

# Aijun Du

## List of Publications by Citations

**Source:** <https://exaly.com/author-pdf/4008967/ajun-du-publications-by-citations.pdf>

**Version:** 2024-04-27

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

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	Hydrogen evolution by a metal-free electrocatalyst. <i>Nature Communications</i> , <b>2014</b> , 5, 3783	17.4	1572
335	TiC MXene co-catalyst on metal sulfide photo-absorbers for enhanced visible-light photocatalytic hydrogen production. <i>Nature Communications</i> , <b>2017</b> , 8, 13907	17.4	1073
334	Nanoporous graphitic-C <sub>3</sub> N <sub>4</sub> @carbon metal-free electrocatalysts for highly efficient oxygen reduction. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 20116-9	16.4	869
333	Single Atom (Pd/Pt) Supported on Graphitic Carbon Nitride as an Efficient Photocatalyst for Visible-Light Reduction of Carbon Dioxide. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 6292-7	16.4	735
332	Defect Graphene as a Trifunctional Catalyst for Electrochemical Reactions. <i>Advanced Materials</i> , <b>2016</b> , 28, 9532-9538	24	711
331	A Heterostructure Coupling of Exfoliated Ni-Fe Hydroxide Nanosheet and Defective Graphene as a Bifunctional Electrocatalyst for Overall Water Splitting. <i>Advanced Materials</i> , <b>2017</b> , 29, 1700017	24	651
330	2D MXenes: A New Family of Promising Catalysts for the Hydrogen Evolution Reaction. <i>ACS Catalysis</i> , <b>2017</b> , 7, 494-500	13.1	548
329	Hybrid graphene and graphitic carbon nitride nanocomposite: gap opening, electron-hole puddle, interfacial charge transfer, and enhanced visible light response. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 4393-7	16.4	490
328	Metal-Free Single Atom Catalyst for N Fixation Driven by Visible Light. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 14161-14168	16.4	460
327	Graphene Defects Trap Atomic Ni Species for Hydrogen and Oxygen Evolution Reactions. <i>Chem</i> , <b>2018</b> , 4, 285-297	16.2	436
326	Understanding the Enhancement in Photoelectrochemical Properties of Photocatalytically Prepared TiO <sub>2</sub> -Reduced Graphene Oxide Composite. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 6004-6009	23.8	377
325	Graphdiyne: a versatile nanomaterial for electronics and hydrogen purification. <i>Chemical Communications</i> , <b>2011</b> , 47, 11843-5	5.8	289
324	Organic/inorganic bismuth (III)-based material: A lead-free, air-stable and solution-processable light-absorber beyond organolead perovskites. <i>Nano Research</i> , <b>2016</b> , 9, 692-702	10	283
323	Multifunctional porous graphene for nanoelectronics and hydrogen storage: new properties revealed by first principle calculations. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 2876-7	16.4	277
322	Charge Mediated Semiconducting-to-Metallic Phase Transition in Molybdenum Disulfide Monolayer and Hydrogen Evolution Reaction in New 1T' Phase. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 13124-13128	33.8	248
321	Charge-controlled switchable CO <sub>2</sub> capture on boron nitride nanomaterials. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 8246-53	16.4	239
320	First-principles prediction of metal-free magnetism and intrinsic half-metallicity in graphitic carbon nitride. <i>Physical Review Letters</i> , <b>2012</b> , 108, 197207	7.4	234

319	Hybrid Graphene/Titania Nanocomposite: Interface Charge Transfer, Hole Doping, and Sensitization for Visible Light Response. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 894-9	6.4	230
318	Synergistic crystal facet engineering and structural control of WO <sub>3</sub> films exhibiting unprecedented photoelectrochemical performance. <i>Nano Energy</i> , <b>2016</b> , 24, 94-102	17.1	193
317	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 6918-6922	3.8	184
316	A General Two-Step Strategy-Based High-Throughput Screening of Single Atom Catalysts for Nitrogen Fixation. <i>Small Methods</i> , <b>2019</b> , 3, 1800376	12.8	175
315	Graphene-like Two-Dimensional Ionic Boron with Double Dirac Cones at Ambient Condition. <i>Nano Letters</i> , <b>2016</b> , 16, 3022-8	11.5	170
314	Rapid microwave-assisted synthesis of Mn <sub>3</sub> O <sub>4</sub> /graphene nanocomposite and its lithium storage properties. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 3600		168
313	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> , <b>2018</b> , 122, 16842-16847	3.8	163
312	Understanding the Roles of Oxygen Vacancies in Hematite-Based Photoelectrochemical Processes. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 1030-1034	16.4	159
311	Dots versus antidots: computational exploration of structure, magnetism, and half-metallicity in boron-nitride nanostructures. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 17354-9	16.4	158
310	First-principle studies of electronic structure and C-doping effect in boron nitride nanoribbon. <i>Chemical Physics Letters</i> , <b>2007</b> , 447, 181-186	2.5	158
309	First-Principles Prediction of a Room-Temperature Ferromagnetic Janus VSSe Monolayer with Piezoelectricity, Ferroelasticity, and Large Valley Polarization. <i>Nano Letters</i> , <b>2019</b> , 19, 1366-1370	11.5	155
308	New Iron-Cobalt Oxide Catalysts Promoting BiVO <sub>4</sub> Films for Photoelectrochemical Water Splitting. <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1802685	15.6	150
307	Strain engineering of selective chemical adsorption on monolayer MoS <sub>2</sub> . <i>Nanoscale</i> , <b>2014</b> , 6, 5156-61	7.7	148
306	Lithium-Catalyzed Dehydrogenation of Ammonia Borane within Mesoporous Carbon Framework for Chemical Hydrogen Storage. <i>Advanced Functional Materials</i> , <b>2009</b> , 19, 265-271	15.6	148
305	Dirac State in the FeB Monolayer with Graphene-Like Boron Sheet. <i>Nano Letters</i> , <b>2016</b> , 16, 6124-6129	11.5	147
304	Hydrogenated borophene as a stable two-dimensional Dirac material with an ultrahigh Fermi velocity. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 27284-27289	3.6	136
303	Anti-fouling graphene-based membranes for effective water desalination. <i>Nature Communications</i> , <b>2018</b> , 9, 683	17.4	135
302	An Intrinsically Non-flammable Electrolyte for High-Performance Potassium Batteries. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 3638-3644	16.4	134

