Mingwen Zhao

List of Publications by Year in Descending Order

348 papers	10,633 citations	52 h-index	87 g-index
365 ext. papers	12,187 ext. citations	5.2 avg, IF	6.66 L-index

#	Paper	IF	Citations
348	pH-switchable nanozyme cascade catalysis: a strategy for spatial-temporal modulation of pathological wound microenvironment to rescue stalled healing in diabetic ulcer.. *Journal of Nanobiotechnology*, **2022**, 20, 12	9.4	6
347	Nanophysical Antimicrobial Strategies: A Rational Deployment of Nanomaterials and Physical Stimulations in Combating Bacterial Infections.. *Advanced Science*, **2022**, e2105252	13.6	4
346	Highly-anisotropic plasmons in two-dimensional hyperbolic copper borides.. *Optics Express*, **2022**, 30, 5596-5607	3.3	0
345	Ultrafine zirconium boride nanoparticles constructed bidirectional catalyst for ultrafast and long-lived lithium-sulfur batteries. *Energy Storage Materials*, **2022**, 45, 130-141	19.4	6
344	Efficient anisotropic desalination by layer-stacked black phosphorus carbide (⊞PC) membrane. *Desalination*, **2022**, 522, 115422	10.3	0
343	Sub-nanometer-sized carbon nanoparticle shows higher biocompatibility to DNA than nanometer-sized nanoparticles. *Journal Physics D: Applied Physics*, **2022**, 55, 295401	3	
342	Robust broadband directional plasmons in a MoOCl2 monolayer. *Physical Review B*, **2021**, 104,	3.3	1
341	Two-dimensional XC-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	3.6	
340	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	5	13
339	New Spiral Form of Carbon Nitride with Ultrasoftness and Tunable Electronic Structures. *ACS Omega*, **2021**, 6, 516-522	3.9	1
338	Defect-Induced Double-Stranded DNA Unwinding on Graphene. *Journal of Physical Chemistry B*, **2021**, 125, 2833-2840	3.4	4
337	Monolayer FeGeX (X = S, Se, and Te) as Highly Efficient Electrocatalysts for Lithium-Sulfur Batteries. *ACS Applied Materials & Interfaces*, **2021**, 13, 11845-11851	9.5	8
336	Prediction of crossing nodal-lines and large intrinsic spin Hall conductivity in topological Dirac semimetal Ta3As family. *Npj Computational Materials*, **2021**, 7,	10.9	3
335	Direct Z-scheme photocatalytic CO2 conversion to solar fuels in a two-dimensional C2N/aza-CMP heterostructure. *Applied Surface Science*, **2021**, 541, 148630	6.7	7
334	In-situ Nano-Crystallization and Solvation Modulation to Promote Highly Stable Anode Involving Alloy/De-alloy for Potassium Ion Batteries. *Angewandte Chemie - International Edition*, **2021**, 60, 15381-15389	16.4	24
333	In-situ Nano-Crystallization and Solvation Modulation to Promote Highly Stable Anode Involving Alloy/De-alloy for Potassium Ion Batteries. *Angewandte Chemie*, **2021**, 133, 15509-15517	3.6	2
332	Efficient isotropic water desalination in anisotropic lamellar nano-channels formed by layered black phosphorus membrane. *Desalination*, **2021**, 504, 114962	10.3	6

331	Frontispiece: In-situ Nano-Crystallization and Solvation Modulation to Promote Highly Stable Anode Involving Alloy/De-alloy for Potassium Ion Batteries. *Angewandte Chemie - International Edition*, **2021**, 60,	16.4	1
330	Two-dimensional transition metal borides as highly efficient N2 fixation catalysts. *Applied Surface Science*, **2021**, 536, 147742	6.7	19
329	Anomalous plasmons in a two-dimensional Dirac nodal-line Lieb lattice. *Nanoscale Advances*, **2021**, 3, 1127-1135	5.1	2
328	Multi-functional photocatalytic activity of transition-metal tetraaza[14]annulene frameworks. *Journal of Materials Chemistry A*, **2021**, 9, 4221-4229	13	3
