 | Mechanism of Transition-Metal Nanoparticle Catalytic Graphene Cutting. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 1192-7 | 6.4 | 31 |
| 178 | Magnetic Manipulation and Half-Metal Prediction of One-Dimensional Bimetallic Organic Sandwich Molecular Wires [CpTM1CpTM2][TM1 = Ti, Cr, Fe; TM2 = ScCo]. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 2948-2953 | 3.8 | 31 |
| 177 | Perspective on theoretical methods and modeling relating to electro-catalysis processes. <i>Chemical Communications</i> , 2020 , 56, 9937-9949 | 5.8 | 30 |
| 176 | Property-Oriented Material Design Based on a Data-Driven Machine Learning Technique. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 3920-3927 | 6.4 | 30 |

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| 175 | Optimally stuffed fullerene structures of silicon nanoclusters. <i>Physical Review B</i> , 2005 , 71, | 3.3 | 30 |
| 174 | Thermal properties of medium-sized Ge clusters. <i>Solid State Communications</i> , 2001 , 117, 593-598 | 1.6 | 30 |
| 173 | Thermal behavior of Cu ₁₀ bimetallic clusters. <i>Solid State Communications</i> , 2001 , 119, 13-18 | 1.6 | 30 |
| 172 | Dielectric and ferroelectric sensing based on molecular recognition in Cu(1,10-phenothroline)SeO ₃ (diol) systems. <i>Nature Communications</i> , 2017 , 8, 14551 | 17.4 | 29 |
| 171 | Anchoring of black phosphorus quantum dots onto WO nanowires to boost photocatalytic CO conversion into solar fuels. <i>Chemical Communications</i> , 2020 , 56, 7777-7780 | 5.8 | 29 |
| 170 | Arsenene-Based Heterostructures: Highly Efficient Bifunctional Materials for Photovoltaics and Photocatalytics. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 42856-42861 | 9.5 | 29 |
| 169 | Structural, electronic, and magnetic properties of TMZn ₁₁ O ₁₂ and TM ₂ Zn ₁₀ O ₁₂ clusters (TM=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu). <i>Chemical Physics Letters</i> , 2009 , 474, 336-341 | 2.5 | 29 |
| 168 | Insight into the catalytic activity of MXenes for hydrogen evolution reaction. <i>Science Bulletin</i> , 2018 , 63, 1397-1403 | 10.6 | 29 |
| 167 | Ab initio study of bond characteristics and magnetic properties of mixed-sandwich VnBzmCpk clusters. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 2319-23 | 2.8 | 28 |
| 166 | Optical properties of boron nitride nanoribbons: Excitonic effects. <i>Applied Physics Letters</i> , 2011 , 99, 063114 | 3.4 | 28 |
| 165 | A transferable nonorthogonal tight-binding model of germanium: application to small clusters. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2000 , 275, 281-286 | 2.3 | 28 |
| 164 | Bi ₂ OS ₂ : a direct-gap two-dimensional semiconductor with high carrier mobility and surface electron states. <i>Materials Horizons</i> , 2018 , 5, 1058-1064 | 14.4 | 28 |
| 163 | Vacancy-defect modulated pathway of photoreduction of CO on single atomically thin AgInPS sheets into olefiant gas. <i>Nature Communications</i> , 2021 , 12, 4747 | 17.4 | 28 |
| 162 | Role of Water and Defects in Photo-Oxidative Degradation of Methylammonium Lead Iodide Perovskite. <i>Small Methods</i> , 2019 , 3, 1900154 | 12.8 | 27 |
| 161 | Rational Hydrogenation for Enhanced Mobility and High Reliability on ZnO-based Thin Film Transistors: From Simulation to Experiment. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 5408-15 | 9.5 | 27 |
| 160 | Repairing atomic vacancies in single-layer MoSe ₂ field-effect transistor and its defect dynamics. <i>Npj Quantum Materials</i> , 2017 , 2, | 5 | 27 |
| 159 | Quasi-particle energies and optical excitations of hydrogenated and fluorinated germanene. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 4542-50 | 3.6 | 27 |
| 158 | Comparative DFT study of structure and magnetism of TM(n)O(m) (TM = Sc-Mn, n = 1-2, m = 1-6) clusters. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 2471-7 | 3.6 | 27 |

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|-----|---|------|----|
| 157 | Fluorination induced half metallicity in two-dimensional few zinc oxide layers. <i>Journal of Chemical Physics</i> , 2010 , 132, 204703 | 3.9 | 27 |
| 156 | Structures and magnetic properties of Pdn clusters (n=3-19) doped by Mn atoms. <i>Physical Review A</i> , 2011 , 84, | 2.6 | 27 |
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