301	Towards lead-free perovskite photovoltaics and optoelectronics by ab-initio simulations. <i>Scientific Reports</i> , <b>2017</b> , 7, 14025	4.9	133
300	Transition-Metal Single Atoms Anchored on Graphdiyne as High-Efficiency Electrocatalysts for Water Splitting and Oxygen Reduction. <i>Small Methods</i> , <b>2019</b> , 3, 1800419	12.8	133
299	Auxetic and Ferroelastic Borophane: A Novel 2D Material with Negative Poisson's Ratio and Switchable Dirac Transport Channels. <i>Nano Letters</i> , <b>2016</b> , 16, 7910-7914	11.5	121
298	Metallic and carbon nanotube-catalyzed coupling of hydrogenation in magnesium. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 15650-4	16.4	114
297	Edge-Rich Fe-N Active Sites in Defective Carbon for Oxygen Reduction Catalysis. <i>Advanced Materials</i> , <b>2020</b> , 32, e2000966	24	113
296	Tuning oxygen vacancies in two-dimensional iron-cobalt oxide nanosheets through hydrogenation for enhanced oxygen evolution activity. <i>Nano Research</i> , <b>2018</b> , 11, 3509-3518	10	110
295	Activating Catalytic Inert Basal Plane of Molybdenum Disulfide to Optimize Hydrogen Evolution Activity via Defect Doping and Strain Engineering. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 16761-16766	28	109
294	Metal-free graphitic carbon nitride as mechano-catalyst for hydrogen evolution reaction. <i>Journal of Catalysis</i> , <b>2015</b> , 332, 149-155	7.3	106
293	In Situ Formation of Oxygen Vacancies Achieving Near-Complete Charge Separation in Planar BiVO Photoanodes. <i>Advanced Materials</i> , <b>2020</b> , 32, e2001385	24	103
292	Molten-Salt-Mediated Synthesis of an Atomic Nickel Co-catalyst on TiO for Improved Photocatalytic H Evolution. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 7230-7234	16.4	102
291	C-BN single-walled nanotubes from hybrid connection of BN/C nanoribbons: prediction by ab initio density functional calculations. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 1682-3	16.4	100
290	The role of Ti as a catalyst for the dissociation of hydrogen on a Mg(0001) surface. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 18037-41	3.4	100
289	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> , <b>2019</b> , 21, 1546-1551	3.6	94
288	Hydrogen spillover mechanism on a Pd-doped Mg surface as revealed by ab initio density functional calculation. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 10201-4	16.4	94
287	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> , <b>2021</b> , 33, e2006313	24	91
286	Mo-based 2D MOF as a highly efficient electrocatalyst for reduction of N <sub>2</sub> to NH <sub>3</sub> : a density functional theory study. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 14510-14518	13	90
285	Carbon nanodot decorated graphitic carbon nitride: new insights into the enhanced photocatalytic water splitting from ab initio studies. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 31140-4	3.6	90
284	Nanosheets Co <sub>3</sub> O <sub>4</sub> Interleaved with Graphene for Highly Efficient Oxygen Reduction. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2015</b> , 7, 21373-80	9.5	87

283	A single boron atom doped boron nitride edge as a metal-free catalyst for N fixation. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 1110-1116	3.6	84
282	Modelling carbon membranes for gas and isotope separation. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 4832-43	3.6	84
281	First principle studies of zigzag AlN nanoribbon. <i>Chemical Physics Letters</i> , <b>2009</b> , 469, 183-185	2.5	83
280	Mg-based nanocomposites with high capacity and fast kinetics for hydrogen storage. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 11697-703	3.4	80
279	Widely tunable and anisotropic charge carrier mobility in monolayer tin(II) selenide using biaxial strain: a first-principles study. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 1247-1254	7.1	78
278	Predicting Single-Layer Technetium Dichalcogenides (TcX <sub>2</sub> = S, Se) with Promising Applications in Photovoltaics and Photocatalysis. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 5385-92	9.5	78
277	Two-Dimensional Boron Hydride Sheets: High Stability, Massless Dirac Fermions, and Excellent Mechanical Properties. <i>Angewandte Chemie</i> , <b>2016</b> , 128, 10448-10451	3.6	77
276	Computational screening of two-dimensional coordination polymers as efficient catalysts for oxygen evolution and reduction reaction. <i>Journal of Catalysis</i> , <b>2017</b> , 352, 579-585	7.3	77
275	Two-Dimensional Boron Hydride Sheets: High Stability, Massless Dirac Fermions, and Excellent Mechanical Properties. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 10292-5	16.4	76
274	Porous Polyethersulfone-Supported Zeolitic Imidazolate Framework Membranes for Hydrogen Separation. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 13264-13270	3.8	75
273	A density functional theory study on CO <sub>2</sub> capture and activation by graphene-like boron nitride with boron vacancy. <i>Catalysis Today</i> , <b>2011</b> , 175, 271-275	5.3	74
272	Strong Coupling of MoS Nanosheets and Nitrogen-Doped Graphene for High-Performance Pseudocapacitance Lithium Storage. <i>Small</i> , <b>2018</b> , 14, e1704410	11	72
271	Computational Dissection of Two-Dimensional Rectangular Titanium Mononitride TiN: Auxetics and Promises for Photocatalysis. <i>Nano Letters</i> , <b>2017</b> , 17, 4466-4472	11.5	71
270	Spin-polarization and ferromagnetism of graphitic carbon nitride materials. <i>Journal of Materials Chemistry C</i> , <b>2013</b> , 1, 6265	7.1	71
269	Transition metal dichalcogenides bilayer single crystals by reverse-flow chemical vapor epitaxy. <i>Nature Communications</i> , <b>2019</b> , 10, 598	17.4	69
268	Asymmetrically Decorated, Doped Porous Graphene As an Effective Membrane for Hydrogen Isotope Separation. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 6672-6676	3.8	69
267	Single layer lead iodide: computational exploration of structural, electronic and optical properties, strain induced band modulation and the role of spin-orbital-coupling. <i>Nanoscale</i> , <b>2015</b> , 7, 15168-74	7.7	67
266	Gas sensing and capturing based on two-dimensional layered materials: Overview from theoretical perspective. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2018</b> , 8, e1361	7.9	67