327	Photo-assisted high performance single atom electrocatalysis of the N2 reduction reaction by a Mo-embedded covalent organic framework. *Journal of Materials Chemistry A*, **2021**, 9, 19949-19957	13	6
326	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	7.7	9
325	Interface-enhanced CO2 capture via the synthetic effects of a nanomaterial-supported ionic liquid thin film. *Nanoscale Advances*, **2021**, 3, 1397-1403	5.1	7
324	Giant negative Poisson's ratio in two-dimensional V-shaped materials. *Nanoscale Advances*, **2021**, 3, 4554-4560	5.1	1
323	Floquet-Dirac fermions in monolayer graphene by Wannier functions. *Journal of Physics Condensed Matter*, **2021**,	1.8	1
322	Prediction of intrinsic topological superconductivity in Mn-doped GeTe monolayer from first-principles. *Npj Computational Materials*, **2021**, 7,	10.9	2
321	Construction and electrochemical mechanism investigation of hierarchical core–shell like composite as high performance anode for potassium ion batteries. *Nano Research*, **2021**, 14, 3552-3561	10	8
320	Stable multifunctional single-atom catalysts adsorbed on pyrazine-modified graphyne. *Applied Surface Science*, **2021**, 553, 149464	6.7	11
319	Highly Efficient Photocatalytic CO Reduction in Two-Dimensional Ferroelectric CuInPS Bilayers. *ACS Applied Materials & Interfaces*, **2021**, 13, 34486-34494	9.5	11
318	Spin-Gapless States in Two-Dimensional Molecular Ferromagnet Fe(TCNQ). *Journal of Physical Chemistry Letters*, **2021**, 12, 7921-7927	6.4	0
317	Laser-driven anisotropic and nonlinear Rashba spin splitting in GaAs monolayer. *Physical Review B*, **2021**, 104,	3.3	1
316	Bi-atom active sites embedded in a two-dimensional covalent organic framework for efficient nitrogen reduction reaction. *Applied Surface Science*, **2021**, 563, 150352	6.7	6
315	Regulating polysulfide intermediates by ultrathin Co-Bi nanosheet electrocatalyst in lithium–sulfur batteries. *Nano Today*, **2021**, 40, 101246	17.9	15
314	Transition-metal monochalcogenide nanowires: highly efficient bi-functional catalysts for the oxygen evolution/reduction reactions. *Nanoscale*, **2020**, 12, 12883-12890	7.7	3

313	Ferroelectricity and multiferroicity in two-dimensional ScPSe and ScCrPSe monolayers. *Physical Chemistry Chemical Physics*, **2020**, 22, 7489-7496	3.6	9
312	Synergistic trifunctional electrocatalysis of pyridinic nitrogen and single transition-metal atoms anchored on pyrazine-modified graphdiyne. *Science Bulletin*, **2020**, 65, 995-1002	10.6	16
311	Tunable Valley Polarization in a Multiferroic CuCrP2Te6 Monolayer. *Physica Status Solidi - Rapid Research Letters*, **2020**, 14, 2000008	2.5	4
310	Anisotropic protein diffusion on nanosurface. *Nanoscale*, **2020**, 12, 5209-5216	7.7	10
309	Multifunctional electrocatalytic activity of coronene-based two-dimensional metal-organic frameworks: TM-PTC. *Applied Surface Science*, **2020**, 511, 145393	6.7	10
308	Orientational DNA binding and directed transport on nanomaterial heterojunctions. *Nanoscale*, **2020**, 12, 5217-5226	7.7	16
307	High-efficiency helium separation through an inorganic graphenylene membrane: a theoretical study. *Physical Chemistry Chemical Physics*, **2020**, 22, 9789-9795	3.6	14
306	Understanding CO capture kinetics and energetics by ionic liquids with molecular dynamics simulation.. *RSC Advances*, **2020**, 10, 13968-13974	3.7	6
305	Low-loss hyperbolic dispersion and anisotropic plasmonic excitation in nodal-line semimetallic yttrium nitride. *Optics Express*, **2020**, 28, 22076-22087	3.3	3
304	Inversion/Mirror Symmetry-Protected Dirac Cones in Distorted Ruby Lattices. *Chinese Physics Letters*, **2020**, 37, 127102	1.8	0
