

Aijun Du

List of Publications by Year in Descending Order

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Version: 2024-04-27

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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.

336
papers

21,396
citations

69
h-index

137
g-index

356
ext. papers

25,674
ext. citations

7.9
avg, IF

7.55
L-index

#	Paper	IF	Citations
336	hcp-phased Ni nanoparticles with generic catalytic hydrogenation activities toward different functional groups. <i>Science China Materials</i> , 2022 , 65, 1252	7.1	1
335	Vacancy engineering of oxidized Nb ₂ CT _x MXenes for a biased nitrogen fixation. <i>Green Energy and Environment</i> , 2022 ,	5.7	1
334	Controlling the Interfacial Charge Polarization of MOF-Derived 0D-2D vdW Architectures as a Unique Strategy for Bifunctional Oxygen Electrocatalysis.. <i>ACS Applied Materials & Interfaces</i> , 2022 ,	9.5	8
333	Coupling Fe ₃ O ₄ /Fe _{1-x} S@Carbon with carbon-coated MoS ₂ nanosheets as a superior anode for sodium-ion batteries. <i>Chemical Engineering Journal</i> , 2022 , 427, 131652	14.7	4
332	In-situ conversion growth of carbon-coated MoS ₂ /N-doped carbon nanotubes as anodes with superior capacity retention for sodium-ion batteries. <i>Journal of Materials Science and Technology</i> , 2022 , 102, 8-15	9.1	3
331	Carbon-coated MoS ₂ nanosheets@CNTs-Ti ₃ C ₂ MXene quaternary composite with the superior rate performance for sodium-ion batteries. <i>Journal of Materials Science and Technology</i> , 2022 , 100, 101-109	9.1	4
330	Nanostructure Shape-Effects in ZnO heterogeneous photocatalysis. <i>Journal of Colloid and Interface Science</i> , 2022 , 606, 588-599	9.3	5
329	K-Functionalized Carbon Quantum Dots-Induced Interface Assembly of Carbon Nanocages for Ultrastable Potassium Storage Performance.. <i>Small Methods</i> , 2022 , e2101627	12.8	0
328	N/P-Doped MoS ₂ Monolayers as Promising Materials for Controllable CO ₂ Capture and Separation under Reduced Electric Fields: A Theoretical Modeling. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 203-211	3.8	0
327	Controllable Acceleration and Deceleration of Charge Carrier Transport in Metal-Halide Perovskite Single-Crystal by Cs-Cation Induced Bandgap Engineering.. <i>Small</i> , 2022 , e2107680	11	1
326	Versatile Gold Telluride Iodide Monolayer as a Potential Photocatalyst for Water Splitting. <i>Nanomaterials</i> , 2022 , 12, 1915	5.4	0
325	Atomically Dispersed Heteronuclear Dual-Atom Catalysts: A New Rising Star in Atomic Catalysis.. <i>Small</i> , 2021 , e2106091	11	9
324	Two-Dimensional Janus Antimony Selenium Telluride with Large Rashba Spin Splitting and High Electron Mobility. <i>ACS Omega</i> , 2021 , 6, 31919-31925	3.9	1
323	Surface-Dependent Intermediate Adsorption Modulation on Iridium-Modified Black Phosphorus Electrocatalysts for Efficient pH-Universal Water Splitting. <i>Advanced Materials</i> , 2021 , 33, e2104638	24	14
322	Leaf-inspired design of mesoporous Sb ₂ S ₃ /N-doped Ti ₃ C ₂ T _x composite towards fast sodium storage. <i>Science China Chemistry</i> , 2021 , 64, 964-973	7.9	20
321	Sn ²⁺ -Regulated Synthesis of a Bone-like Fe ₃ O ₄ @N-Doped Carbon Composite as the Anode for High-Performance Lithium Storage. <i>ACS Applied Energy Materials</i> , 2021 , 4, 3785-3793	6.1	5
320	Regulating the interfacial behavior of carbon nanotubes for fast lithium storage. <i>Electrochimica Acta</i> , 2021 , 388, 138591	6.7	3