265	Understanding the activity and selectivity of single atom catalysts for hydrogen and oxygen evolution via ab initial study. <i>Catalysis Science and Technology</i> , <b>2018</b> , 8, 996-1001	5.5	67
264	Carbon Dioxide Capture and Gas Separation on B80 Fullerene. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 2170-2177	3.8	67
263	Atomically embedded asymmetrical dual-metal dimers on N-doped graphene for ultra-efficient nitrogen reduction reaction. <i>Journal of Catalysis</i> , <b>2020</b> , 388, 77-83	7.3	66
262	A water-dielectric capacitor using hydrated graphene oxide film. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 21085		66
261	First-Principles Prediction of Spin-Polarized Multiple Dirac Rings in Manganese Fluoride. <i>Physical Review Letters</i> , <b>2017</b> , 119, 016403	7.4	64
260	Tailoring Crystal Structure of FA <sub>0.83</sub> Cs <sub>0.17</sub> PbI <sub>3</sub> Perovskite Through Guanidinium Doping for Enhanced Performance and Tunable Hysteresis of Planar Perovskite Solar Cells. <i>Advanced Functional Materials</i> , <b>2019</b> , 29, 1806479	15.6	64
259	An Unusual Red Carbon Nitride to Boost the Photoelectrochemical Performance of Wide Bandgap Photoanodes. <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1805698	15.6	63
258	Stable Copper Nanoparticle Photocatalysts for Selective Epoxidation of Alkenes with Visible Light. <i>ACS Catalysis</i> , <b>2017</b> , 7, 4975-4985	13.1	62
257	Electric field controlled CO capture and CO/N separation on MoS monolayers. <i>Nanoscale</i> , <b>2017</b> , 9, 19-24	7.7	61
256	Single Pt atom decorated graphitic carbon nitride as an efficient photocatalyst for the hydrogenation of nitrobenzene into aniline. <i>Nano Research</i> , <b>2019</b> , 12, 1817-1823	10	61
255	Hindered Formation of Photoinactive $\delta$ -FAPbI Phase and Hysteresis-Free Mixed-Cation Planar Heterojunction Perovskite Solar Cells with Enhanced Efficiency via Potassium Incorporation. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 2113-2120	6.4	61
254	2D-3D Mixed Organic-Inorganic Perovskite Layers for Solar Cells with Enhanced Efficiency and Stability Induced by $\gamma$ -Propylammonium Iodide Additives. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 29753-29764	9.5	60
253	Two-dimensional GeP as a high capacity electrode material for Li-ion batteries. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 25886-25890	3.6	57
252	H <sub>2</sub> purification by functionalized graphdiyne $\pi$ -role of nitrogen doping. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 6767-6771	13	56
251	First-Principle Studies of the Formation and Diffusion of Hydrogen Vacancies in Magnesium Hydride. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 8360-8365	3.8	56
250	Ab initio studies of hydrogen desorption from low index magnesium hydride surface. <i>Surface Science</i> , <b>2006</b> , 600, 1854-1859	1.8	56
249	Electronic and optical properties of lead-free hybrid double perovskites for photovoltaic and optoelectronic applications. <i>Scientific Reports</i> , <b>2019</b> , 9, 718	4.9	55
248	Predicting Two-Dimensional CB/CN van der Waals p-n Heterojunction with Strong Interlayer Electron Coupling and Enhanced Photocurrent. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 858-862	6.4	55