303	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	10.6	18
302	Metal-free highly efficient photocatalysts for overall water splitting: CN multilayers. *Nanoscale*, **2020**, 12, 306-315	7.7	24
301	Tunable ferroelectricity and antiferromagnetism via ferroelastic switching in an FeOOH monolayer. *Journal of Materials Chemistry C*, **2020**, 8, 13982-13989	7.1	6
300	Tunable valley splitting and anomalous valley Hall effect in VTe2/Ga2S3 heterostructures. *Journal of Materials Chemistry C*, **2020**, 8, 14895-14901	7.1	6
299	Stable Multifunctional Single-Atom Catalysts Resulting from the Synergistic Effect of Anchored Transition-Metal Atoms and Host Covalent□Organic Frameworks. *Journal of Physical Chemistry C*, **2020**, 124, 17675-17683	3.8	22
298	Serendipity for Topological Insulator as Multifunctional Electrocatalyst. *ACS Applied Energy Materials*, **2020**, 3, 8929-8936	6.1	0
297	Computational studies on triphenyldiyne as a two-dimensional visible-light-driven photocatalyst for overall water splitting. *Physical Chemistry Chemical Physics*, **2020**, 22, 20061-20068	3.6	2
296	Mild lipid extraction and anisotropic cell membrane penetration of □phase phosphorene carbide nanoribbons by molecular dynamics simulation studies. *Physical Chemistry Chemical Physics*, **2020**, 22, 23268-23275	3.6	6

295	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	5.1	4
294	Prediction of a ternary two-dimensional pentagonal Zn2C2P2 monolayer for photocatalytic water splitting with high carriers mobility. *Applied Surface Science*, **2020**, 518, 146197	6.7	6
293	Bifunctional HER/OER or OER/ORR Catalytic Activity of Two-Dimensional TM3(HITP)2 with TM = Fe□n. *Journal of Physical Chemistry C*, **2020**, 124, 9350-9359	3.8	32
292	Enhancing superconductivity in bulk □i2Pd by negative pressure induced by quantum electronic stress. *Physical Review B*, **2019**, 100,	3.3	2
291	Bifunctional Electrocatalytic Activity of Bis(iminothiolato)nickel Monolayer for Overall Water Splitting. *Journal of Physical Chemistry C*, **2019**, 123, 25651-25656	3.8	11
290	Dirac cones in a snub trihexagonal tiling lattice with reflective symmetry breaking. *Journal of Physics Condensed Matter*, **2019**, 31, 155001	1.8	1
289	Valley polarization and ferroelectricity in a two-dimensional GaAsC monolayer. *Physical Chemistry Chemical Physics*, **2019**, 21, 3954-3959	3.6	6
288	Intrinsic multiferroicity in two-dimensional VOCl monolayers. *Nanoscale*, **2019**, 11, 1103-1110	7.7	36
287	Porous-hollow nanorods constructed from alternate intercalation of carbon and MoS2 monolayers for lithium and sodium storage. *Nano Research*, **2019**, 12, 1912-1920	10	25
286	Tuning the electronic and magnetic properties of MoS nanotubes with vacancy defects.. *RSC Advances*, **2019**, 9, 17203-17210	3.7	7
285	Tungsten boride: a 2D multiple Dirac semimetal for the hydrogen evolution reaction. *Journal of Materials Chemistry C*, **2019**, 7, 8868-8873	7.1	30
284	Hydrogen Confined in a Single Wall Carbon Nanotube Becomes a Metallic and Superconductive Nanowire under High Pressure. *Nano Letters*, **2019**, 19, 2537-2542	11.5	8
283	Two-dimensional graphyne-like carbon nitrides: Moderate band gaps, high carrier mobility, high flexibility and type-II band alignment. *Carbon*, **2019**, 149, 234-241	10.4	25
282	Strain-tunable CO storage by black phosphorene and □PC from combined first principles and molecular dynamics studies. *Physical Chemistry Chemical Physics*, **2019**, 21, 20107-20117	3.6	7