319	A Highly Efficient Conjoined-twin Porphyrin-based Complex for the Electrochemical Reduction of CO to Ethanol. <i>ChemNanoMat</i> , 2021 , 7, 935-941	3.5	0
318	High-Performance Perovskite Composite Electrocatalysts Enabled by Controllable Interface Engineering. <i>Small</i> , 2021 , 17, e2101573	11	44
317	Unravelling the Reaction Mechanisms of N Fixation on Molybdenum Nitride: A Full DFT Study from the Pristine Surface to Heteroatom Anchoring. <i>ChemSusChem</i> , 2021 , 14, 3257-3266	8.3	7
316	Computational Design and Experimental Validation of the Optimal Bimetal-Doped SrCoO Perovskite as Solid Oxide Fuel Cell Cathode. <i>Journal of the American Chemical Society</i> , 2021 , 143, 9507-9514	16.4	14
315	B-incorporated, N-doped hierarchically porous carbon nanosheets as anodes for boosted potassium storage capability. <i>Chinese Chemical Letters</i> , 2021 , 33, 480-480	8.1	4
314	High capacity and mobility in germanium sulfide/graphene (GeS/Gr) van der Waals heterostructure as anode materials for sodium-ion batteries: A first-principles investigation. <i>Applied Surface Science</i> , 2021 , 536, 147779	6.7	7
313	Theoretical insights into the performance of single and double transition metal atoms doped on N-graphenes for N ₂ electroreduction. <i>Applied Surface Science</i> , 2021 , 537, 148012	6.7	12
312	First principles studies of mononuclear and dinuclear Pacman complexes for electrocatalytic reduction of CO ₂ . <i>Catalysis Science and Technology</i> , 2021 , 11, 637-645	5.5	3
311	Prediction of room-temperature ferromagnetism and large perpendicular magnetic anisotropy in a planar hypercoordinate FeB monolayer. <i>Nanoscale Horizons</i> , 2021 , 6, 43-48	10.8	19
310	Two-dimensional vanadium tetrafluoride with antiferromagnetic ferroelasticity and bidirectional negative Poisson's ratio. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 95-100	7.1	8
309	N ₂ electrochemical reduction on two dimensional transition metal monoborides: A density functional theory study. <i>International Journal of Quantum Chemistry</i> , 2021 , 121, e26548	2.1	1
308	Manipulating the Solvation Structure of Nonflammable Electrolyte and Interface to Enable Unprecedented Stability of Graphite Anodes beyond 2 Years for Safe Potassium-Ion Batteries. <i>Advanced Materials</i> , 2021 , 33, e2006313	24	91
307	Ultrasml SnO ₂ nanocrystals sandwiched into polypyrrole and Ti ₃ C ₂ T _x MXene for highly effective sodium storage. <i>Materials Chemistry Frontiers</i> , 2021 , 5, 825-833	7.8	13
306	Exploring Aluminum-Ion Insertion into Magnesium-Doped Manjiroite (MnO ₂) Nanorods in Aqueous Solution. <i>ChemElectroChem</i> , 2021 , 8, 1048-1054	4.3	1
305	Integrating SnS ₂ Quantum Dots with Nitrogen-Doped Ti ₃ C ₂ T _x MXene Nanosheets for Robust Sodium Storage Performance. <i>ACS Applied Energy Materials</i> , 2021 , 4, 846-854	6.1	17
304	First-principles prediction of polar half-metallicity and out-of-plane piezoelectricity in two-dimensional quintuple layered cobalt selenide. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 12046-12050	7.1	2
303	Unlocking the potential of ruthenium catalysts for nitrogen fixation with subsurface oxygen. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 6575-6582	13	5
302	Tuning CO binding strength via engineering the copper/borophene interface for highly efficient conversion of CO into ethanol. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 13192-13199	13	7