247	Strong affinity of polysulfide intermediates to multi-functional binder for practical application in lithium-sulfur batteries. <i>Nano Energy</i> , <b>2016</b> , 26, 722-728	17.1	55
246	Ultrathin Cobaltosic Oxide Nanosheets as an Effective Sulfur Encapsulation Matrix with Strong Affinity Toward Polysulfides. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 4320-4325	9.5	55
245	Electrocatalytically switchable CO <sub>2</sub> capture: first principle computational exploration of carbon nanotubes with pyridinic nitrogen. <i>ChemSusChem</i> , <b>2014</b> , 7, 435-41	8.3	55
244	A density functional theory study of CO <sub>2</sub> and N <sub>2</sub> adsorption on aluminium nitride single walled nanotubes. <i>Journal of Materials Chemistry</i> , <b>2010</b> , 20, 10426		54
243	Understanding the Roles of Oxygen Vacancies in Hematite-Based Photoelectrochemical Processes. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 1042-1046	3.6	54
242	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> , <b>2021</b> , 143, 1203-1215	16.4	54
241	Sodium and Lithium Storage Properties of Spray-Dried Molybdenum Disulfide-Graphene Hierarchical Microspheres. <i>Scientific Reports</i> , <b>2015</b> , 5, 11989	4.9	53
240	Single Layer Bismuth Iodide: Computational Exploration of Structural, Electrical, Mechanical and Optical Properties. <i>Scientific Reports</i> , <b>2015</b> , 5, 17558	4.9	53
239	Electronic Functionality in Graphene-Based Nanoarchitectures: Discovery and Design via First-Principles Modeling. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 73-80	6.4	53
238	Tailoring the Interfacial Interactions of van der Waals 1T-MoS <sub>2</sub> /C Heterostructures for High-Performance Hydrogen Evolution Reaction Electrocatalysis. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 17923-17927	16.4	53
237	Computation-Aided Design of Single-Atom Catalysts for One-Pot CO Capture, Activation, and Conversion. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 36866-36872	9.5	53
236	Combined electrophoretic deposition-anodization method to fabricate reduced graphene oxide-coated TiO <sub>2</sub> nanotube films. <i>RSC Advances</i> , <b>2012</b> , 2, 8164	3.7	52
235	Identifying Copper Vacancies and Their Role in the CuO Based Photocathode for Water Splitting. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 17604-17609	16.4	51
234	Van der Waals-corrected density functional theory: benchmarking for hydrogen-nanotube and nanotube-nanotube interactions. <i>Nanotechnology</i> , <b>2005</b> , 16, 2118-23	3.4	51
233	Single-atom supported on graphene grain boundary as an efficient electrocatalyst for hydrogen evolution reaction. <i>Chemical Engineering Science</i> , <b>2019</b> , 194, 58-63	4.4	50
232	A Directional Synthesis for Topological Defect in Carbon. <i>Chem</i> , <b>2020</b> , 6, 2009-2023	16.2	49
231	Versatile Single-Layer Sodium Phosphidostannate(II): Strain-Tunable Electronic Structure, Excellent Mechanical Flexibility, and an Ideal Gap for Photovoltaics. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 2682-7	6.4	48
230	Metal-doped graphitic carbon nitride (g-C <sub>3</sub> N <sub>4</sub> ) as selective NO <sub>2</sub> sensors: A first-principles study. <i>Applied Surface Science</i> , <b>2018</b> , 455, 1116-1122	6.7	48

229	First-principle study of adsorption of hydrogen on Ti-doped Mg(0001) surface. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 21747-50	3.4	48
228	Catalytic effects of subsurface carbon in the chemisorption of hydrogen on a Mg(0001) surface: an ab-initio study. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 1814-9	3.4	48
227	Endohedral metallofullerenes (M@C60) as efficient catalysts for highly active hydrogen evolution reaction. <i>Journal of Catalysis</i> , <b>2017</b> , 354, 231-235	7.3	46
226	Adsorption of Carbon Dioxide and Nitrogen on Single-Layer Aluminum Nitride Nanostructures Studied by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 7846-7849	3.8	46
225	Electrochemical reduction of carbon dioxide on precise number of Fe atoms anchored graphdiyne. <i>Journal of CO2 Utilization</i> , <b>2020</b> , 37, 272-277	7.6	46
224	Predicting a new class of metal-organic frameworks as efficient catalyst for bi-functional oxygen evolution/reduction reactions. <i>Journal of Catalysis</i> , <b>2018</b> , 367, 206-211	7.3	45
223	Predicting a new phase (T'') of two-dimensional transition metal di-chalcogenides and strain-controlled topological phase transition. <i>Nanoscale</i> , <b>2016</b> , 8, 4969-75	7.7	44
222	High-Performance Perovskite Composite Electrocatalysts Enabled by Controllable Interface Engineering. <i>Small</i> , <b>2021</b> , 17, e2101573	11	44
221	Novel two-dimensional MOF as a promising single-atom electrocatalyst for CO2 reduction: A theoretical study. <i>Applied Surface Science</i> , <b>2020</b> , 500, 143993	6.7	43
220	Simplest MOF Units for Effective Photodriven Hydrogen Evolution Reaction. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 9159-9166	16.4	43
219	First-Principles Study of Electrocatalytically Reversible CO Capture on Graphene-like C N. <i>ChemPhysChem</i> , <b>2018</b> , 19, 2788-2795	3.2	42
218	Novel Excitonic Solar Cells in Phosphorene-TiO2 Heterostructures with Extraordinary Charge Separation Efficiency. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 1880-7	6.4	41
217	Graphene-covered perovskites: an effective strategy to enhance light absorption and resist moisture degradation. <i>RSC Advances</i> , <b>2015</b> , 5, 82346-82350	3.7	40
216	High capacity and reversible hydrogen storage on two dimensional C 2 N monolayer membrane. <i>International Journal of Hydrogen Energy</i> , <b>2018</b> , 43, 9895-9901	6.7	40
215	Molecule-Induced Conformational Change in Boron Nitride Nanosheets with Enhanced Surface Adsorption. <i>Advanced Functional Materials</i> , <b>2016</b> , 26, 8202-8210	15.6	39
214	Gas Protection of Two-Dimensional Nanomaterials from High-Energy Impacts. <i>Scientific Reports</i> , <b>2016</b> , 6, 35532	4.9	39
213	Dual-Ion-Diffusion Induced Degradation in Lead-Free Cs2AgBiBr6 Double Perovskite Solar Cells. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 2002342	15.6	39
212	Doped phosphorene for hydrogen capture: A DFT study. <i>Applied Surface Science</i> , <b>2018</b> , 433, 249-255	6.7	38