281	First-principles design of highly-efficient earth-abundant electrocatalysts for hydrogen evolution reaction: TiF3 and its analogs. *Applied Surface Science*, **2019**, 495, 143623	6.7	6
280	Spontaneous full photocatalytic water splitting on 2D MoSe/SnSe and WSe/SnSe vdW heterostructures. *Nanoscale*, **2019**, 11, 14836-14843	7.7	73
279	Reversible out-of-plane spin texture in a two-dimensional ferroelectric material for persistent spin helix. *Physical Review Materials*, **2019**, 3,	3.2	21
278	Hyperbolic dispersion and negative refraction in a metal-organic framework Cu-BHT. *Physical Review Materials*, **2019**, 3,	3.2	7

277	Tunable broadband hyperbolic light dispersion in metal diborides. *Optics Express*, **2019**, 27, 36911-36922	3.3	6
276	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	13	18
275	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	3.6	1
274	Prediction of a flexible anode material for Li/Na ion batteries: Phosphorous carbide monolayer (PC). *Carbon*, **2019**, 141, 444-450	10.4	40
273	A Photoresponsive Rutile TiO Heterojunction with Enhanced Electron-Hole Separation for High-Performance Hydrogen Evolution. *Advanced Materials*, **2019**, 31, e1806596	24	137
272	Promotion of Overall Water Splitting Activity Over a Wide pH Range by Interfacial Electrical Effects of Metallic NiCo-nitrides Nanoparticle/NiCoO Nanoflake/graphite Fibers. *Advanced Science*, **2019**, 6, 1801829	13.6	78
271	An unprecedented high-temperature-tolerance 2D laminar MXene membrane for ultrafast hydrogen sieving. *Journal of Membrane Science*, **2019**, 569, 117-123	9.6	47
270	Strain-induced tunable negative differential resistance in triangle graphene spirals. *Nanotechnology* , **2018**, 29, 205202	3.4	3
269	Novel Conductive Metal-Organic Framework for a High-Performance Lithium-Sulfur Battery Host: 2D Cu-Benzenehexathial (BHT). *ACS Applied Materials & Interfaces*, **2018**, 10, 15012-15020	9.5	71
268	Topological states in a two-dimensional metal alloy in Si surface: BiAg/Si(111)-4 surface. *Physical Review B*, **2018**, 97,	3.3	7
267	Kane Fermion in a Two-Dimensional Conjugated Bis(iminothiolato)nickel Monolayer. *Journal of Physical Chemistry Letters*, **2018**, 9, 614-619	6.4	14
266	Promising half-metallicity in ductile NbF: a first-principles prediction. *Physical Chemistry Chemical Physics*, **2018**, 20, 4781-4786	3.6	6
265	ZrSi: an antiferromagnetic Dirac MXene. *Physical Chemistry Chemical Physics*, **2018**, 20, 3946-3952	3.6	10
264	Two-Dimensional Metal Organic Half-metallic Antiferromagnet: CoFePz. *Journal of Physical Chemistry C*, **2018**, 122, 1846-1851	3.8	14
263	Negative Poisson's ratio and high-mobility transport anisotropy in SiC siligraphene. *Nanoscale*, **2018** , 10, 2108-2114	7.7	41
262	Silicene and germanene on InSe substrates: structures and tunable electronic properties. *Physical Chemistry Chemical Physics*, **2018**, 20, 11369-11377	3.6	32
261	Direct Z-scheme photocatalytic overall water splitting on 2D CdS/InSe heterostructures. *Journal Physics D: Applied Physics*, **2018**, 51, 395501	3	30
260	Valley-selective circular dichroism and high carrier mobility of graphene-like BCN. *Nanoscale*, **2018**, 10, 13179-13186	7.7	22

259	PNTCDA: a promising versatile organic electrode material for alkali-metal ion batteries. *Journal of Materials Chemistry A*, **2018**, 6, 24869-24876	13	6
258	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	3.8	32
257	Conductive and Polar Titanium Boride as a Sulfur Host for Advanced Lithium–Sulfur Batteries. *Chemistry of Materials*, **2018**, 30, 6969-6977	9.6	75