301	Prediction of two-dimensional ferroelectric metal Mxenes. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 11343-11348	7.1	2
300	First-principles prediction of ferroelasticity tuned anisotropic auxeticity and carrier mobility in two-dimensional AgO. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 3155-3160	7.1	5
299	Exploring Aluminum-Ion Insertion into Magnesium-Doped Manjiroite (MnO ₂) Nanorods in Aqueous Solution. <i>ChemElectroChem</i> , 2021 , 8, 995-995	4.3	
298	Thermal Reductive Perforation of Graphene Cathode for High-Performance Aluminum-Ion Batteries. <i>Advanced Functional Materials</i> , 2021 , 31, 2010569	15.6	15
297	Boron-rich boron nitride nanomaterials as efficient metal-free catalysts for converting CO ₂ into valuable fuel. <i>Applied Surface Science</i> , 2021 , 555, 149652	6.7	4
296	Controllable CO electrocatalytic reduction via ferroelectric switching on single atom anchored InSe monolayer. <i>Nature Communications</i> , 2021 , 12, 5128	17.4	30
295	Purely one-dimensional ferroelectricity and antiferroelectricity from van der Waals niobium oxide trihalides. <i>Npj Computational Materials</i> , 2021 , 7,	10.9	2
294	Rhodium-molybdenum oxide electrocatalyst with dual active sites for electrochemical ammonia synthesis under neutral pH condition. <i>Journal of Electroanalytical Chemistry</i> , 2021 , 896, 115157	4.1	1
293	CO Capture, Separation and Reduction on Boron-Doped MoS ₂ , MoSe and Heterostructures with Different Doping Densities: A Theoretical Study. <i>ChemPhysChem</i> , 2021 , 22, 2392-2400	3.2	1
292	Predicting MnB ₆ monolayer with room temperature ferromagnetism and high magnetic anisotropy. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 134, 114930	3	1
291	Interfacing 2D VS ₂ with Janus MoSSe: Antiferromagnetic electric polarization and charge transfer driven Half-metallicity. <i>Applied Surface Science</i> , 2021 , 570, 151129	6.7	1
290	Techniques enabling inorganic materials into wearable fiber/yarn and flexible lithium-ion batteries. <i>Energy Storage Materials</i> , 2021 , 43, 62-84	19.4	6
289	Numerical investigation of microstructure and failure of lithiated silicon under biaxial tension. <i>Computational Materials Science</i> , 2021 , 200, 110764	3.2	
288	Tuning the Intermolecular Electron Transfer of Low-Dimensional and Metal-Free BCN/C Electrocatalysts via Interfacial Defects for Efficient Hydrogen and Oxygen Electrochemistry. <i>Journal of the American Chemical Society</i> , 2021 , 143, 1203-1215	16.4	54
287	Graphynes as emerging 2D-platforms for electronic and energy applications: a computational perspective. <i>Materials Chemistry Frontiers</i> , 2021 , 5, 6392-6412	7.8	2
286	Tunable magnetic anisotropy in 2D magnets via molecular adsorption. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 14948-14953	7.1	9
285	Direct conversion of metal organic frameworks into ultrafine phosphide nanocomposites in multicomponent plasma for wide pH hydrogen evolution. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 10402-10408	13.7	7
284	In Situ Formation of Oxygen Vacancies Achieving Near-Complete Charge Separation in Planar BiVO ₄ Photoanodes. <i>Advanced Materials</i> , 2020 , 32, e2001385	24	103