211	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> , <b>2019</b> , 10, 2567-2573	6.4	37
210	WO3 nanolayer coated 3D-graphene/sulfur composites for high performance lithium/sulfur batteries. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 4596-4603	13	36
209	In-plane graphene/boron-nitride heterostructures as an efficient metal-free electrocatalyst for the oxygen reduction reaction. <i>Nanoscale</i> , <b>2016</b> , 8, 14084-91	7.7	36
208	Charge- and Electric-Field-Controlled Switchable Carbon Dioxide Capture and Gas Separation on a C2N Monolayer. <i>Energy Technology</i> , <b>2018</b> , 6, 205-212	3.5	35
207	Two-Dimensional Titanium Carbonitride Mxene for High-Performance Sodium Ion Batteries. <i>ACS Applied Nano Materials</i> , <b>2018</b> , 1, 6854-6863	5.6	35
206	Graphyne and Graphdiyne: Versatile Catalysts for Dehydrogenation of Light Metal Complex Hydrides. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 21643-21650	3.8	34
205	Rhombohedral Lanthanum Manganite: A New Class of Dirac Half-Metal with Promising Potential in Spintronics. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 36088-36093	9.5	34
204	Modelling CO <sub>2</sub> adsorption and separation on experimentally-realized B <sub>40</sub> fullerene. <i>Computational Materials Science</i> , <b>2015</b> , 108, 38-41	3.2	33
203	Versatile two-dimensional silicon diphosphide (SiP) for photocatalytic water splitting. <i>Nanoscale</i> , <b>2018</b> , 10, 6369-6374	7.7	33
202	CO <sub>2</sub> capture and gas separation on boron carbon nanotubes. <i>Chemical Physics Letters</i> , <b>2013</b> , 575, 59-66	2.5	33
201	Atomically dispersed asymmetric Cu <sub>2</sub> S pair on 2D carbon nitride synergistically boosts the conversion of CO into C <sub>2</sub> products. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 599-606	13	33
200	Distorted Janus Transition Metal Dichalcogenides: Stable Two-Dimensional Materials with Sizable Band Gap and Ultrahigh Carrier Mobility. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 19153-19160	3.8	32
199	Insights into the nature of the coupling interactions between uracil corrosion inhibitors and copper: A DFT and molecular dynamics study. <i>Corrosion Science</i> , <b>2012</b> , 61, 101-110	6.8	32
198	Reversible Intercalation of Multivalent Al Ions into Potassium-Rich Cryptomelane Nanowires for Aqueous Rechargeable Al-Ion Batteries. <i>ChemSusChem</i> , <b>2019</b> , 12, 3753-3760	8.3	31
197	Plasmonic nanostructures to enhance catalytic performance of zeolites under visible light. <i>Scientific Reports</i> , <b>2014</b> , 4, 3805	4.9	31
196	Gradient-Concentration Design of Stable Core-Shell Nanostructure for Acidic Oxygen Reduction Electrocatalysis. <i>Advanced Materials</i> , <b>2020</b> , 32, e2003493	24	30
195	Vertically-aligned carbon nanotube membranes for hydrogen separation. <i>RSC Advances</i> , <b>2012</b> , 2, 5329	3.7	30
194	A zinc bromine supercapattery system combining triple functions of capacitive, pseudocapacitive and battery-type charge storage. <i>Materials Horizons</i> , <b>2020</b> , 7, 495-503	14.4	30

193	Silicon-doped graphene edges: an efficient metal-free catalyst for the reduction of CO <sub>2</sub> into methanol and ethanol. <i>Catalysis Science and Technology</i> , <b>2019</b> , 9, 6800-6807	5.5	30
192	Controllable CO electrocatalytic reduction via ferroelectric switching on single atom anchored InSe monolayer. <i>Nature Communications</i> , <b>2021</b> , 12, 5128	17.4	30
191	Reversible gas capture using a ferroelectric switch and 2D molecule multiferroics on the In <sub>2</sub> Se <sub>3</sub> monolayer. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 7331-7338	13	29
190	An amorphous dual action electrocatalyst based on oxygen doped cobalt sulfide for the hydrogen and oxygen evolution reactions. <i>RSC Advances</i> , <b>2017</b> , 7, 54995-55004	3.7	29
189	Tetragonal bismuth bilayer: a stable and robust quantum spin hall insulator. <i>2D Materials</i> , <b>2015</b> , 2, 045019	19	29
188	The catalytic role of an isolated-Ti atom in the hydrogenation of Ti-doped Al(001) surface: An ab initio density functional theory calculation. <i>Chemical Physics Letters</i> , <b>2007</b> , 450, 80-85	2.5	29
187	Grafting Cobalt Diselenide on Defective Graphene for Enhanced Oxygen Evolution Reaction. <i>IScience</i> , <b>2018</b> , 7, 145-153	6.1	29
186	Predicting a graphene-like WB nanosheet with a double Dirac cone, an ultra-high Fermi velocity and significant gap opening by spin-orbit coupling. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 5449-5453	3.6	28
185	Neutral and charged boron-doped fullerenes for CO <sub>2</sub> adsorption. <i>Beilstein Journal of Nanotechnology</i> , <b>2014</b> , 5, 413-8	3	28
184	Development of cross-linked dextrin as aqueous binders for silicon based anodes. <i>Journal of Power Sources</i> , <b>2020</b> , 450, 227671	8.9	28
183	Molten-Salt-Mediated Synthesis of an Atomic Nickel Co-catalyst on TiO <sub>2</sub> for Improved Photocatalytic H <sub>2</sub> Evolution. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 7297-7301	3.6	27
182	Adsorption behavior of CO <sub>2</sub> on pristine and doped phosphorenes: A dispersion corrected DFT study. <i>Journal of CO<sub>2</sub> Utilization</i> , <b>2018</b> , 24, 463-470	7.6	27
181	In silico engineering of graphene-based van der Waals heterostructured nanohybrids for electronics and energy applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2016</b> , 6, 551-570	7.9	27
180	Multiferroic and Ferroic Topological Order in Ligand-Functionalized Germanene and Arsenene. <i>Physical Review Applied</i> , <b>2018</b> , 10,	4.3	27
179	Stacking-Dependent Interlayer Magnetic Coupling in 2D CrI <sub>3</sub> /CrGeTe <sub>3</sub> Nanostructures for Spintronics. <i>ACS Applied Nano Materials</i> , <b>2020</b> , 3, 1282-1288	5.6	27
178	Boron Radicals Identified as the Source of the Unexpected Catalysis by Boron Nitride Nanosheets. <i>ACS Nano</i> , <b>2019</b> , 13, 1394-1402	16.7	27
177	Plasma-induced on-surface sulfur vacancies in NiCo <sub>2</sub> S <sub>4</sub> enhance the energy storage performance of supercapatteries. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 9278-9291	13	27
176	Galvanic replacement of liquid metal galinstan with Pt for the synthesis of electrocatalytically active nanomaterials. <i>Nanoscale</i> , <b>2019</b> , 11, 9705-9715	7.7	26