256	Electronic properties of a π-conjugated Cairo pentagonal lattice: Direct band gap, ultrahigh carrier mobility, and slanted Dirac cones. *Physical Review B*, **2018**, 98,	3.3	13
255	Anchoring effects of S-terminated Ti2C MXene for lithium-sulfur batteries: A first-principles study. *Applied Surface Science*, **2018**, 455, 522-526	6.7	83
254	Irradiation resistance study of binderless nanopore-isotropic graphite for use in molten salt nuclear reactors. *Nuclear Engineering and Design*, **2018**, 335, 231-240	1.8	4
253	Predicting a graphene-like WB nanosheet with a double Dirac cone, an ultra-high Fermi velocity and significant gap opening by spin-orbit coupling. *Physical Chemistry Chemical Physics*, **2017**, 19, 5449-5453	3.6	28
252	Ultrabroadband MoS Photodetector with Spectral Response from 445 to 2717 nm. *Advanced Materials*, **2017**, 29, 1605972	24	166
251	Strain-Modulated Electronic Structure and Infrared Light Adsorption in Palladium Diselenide Monolayer. *Scientific Reports*, **2017**, 7, 39995	4.9	31
250	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	10	12
249	Tuning of Interlayer Coupling in Large-Area Graphene/WSe2 van der Waals Heterostructure via Ion Irradiation: Optical Evidences and Photonic Applications. *ACS Photonics*, **2017**, 4, 1531-1538	6.3	55
248	Efficient hydrogen isotopologues separation through a tunable potential barrier: The case of a CN membrane. *Scientific Reports*, **2017**, 7, 1483	4.9	14
247	Dirac node lines in two-dimensional Lieb lattices. *Nanoscale*, **2017**, 9, 8740-8746	7.7	27
246	Cu3N and its analogs: a new class of electrodes for lithium ion batteries. *Journal of Materials Chemistry A*, **2017**, 5, 8762-8768	13	25
245	A niobium and tantalum co-doped perovskite cathode for solid oxide fuel cells operating below 500 °C. *Nature Communications*, **2017**, 8, 13990	17.4	144
244	Low-energy transmission electron diffraction and imaging of large-area graphene. *Science Advances* , **2017**, 3, e1603231	14.3	18
243	Half-metallic TiF3: a potential anode material for Li-ion spin batteries. *Journal of Materials Chemistry A*, **2017**, 5, 21486-21490	13	13
242	Theoretical Discovery of a Superconducting Two-Dimensional Metal-Organic Framework. *Nano Letters*, **2017**, 17, 6166-6170	11.5	56

241	Efficient He/He separation in a nanoporous graphenylene membrane. *Physical Chemistry Chemical Physics*, **2017**, 19, 21522-21526	3.6	9
240	Theoretical Design of Highly Efficient CO2/N2 Separation Membranes Based on Electric Quadrupole Distinction. *Journal of Physical Chemistry C*, **2017**, 121, 17925-17931	3.8	14
239	Metal-free Ternary BCN Nanosheets with Synergetic Effect of Band Gap Engineering and Magnetic Properties. *Scientific Reports*, **2017**, 7, 6617	4.9	26
238	Chern Insulator and Chern Half-Metal States in the Two-Dimensional Spin-Gapless Semiconductor MnCS. *Journal of Physical Chemistry Letters*, **2017**, 8, 3770-3775	6.4	24
237	A promising alkali-metal ion battery anode material: 2D metallic phosphorus carbide (□-PC). *Electrochimica Acta*, **2017**, 258, 582-590	6.7	26
236	Tunable Dirac cones in two-dimensional covalent organic materials: C2N6S3 and its analogs. *RSC Advances*, **2017**, 7, 52065-52070	3.7	6
235	Dirac cones and highly anisotropic electronic structure of super-graphyne. *Carbon*, **2017**, 113, 40-45	10.4	23
234	Tunable topological states in electron-doped HTT-Pt. *Physical Review B*, **2016**, 93,	3.3	32
233	Electron spin-polarization and spin-gapless states in an oxidized carbon nitride monolayer. *RSC Advances*, **2016**, 6, 108280-108285	3.7	
232	Highly Efficient Quantum Sieving in Porous Graphene-like Carbon Nitride for Light Isotopes Separation. *Scientific Reports*, **2016**, 6, 19952	4.9	39