283	Atomically embedded asymmetrical dual-metal dimers on N-doped graphene for ultra-efficient nitrogen reduction reaction. <i>Journal of Catalysis</i> , 2020 , 388, 77-83	7.3	66
282	The importance of atomic charge distributions of solid boron material in N ₂ electrochemical reduction. <i>Applied Surface Science</i> , 2020 , 526, 146606	6.7	10
281	Potassium Doping to Enhance Green Photoemission of Light-Emitting Diodes Based on CsPbBr ₃ Perovskite Nanocrystals. <i>Advanced Optical Materials</i> , 2020 , 8, 2000742	8.1	14
280	Remarkably improved oxygen evolution reaction activity of cobalt oxides by an Fe ion solution immersion process. <i>Inorganic Chemistry Frontiers</i> , 2020 , 7, 3327-3339	6.8	13
279	A Directional Synthesis for Topological Defect in Carbon. <i>CheM</i> , 2020 , 6, 2009-2023	16.2	49
278	Multiferroic decorated FeO monolayer predicted from first principles. <i>Nanoscale</i> , 2020 , 12, 14847-14852	7.7	16
277	Computational Screening of Transition Metal Porphyrins for the Electrochemical Reduction of Carbon Dioxide. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 7708-7715	3.8	14
276	Polymorphism of low dimensional boron nanomaterials driven by electrostatic gating: a computational discovery. <i>Nanoscale</i> , 2020 , 12, 10543-10549	7.7	2
275	Synergistic trifunctional electrocatalysis of pyridinic nitrogen and single transition-metal atoms anchored on pyrazine-modified graphdiyne. <i>Science Bulletin</i> , 2020 , 65, 995-1002	10.6	16
274	Reversible gas capture using a ferroelectric switch and 2D molecule multiferroics on the In ₂ Se ₃ monolayer. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 7331-7338	13	29
273	Edge-Rich Fe-N Active Sites in Defective Carbon for Oxygen Reduction Catalysis. <i>Advanced Materials</i> , 2020 , 32, e2000966	24	113
272	Gradient-Concentration Design of Stable Core-Shell Nanostructure for Acidic Oxygen Reduction Electrocatalysis. <i>Advanced Materials</i> , 2020 , 32, e2003493	24	30
271	Water Splitting: In Situ Formation of Oxygen Vacancies Achieving Near-Complete Charge Separation in Planar BiVO ₄ Photoanodes (Adv. Mater. 26/2020). <i>Advanced Materials</i> , 2020 , 32, 2070198	24	2
270	Computational screening of MN (M = Ti-Cu) based metal organic frameworks for CO reduction using the d-band centre as a descriptor. <i>Nanoscale</i> , 2020 , 12, 6188-6194	7.7	25
269	Molten-Salt-Mediated Synthesis of an Atomic Nickel Co-catalyst on TiO for Improved Photocatalytic H ₂ Evolution. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 7230-7234	16.4	102
268	Molten-Salt-Mediated Synthesis of an Atomic Nickel Co-catalyst on TiO ₂ for Improved Photocatalytic H ₂ Evolution. <i>Angewandte Chemie</i> , 2020 , 132, 7297-7301	3.6	27
267	Bandstructure engineering in 2D materials using Ferroelectric materials. <i>Applied Surface Science</i> , 2020 , 513, 145817	6.7	7
266	Metal-free graphene/boron nitride heterointerface for CO ₂ reduction: Surface curvature controls catalytic activity and selectivity. <i>EcoMat</i> , 2020 , 2, e12013	9.4	7