175	Two-dimensional ferroelectric topological insulators in functionalized atomically thin bismuth layers. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	26
174	Conduction-band valley spin splitting in single-layer H-Tl <sub>2</sub> O. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	26
173	A computational study of carbon dioxide adsorption on solid boron. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 12695-702	3.6	26
172	Fabricating highly efficient heterostructured CuBi <sub>2</sub> O <sub>4</sub> photocathodes for unbiased water splitting. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 2498-2504	13	26
171	Transition Metal Diborides: A New Type of High-performance Electrocatalysts for Nitrogen Reduction. <i>ChemCatChem</i> , <b>2019</b> , 11, 2624-2633	5.2	25
170	Mo-doped boron nitride monolayer as a promising single-atom electrocatalyst for CO conversion. <i>Beilstein Journal of Nanotechnology</i> , <b>2019</b> , 10, 540-548	3	25
169	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> , <b>2020</b> , 12, 6188-6194	7.7	25
168	Non-covalent surface modification of boron nitride nanotubes for enhanced catalysis. <i>Chemical Communications</i> , <b>2014</b> , 50, 225-7	5.8	25
167	Ultralarge interlayer distance and C,N-codoping enable superior sodium storage capabilities of MoS <sub>2</sub> nanoions. <i>Chemical Engineering Journal</i> , <b>2019</b> , 378, 122249	14.7	24
166	Decorating platinum on nitrogen-doped graphene sheets: Control of the platinum particle size distribution for improved photocatalytic H <sub>2</sub> generation. <i>Chemical Engineering Science</i> , <b>2019</b> , 194, 85-93	4.4	24
165	Highly compact and uniform CH <sub>3</sub> NH <sub>3</sub> Sn <sub>0.5</sub> Pb <sub>0.5</sub> I <sub>3</sub> films for efficient panchromatic planar perovskite solar cells. <i>Science Bulletin</i> , <b>2016</b> , 61, 1558-1562	10.6	23
164	Group 14 element-based non-centrosymmetric quantum spin Hall insulators with large bulk gap. <i>Nano Research</i> , <b>2015</b> , 8, 3412-3420	10	22
163	Boosting oxygen reduction and hydrogen evolution at the edge sites of a web-like carbon nanotube-graphene hybrid. <i>Carbon</i> , <b>2016</b> , 107, 739-746	10.4	22
162	Theoretical study of two states reactivity of methane activation on iron atom and iron dimer. <i>Fuel</i> , <b>2012</b> , 96, 291-297	7.1	22
161	Chemically modified ribbon edge stimulated H <sub>2</sub> dissociation: a first-principles computational study. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 8054-7	3.6	22
160	Formation of single-walled carbon nanotube via the interaction of graphene nanoribbons: ab initio density functional calculations. <i>Nano Letters</i> , <b>2007</b> , 7, 3349-54	11.5	22
159	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> , <b>2019</b> , 123, 3703-3710	3.8	21
158	Plasma modification of a Ni based metal-organic framework for efficient hydrogen evolution. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 8129-8135	13	21