231	Spin-polarized Dirac cones and topological nontriviality in a metal-organic framework Ni2C24S6H12. *Physical Chemistry Chemical Physics*, **2016**, 18, 8059-64	3.6	38
230	Gas Adsorption Effects on the Electronic Properties of Two-Dimensional Nickel Bis(dithiolene) Complex. *Journal of Physical Chemistry C*, **2016**, 120, 3846-3852	3.8	29
229	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	2.3	2
228	Energetics of carbon and nitrogen impurities and their interactions with vacancy in vanadium. *Chinese Physics B*, **2016**, 25, 036104	1.2	5
227	Tunable C2N Membrane for High Efficient Water Desalination. *Scientific Reports*, **2016**, 6, 29218	4.9	53
226	Intrinsic current□oltage characteristics of metal-carbon nanotube networks: A first-principles study. *Organic Electronics*, **2016**, 31, 278-286	3.5	3
225	Prediction of an ultrasoft graphene allotrope with Dirac cones. *Carbon*, **2016**, 105, 323-329	10.4	42
224	Germanium sulfide nanosheet: a universal anode material for alkali metal ion batteries. *Journal of Materials Chemistry A*, **2016**, 4, 8905-8912	13	139

223	Band inversion and topological aspects in a TiNI monolayer. *Physical Chemistry Chemical Physics*, **2016**, 18, 22154-9	3.6	17
222	Kinetics of Nonlinear Optical Response at Insulator–Metal Transition in Vanadium Dioxide. *Advanced Optical Materials*, **2015**, 3, 64-70	8.1	6
221	High activity and durability of novel perovskite electrocatalysts for water oxidation. *Materials Horizons*, **2015**, 2, 495-501	14.4	119
220	Stacking dependent electronic properties of the nanofilms composing of super-aligned single-walled carbon nanotubes. *Journal Physics D: Applied Physics*, **2015**, 48, 215307	3	
219	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	17.1	125
218	Prediction of quantum anomalous Hall effect on graphene nanomesh. *RSC Advances*, **2015**, 5, 9875-9880	3.7	24
217	Driving a GaAs film to a large-gap topological insulator by tensile strain. *Scientific Reports*, **2015**, 5, 8441	4.9	50
216	Electron spin-polarization and band gap engineering in carbon-modified graphitic carbon nitrides. *Journal of Materials Chemistry C*, **2015**, 3, 10886-10891	7.1	12
215	Prediction of a large-gap quantum-spin-Hall insulator: Diamond-like GaBi bilayer. *Nano Research*, **2015**, 8, 3823-3829	10	9
214	Hydrogenation-induced large-gap quantum-spin-Hall insulator states in a germanium–tin dumbbell structure. *RSC Advances*, **2015**, 5, 72462-72468	3.7	12
213	Phagraphene: A Low-Energy Graphene Allotrope Composed of 5-6-7 Carbon Rings with Distorted Dirac Cones. *Nano Letters*, **2015**, 15, 6182-6	11.5	325
212	Efficient helium separation of graphitic carbon nitride membrane. *Carbon*, **2015**, 95, 51-57	10.4	88
211	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, 8122-8	11.5	26
210	Spin-gapless semiconducting graphitic carbon nitrides: A theoretical design from first principles. *Carbon*, **2015**, 84, 1-8	10.4	61
209	From UV to near-infrared, WS2 nanosheet: a novel photocatalyst for full solar light spectrum photodegradation. *Advanced Materials*, **2015**, 27, 363-9	24	402
208	Strain-driven band inversion and topological aspects in Antimonene. *Scientific Reports*, **2015**, 5, 16108	4.9	166
207	Robust half-metallicity and topological aspects in two-dimensional Cu-TPyB. *Scientific Reports*, **2015**, 5, 14098	4.9	24
206	Chemical Weathering–Exfoliation of Atom-Thick Transition Metal Dichalcogenides and Their Ultrafast Saturable Absorption Properties. *Advanced Functional Materials*, **2015**, 25, 5292-5299	15.6	60