265	An Intrinsically Non-flammable Electrolyte for High-Performance Potassium Batteries. <i>Angewandte Chemie</i> , 2020 , 132, 3667-3673	3.6	6
264	Dimensionality-Controlled Surface Passivation for Enhancing Performance and Stability of Perovskite Solar Cells via Triethylenetetramine Vapor. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 6651-6661	9.5	18
263	Electric-controlled half-metallicity in magnetic van der Waals heterobilayer. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 7034-7040	7.1	16
262	The effect of ethylene-amine ligands enhancing performance and stability of perovskite solar cells. <i>Journal of Power Sources</i> , 2020 , 463, 228210	8.9	12
261	Molecular dynamic investigation of the structure and stress in crystalline and amorphous silicon during lithiation. <i>Computational Materials Science</i> , 2020 , 183, 109811	3.2	5
260	Highly stable two-dimensional gold selenide with large in-plane anisotropy and ultrahigh carrier mobility. <i>Nanoscale Horizons</i> , 2020 , 5, 366-371	10.8	15
259	Atomically dispersed asymmetric Cu ₂ B pair on 2D carbon nitride synergistically boosts the conversion of CO into C ₂ products. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 599-606	13	33
258	Fabricating highly efficient heterostructured CuBi ₂ O ₄ photocathodes for unbiased water splitting. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 2498-2504	13	26
257	Cu ₂ B active sites stabilization through Mott-Schottky effect for promoting highly efficient conversion of carbon monoxide into n-propanol. <i>Journal of Catalysis</i> , 2020 , 382, 49-56	7.3	15
256	Two-dimensional heterojunction SnS ₂ /SnO ₂ photoanode with excellent photoresponse up to near infrared region. <i>Solar Energy Materials and Solar Cells</i> , 2020 , 207, 110342	6.4	6
255	Electrochemical reduction of carbon dioxide on precise number of Fe atoms anchored graphdiyne. <i>Journal of CO₂ Utilization</i> , 2020 , 37, 272-277	7.6	46
254	A zinc bromine Supercapattery system combining triple functions of capacitive, pseudocapacitive and battery-type charge storage. <i>Materials Horizons</i> , 2020 , 7, 495-503	14.4	30
253	Development of cross-linked dextrin as aqueous binders for silicon based anodes. <i>Journal of Power Sources</i> , 2020 , 450, 227671	8.9	28
252	Borophene: A Metal-free and Metallic Electrocatalyst for Efficient Converting CO ₂ into CH ₄ . <i>ChemCatChem</i> , 2020 , 12, 1483-1490	5.2	15
251	Stacking-Dependent Interlayer Magnetic Coupling in 2D CrI ₃ /CrGeTe ₃ Nanostructures for Spintronics. <i>ACS Applied Nano Materials</i> , 2020 , 3, 1282-1288	5.6	27
250	An Intrinsically Non-flammable Electrolyte for High-Performance Potassium Batteries. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 3638-3644	16.4	134
249	First-principles study of a Mn-doped In ₂ Se ₃ monolayer: Coexistence of ferromagnetism and ferroelectricity with robust half-metallicity and enhanced polarization. <i>Physical Review B</i> , 2020 , 102,	3.3	10
248	Solvent Effect on Supramolecular Self-Assembly of Chlorophylls a on Chemically Reduced Graphene Oxide. <i>Langmuir</i> , 2020 , 36, 13575-13582	4	6

247	Tailoring the Interfacial Interactions of van der Waals 1T-MoS/C Heterostructures for High-Performance Hydrogen Evolution Reaction Electrocatalysis. <i>Journal of the American Chemical Society</i> , 2020 , 142, 17923-17927	16.4	53
246	2D atomic crystal molecular superlattices by soft plasma intercalation. <i>Nature Communications</i> , 2020 , 11, 5960	17.4	14
245	Strain induced variation of PFOS adsorption on pristine and defected phosphorene: A DFT study. <i>Applied Surface Science</i> , 2020 , 532, 147452	6.7	5
244	Single Copper Atoms Supported on ZnS as an Efficient Catalyst for Electrochemical Reduction of CO to CH ₃ OH. <i>ChemNanoMat</i> , 2020 , 6, 1806-1811	3.5	5
243	First-principles screening of novel ferroelectric MXene phases with a large piezoelectric response and unusual auxeticity. <i>Nanoscale</i> , 2020 , 12, 21291-21298	7.7	18
242	Tuning band alignment and optical properties of 2D van der Waals heterostructure via ferroelectric polarization switching. <i>Frontiers of Physics</i> , 2020 , 15, 1	3.7	9
241	Dual-Ion-Diffusion Induced Degradation in Lead-Free Cs ₂ AgBiBr ₆ Double Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2020 , 30, 2002342	15.6	39
240	Cobalt porphyrin supported on graphene/Ni (111) surface: Enhanced oxygen evolution/reduction reaction and the role of electron coupling. <i>Catalysis Today</i> , 2020 , 351, 113-118	5.3	11
239	Novel two-dimensional MOF as a promising single-atom electrocatalyst for CO ₂ reduction: A theoretical study. <i>Applied Surface Science</i> , 2020 , 500, 143993	6.7	43
238	Strain engineering of selective chemical adsorption on monolayer black phosphorous. <i>Applied Surface Science</i> , 2020 , 503, 144033	6.7	12
237	Functionalized boron nitride monolayers as promising materials for uranyl ion capture: A first-principles study. <i>Journal of Molecular Structure</i> , 2020 , 1200, 127080	3.4	4
236	Carbon-Phosphorus Bonds-Enriched 3D Graphene by Self-Sacrificing Black Phosphorus Nanosheets for Elevating Capacitive Lithium Storage. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 21720-21729	9.5	21
235	Plasma-induced on-surface sulfur vacancies in NiCo ₂ S ₄ enhance the energy storage performance of supercapatteries. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 9278-9291	13	27
234	Recent progress on the prediction of two-dimensional materials using CALYPSO. <i>Chinese Physics B</i> , 2019 , 28, 107306	1.2	11
233	B80 Fullerene: A Promising Metal-Free Photocatalyst for Efficient Conversion of CO ₂ to HCOOH. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 24193-24199	3.8	10
232	Two-Dimensional CuTe ₂ X (X = Cl, Br, and I): Potential Photocatalysts for Water Splitting under the Visible/Infrared Light. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 25543-25548	3.8	1
231	Single tungsten atom supported on N-doped graphyne as a high-performance electrocatalyst for nitrogen fixation under ambient conditions. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 1546-1551	3.6	94
230	2D boron dichalcogenides from the substitution of Mo with ionic B ₂ pair in MoX ₂ (X = S, Se and Te): high stability, large excitonic effect and high charge carrier mobility. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 1651-1658	7.1	11