157	Nitrogen removal from natural gas using solid boron: A first-principles computational study. <i>Fuel</i> , <b>2013</b> , 109, 575-581	7.1	21
156	Charge carrier exchange at chemically modified graphene edges: a density functional theory study. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 8321		21
155	How to achieve maximum charge carrier loading on heteroatom-substituted graphene nanoribbon edges: density functional theory study. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 13751		21
154	The role of V <sub>2</sub> O <sub>5</sub> on the dehydrogenation and hydrogenation in magnesium hydride: An ab initio study. <i>Applied Physics Letters</i> , <b>2008</b> , 92, 163106	3.4	21
153	Carbon-Phosphorus Bonds-Enriched 3D Graphene by Self-Sacrificing Black Phosphorus Nanosheets for Elevating Capacitive Lithium Storage. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 21720-21729	9.5	21
152	Predicting multiple Dirac-cones and ultrahigh Fermi velocity in perovskite R <sub>c</sub> phase LaCuO <sub>3</sub> . <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 6132-6137	7.1	20
151	Interaction of Water with the Fluorine-Covered Anatase TiO <sub>2</sub> (001) Surface. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 17092-17096	3.8	20
150	Leaf-inspired design of mesoporous Sb <sub>2</sub> S <sub>3</sub> /N-doped Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> composite towards fast sodium storage. <i>Science China Chemistry</i> , <b>2021</b> , 64, 964-973	7.9	20
149	Growth of MoS <sub>2</sub> Nanoflowers with Expanded Interlayer Distance onto N-Doped Graphene for Reversible Lithium Storage. <i>ChemElectroChem</i> , <b>2018</b> , 5, 2263-2270	4.3	20
148	Silicene catalysts for CO hydrogenation: the number of layers controls selectivity. <i>Nanoscale</i> , <b>2019</b> , 11, 7734-7743	7.7	19
147	Synthesis of biphenyl bridged dendritic mesoporous organosilica with extremely high adsorption of pyrene. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 12029-12037	13	19
146	Charged-Controlled Separation of Nitrogen from Natural Gas Using Boron Nitride Fullerene. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 30006-30012	3.8	19
145	The effect of Fe doping on adsorption of CO <sub>2</sub> /N <sub>2</sub> within carbon nanotubes: a density functional theory study with dispersion corrections. <i>Nanotechnology</i> , <b>2009</b> , 20, 375701	3.4	19
144	Prediction of room-temperature ferromagnetism and large perpendicular magnetic anisotropy in a planar hypercoordinate FeB monolayer. <i>Nanoscale Horizons</i> , <b>2021</b> , 6, 43-48	10.8	19
143	Dimensionality-Controlled Surface Passivation for Enhancing Performance and Stability of Perovskite Solar Cells via Triethylenetetramine Vapor. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 6651-6661	9.5	18
142	First-principles screening of novel ferroelectric MXene phases with a large piezoelectric response and unusual auxeticity. <i>Nanoscale</i> , <b>2020</b> , 12, 21291-21298	7.7	18
141	Defective Graphene on the Transition-Metal Surface: Formation of Efficient Bifunctional Catalysts for Oxygen Evolution/Reduction Reactions in Alkaline Media. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 17410-17415	9.5	17
140	Insights into the mechanism of the reaction between tetrachloro-p-benzoquinone and hydrogen peroxide and their implications in the catalytic role of water molecules in producing the hydroxyl radical. <i>ChemPhysChem</i> , <b>2013</b> , 14, 2737-43	3.2	17

139	Methane activation on Fe <sub>4</sub> cluster: A density functional theory study. <i>Chemical Physics Letters</i> , <b>2012</b> , 550, 41-46	2.5	17
138	Addition of diazomethane to armchair single-walled carbon nanotubes and their reaction sequences: A computational study. <i>Chemical Physics Letters</i> , <b>2007</b> , 436, 218-223	2.5	17
137	Band inversion and topological aspects in a TiNi monolayer. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 22154-9	3.6	17
136	Integrating SnS <sub>2</sub> Quantum Dots with Nitrogen-Doped Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> MXene Nanosheets for Robust Sodium Storage Performance. <i>ACS Applied Energy Materials</i> , <b>2021</b> , 4, 846-854	6.1	17
135	Strained graphitic carbon nitride for hydrogen purification. <i>Journal of Membrane Science</i> , <b>2017</b> , 528, 2019-205	3.65	16
134	Multiferroic decorated FeO monolayer predicted from first principles. <i>Nanoscale</i> , <b>2020</b> , 12, 14847-14852	7.7	16
133	Synergistic trifunctional electrocatalysis of pyridinic nitrogen and single transition-metal atoms anchored on pyrazine-modified graphdiyne. <i>Science Bulletin</i> , <b>2020</b> , 65, 995-1002	10.6	16
132	Electric-controlled half-metallicity in magnetic van der Waals heterobilayer. <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 7034-7040	7.1	16
131	Ab initio study of two-dimensional PdPS as an ideal light harvester and promising catalyst for hydrogen evolution reaction. <i>Materials Today Energy</i> , <b>2018</b> , 7, 136-140	7	16
130	Synthesis, structural analysis, and thermal decomposition studies of [(NH <sub>3</sub> ) <sub>2</sub> BH <sub>2</sub> ] <sub>3</sub> B <sub>3</sub> H <sub>8</sub> . <i>RSC Advances</i> , <b>2013</b> , 3, 7460	3.7	16
129	Substantial Band-Gap Tuning and a Strain-Controlled Semiconductor to Gapless/Band-Inverted Semimetal Transition in Rutile Lead/Stannic Dioxide. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 25667-25673	9.5	16
128	Predicting New Two-Dimensional Pd <sub>3</sub> (PS <sub>4</sub> ) <sub>2</sub> as an Efficient Photocatalyst for Water Splitting. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 21927-21932	3.8	16
127	Silicon Nanocages for Selective Carbon Dioxide Conversion under Visible Light. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 9973-9980	3.8	15
126	Ab initio atomistic insights into lead-free formamidinium based hybrid perovskites for photovoltaics and optoelectronics. <i>Computational Materials Science</i> , <b>2019</b> , 169, 109118	3.2	15
125	Enhanced hydrogen separation by vertically-aligned carbon nanotube membranes with zeolite imidazolate frameworks as a selective layer. <i>RSC Advances</i> , <b>2012</b> , 2, 11793	3.7	15
124	Cobalt-doped cadmium selenide colloidal nanowires. <i>Chemical Communications</i> , <b>2011</b> , 47, 11894-6	5.8	15
123	Highly stable two-dimensional gold selenide with large in-plane anisotropy and ultrahigh carrier mobility. <i>Nanoscale Horizons</i> , <b>2020</b> , 5, 366-371	10.8	15
122	Cu <sup>II</sup> active sites stabilization through Mott-Schottky effect for promoting highly efficient conversion of carbon monoxide into n-propanol. <i>Journal of Catalysis</i> , <b>2020</b> , 382, 49-56	7.3	15