205	High hydrogen storage capacity in calcium-decorated silicene nanostructures. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 2072-2078	1.3	9
204	Dumbbell stanane: a large-gap quantum spin hall insulator. *Physical Chemistry Chemical Physics*, **2015**, 17, 16624-9	3.6	24
203	Intrinsic half-metallicity in fractal carbon nitride honeycomb lattices. *Physical Chemistry Chemical Physics*, **2015**, 17, 21837-44	3.6	14
202	Role of edge dehydrogenation in magnetization and spin transport of zigzag graphene nanoribbons with line defects. *Organic Electronics*, **2015**, 27, 212-220	3.5	4
201	A comparative study of SrCo0.8Nb0.2O3□ and SrCo0.8Ta0.2O3□ 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	13	43
200	Tensile strain induced half-metallicity in graphene-like carbon nitride. *Physical Chemistry Chemical Physics*, **2015**, 17, 6028-35	3.6	31
199	Giant topological nontrivial band gaps in chloridized gallium bismuthide. *Nano Letters*, **2015**, 15, 1296-301	11.5	81
198	Strain-induced phase transition and electron spin-polarization in graphene spirals. *Scientific Reports* , **2014**, 4, 5699	4.9	11
197	The stability and electronic structure of Fe atoms embedded in zigzag graphene nanoribbons. *Physica B: Condensed Matter*, **2014**, 441, 28-32	2.8	5
196	A metallic carbon allotrope with superhardness: a first-principles prediction. *Journal of Materials Chemistry C*, **2014**, 2, 2751-2757	7.1	36
195	Theoretical characterization of layered silica nanostructures from first-principles prediction. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 3348-3353	2.3	8
194	Electron spin-polarization and spin lattices in the boron- and nitrogen-doped organic framework COF-5. *Physical Chemistry Chemical Physics*, **2014**, 16, 23286-91	3.6	14
193	Structures, Energetics, and Electronic Properties of Multifarious Stacking Patterns for High-Buckled and Low-Buckled Silicene on the MoS2 Substrate. *Journal of Physical Chemistry C*, **2014**, 118, 19129-19138	4.8	67
192	Two-dimensional topological insulators with binary honeycomb lattices: SiC3 siligraphene and its analogs. *Physical Review B*, **2014**, 89,	3.3	65
191	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	1.1	13
190	Topological insulator states in a honeycomb lattice of s-triazines. *Nanoscale*, **2014**, 6, 11157-62	7.7	65
189	SiC coating: An alternative for the protection of nuclear graphite from liquid fluoride salt. *Journal of Nuclear Materials*, **2014**, 448, 1-3	3.3	43
188	Half-metallicity of C/BN hybrid nanoribbons containing a topological defective interface. *Physica E: Low-Dimensional Systems and Nanostructures*, **2014**, 60, 224-228	3	1

187	Graphyne-based carbon allotropes with tunable properties: From Dirac fermion to semiconductor. *Diamond and Related Materials*, **2014**, 41, 65-72	3.5	28
186	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	3	9
185	A comparative first-principles study of the electronic, mechanical, defect and acoustic properties of Ti2AlC and Ti3AlC. *Journal Physics D: Applied Physics*, **2014**, 47, 215301	3	21
184	Characterization of the effects of 3-MeV proton irradiation on fine-grained isotropic nuclear graphite. *Carbon*, **2014**, 77, 311-318	10.4	23
183	Spin memristive magnetic tunnel junctions with CoO-ZnO nano composite barrier. *Scientific Reports* , **2014**, 4, 3835	4.9	18
182	One-Step Exfoliation and Fluorination of Boron Nitride Nanosheets and a Study of Their Magnetic Properties. *Angewandte Chemie*, **2014**, 126, 3719-3723	3.6	29
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