229	Electronic and optical properties of lead-free hybrid double perovskites for photovoltaic and optoelectronic applications. <i>Scientific Reports</i> , 2019 , 9, 718	4.9	55
228	Single Transition Metal Atom-Doped Graphene Supported on a Nickel Substrate: Enhanced Oxygen Reduction Reactions Modulated by Electron Coupling. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 3703-3710	3.8	21
227	WO ₃ nanolayer coated 3D-graphene/sulfur composites for high performance lithium/sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 4596-4603	13	36
226	Transition metal dichalcogenides bilayer single crystals by reverse-flow chemical vapor epitaxy. <i>Nature Communications</i> , 2019 , 10, 598	17.4	69
225	A single boron atom doped boron nitride edge as a metal-free catalyst for N fixation. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 1110-1116	3.6	84
224	2D-3D Mixed Organic-Inorganic Perovskite Layers for Solar Cells with Enhanced Efficiency and Stability Induced by -Propylammonium Iodide Additives. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 29753-29764	9.5	60
223	Single Pt atom decorated graphitic carbon nitride as an efficient photocatalyst for the hydrogenation of nitrobenzene into aniline. <i>Nano Research</i> , 2019 , 12, 1817-1823	10	61
222	Reversible Intercalation of Multivalent Al Ions into Potassium-Rich Cryptomelane Nanowires for Aqueous Rechargeable Al-Ion Batteries. <i>ChemSusChem</i> , 2019 , 12, 3753-3760	8.3	31
221	Galvanic replacement of liquid metal galinstan with Pt for the synthesis of electrocatalytically active nanomaterials. <i>Nanoscale</i> , 2019 , 11, 9705-9715	7.7	26
220	Transition Metal Diborides: A New Type of High-performance Electrocatalysts for Nitrogen Reduction. <i>ChemCatChem</i> , 2019 , 11, 2624-2633	5.2	25
219	Predicting Novel 2D MB (M = Ti, Hf, V, Nb, Ta) Monolayers with Ultrafast Dirac Transport Channel and Electron-Orbital Controlled Negative Poisson's Ratio. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 2567-2573	6.4	37
218	Mo-based 2D MOF as a highly efficient electrocatalyst for reduction of N ₂ to NH ₃ : a density functional theory study. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 14510-14518	13	90
217	Theoretical discovery of Dirac half metal in experimentally synthesized two dimensional metal semiquinoid frameworks. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 5792-5796	7.1	13
216	Defective Graphene on the Transition-Metal Surface: Formation of Efficient Bifunctional Catalysts for Oxygen Evolution/Reduction Reactions in Alkaline Media. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 17410-17415	9.5	17
215	Silicene catalysts for CO hydrogenation: the number of layers controls selectivity. <i>Nanoscale</i> , 2019 , 11, 7734-7743	7.7	19
214	Plasma modification of a Ni based metal-organic framework for efficient hydrogen evolution. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 8129-8135	13	21
213	Mo-doped boron nitride monolayer as a promising single-atom electrocatalyst for CO conversion. <i>Beilstein Journal of Nanotechnology</i> , 2019 , 10, 540-548	3	25
212	Synthesis of biphenyl bridged dendritic mesoporous organosilica with extremely high adsorption of pyrene. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 12029-12037	13	19

211	Silicon Nanocages for Selective Carbon Dioxide Conversion under Visible Light. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 9973-9980	3.8	15
210	Reversible Intercalation of Multivalent Al ³⁺ Ions into Potassium-Rich Cryptomelane Nanowires for Aqueous Rechargeable Al-Ion Batteries. <i>ChemSusChem</i> , 2019 , 12, 3670-3670	8.3	2
209	Ultralarge interlayer distance and C,N-codoping enable superior sodium storage capabilities of MoS ₂ nanooxions. <i>Chemical Engineering Journal</i> , 2019 , 378, 122249	14.7	24
208	Ab initio atomistic insights into lead-free formamidinium based hybrid perovskites for photovoltaics and optoelectronics. <i>Computational Materials Science</i> , 2019 , 169, 109118	3.2	15
207	Identifying Copper Vacancies and Their Role in the CuO Based Photocathode for Water Splitting. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 17604-17609	16.4	51
206	Intrinsic Ultrahigh Negative Poisson's Ratio in Two-Dimensional Ferroelectric ABP2X6 Materials. <i>Wuli Huaxue Xuebao/Acta Physico-Chimica Sinica</i> , 2019 , 35, 1128-1133	3.8	8
205	Silicon-doped graphene edges: an efficient metal-free catalyst for the reduction of CO ₂ into methanol and ethanol. <i>Catalysis Science and Technology</i> , 2019 , 9, 6800-6807	5.5	30
204	PT-symmetry-protected Dirac states in strain-induced hidden MoS ₂ monolayer. <i>Physical Review B</i> , 2019 , 100,	3.3	6
203	Understanding the Roles of Oxygen Vacancies in Hematite-Based Photoelectrochemical Processes. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 1030-1034	16.4	159
202	Understanding the Roles of Oxygen Vacancies in Hematite-Based Photoelectrochemical Processes. <i>Angewandte Chemie</i> , 2019 , 131, 1042-1046	3.6	54
201	Tailoring Crystal Structure of FA _{0.83} Cs _{0.17} PbI ₃ Perovskite Through Guanidinium Doping for Enhanced Performance and Tunable Hysteresis of Planar Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2019 , 29, 1806479	15.6	64
200	First-Principles Prediction of a Room-Temperature Ferromagnetic Janus VSSe Monolayer with Piezoelectricity, Ferroelasticity, and Large Valley Polarization. <i>Nano Letters</i> , 2019 , 19, 1366-1370	11.5	155
199	Predicting ultrafast Dirac transport channel at the one-dimensional interface of the two-dimensional coplanar ZnO/MoS ₂ heterostructure. <i>Physical Review B</i> , 2019 , 99,	3.3	4
198	Transition-Metal Single Atoms Anchored on Graphdiyne as High-Efficiency Electrocatalysts for Water Splitting and Oxygen Reduction. <i>Small Methods</i> , 2019 , 3, 1800419	12.8	133
197	Boron Radicals Identified as the Source of the Unexpected Catalysis by Boron Nitride Nanosheets. <i>ACS Nano</i> , 2019 , 13, 1394-1402	16.7	27
196	A General Two-Step StrategyBased High-Throughput Screening of Single Atom Catalysts for Nitrogen Fixation. <i>Small Methods</i> , 2019 , 3, 1800376	12.8	175
195	Single-atom supported on graphene grain boundary as an efficient electrocatalyst for hydrogen evolution reaction. <i>Chemical Engineering Science</i> , 2019 , 194, 58-63	4.4	50
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