121	Borophene: A Metal-free and Metallic Electrocatalyst for Efficient Converting CO <sub>2</sub> into CH <sub>4</sub> . <i>ChemCatChem</i> , <b>2020</b> , 12, 1483-1490	5.2	15
120	Thermal Reductive Perforation of Graphene Cathode for High-Performance Aluminum-Ion Batteries. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2010569	15.6	15
119	Potassium Doping to Enhance Green Photoemission of Light-Emitting Diodes Based on CsPbBr <sub>3</sub> Perovskite Nanocrystals. <i>Advanced Optical Materials</i> , <b>2020</b> , 8, 2000742	8.1	14
118	Computational Screening of Transition Metal Porphyrins for the Electrochemical Reduction of Carbon Dioxide. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 7708-7715	3.8	14
117	Field-effect transistors fabricated from diluted magnetic semiconductor colloidal nanowires. <i>Nanoscale</i> , <b>2012</b> , 4, 1263-6	7.7	14
116	Surface-Dependent Intermediate Adsorption Modulation on Iridium-Modified Black Phosphorus Electrocatalysts for Efficient pH-Universal Water Splitting. <i>Advanced Materials</i> , <b>2021</b> , 33, e2104638	24	14
115	2D atomic crystal molecular superlattices by soft plasma intercalation. <i>Nature Communications</i> , <b>2020</b> , 11, 5960	17.4	14
114	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> , <b>2021</b> , 143, 9507-9514	16.4	14
113	Visible light-driven selective hydrogenation of unsaturated aromatics in an aqueous solution by direct photocatalysis of Au nanoparticles. <i>Catalysis Science and Technology</i> , <b>2018</b> , 8, 726-734	5.5	14
112	Theoretical discovery of Dirac half metal in experimentally synthesized two dimensional metal semiquinoid frameworks. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 5792-5796	7.1	13
111	Remarkably improved oxygen evolution reaction activity of cobalt oxides by an Fe ion solution immersion process. <i>Inorganic Chemistry Frontiers</i> , <b>2020</b> , 7, 3327-3339	6.8	13
110	H <sub>2</sub> S Sensing and Splitting on Atom-Functionalized Carbon Nanotubes: A Theoretical Study. <i>Advanced Theory and Simulations</i> , <b>2018</b> , 1, 1700033	3.5	13
109	Versatile two-dimensional stanene-based membrane for hydrogen purification. <i>International Journal of Hydrogen Energy</i> , <b>2017</b> , 42, 5577-5583	6.7	13
108	Ultras-small SnO <sub>2</sub> nanocrystals sandwiched into polypyrrole and Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> MXene for highly effective sodium storage. <i>Materials Chemistry Frontiers</i> , <b>2021</b> , 5, 825-833	7.8	13
107	Strain Mediated Bandgap Reduction, Light Spectrum Broadening, and Carrier Mobility Enhancement of Methylammonium Lead/Tin Iodide Perovskites. <i>Particle and Particle Systems Characterization</i> , <b>2017</b> , 34, 1600288	3.1	12
106	The effect of ethylene-amine ligands enhancing performance and stability of perovskite solar cells. <i>Journal of Power Sources</i> , <b>2020</b> , 463, 228210	8.9	12
105	High-mobility anisotropic transport in few-layer EB films. <i>Nanoscale</i> , <b>2016</b> , 8, 20111-20117	7.7	12
104	Computational study of methyl derivatives of ammonia borane for hydrogen storage. <i>Physical Chemistry Chemical Physics</i> , <b>2008</b> , 10, 6104-6	3.6	12

103	Vacancy mediated desorption of hydrogen from a sodium alanate surface: An ab initio spin-polarized study. <i>Applied Physics Letters</i> , <b>2007</b> , 90, 143119	3.4	12
102	Strain engineering of selective chemical adsorption on monolayer black phosphorous. <i>Applied Surface Science</i> , <b>2020</b> , 503, 144033	6.7	12
101	Theoretical insights into the performance of single and double transition metal atoms doped on N-graphenes for N <sub>2</sub> electroreduction. <i>Applied Surface Science</i> , <b>2021</b> , 537, 148012	6.7	12
100	Density Functional Theory Investigation of Carbon Dots as Hole-transport Material in Perovskite Solar Cells. <i>ChemPhysChem</i> , <b>2018</b> , 19, 3018-3023	3.2	12
99	Recent progress on the prediction of two-dimensional materials using CALYPSO. <i>Chinese Physics B</i> , <b>2019</b> , 28, 107306	1.2	11
98	2D boron dichalcogenides from the substitution of Mo with ionic B <sub>2</sub> pair in MoX <sub>2</sub> (X = S, Se and Te): high stability, large excitonic effect and high charge carrier mobility. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 1651-1658	7.1	11
97	Surface plasmon-enhanced zeolite catalysis under light irradiation and its correlation with molecular polarity of reactants. <i>Chemical Communications</i> , <b>2014</b> , 50, 13893-5	5.8	11
96	Cobalt porphyrin supported on graphene/Ni (111) surface: Enhanced oxygen evolution/reduction reaction and the role of electron coupling. <i>Catalysis Today</i> , <b>2020</b> , 351, 113-118	5.3	11
95	Computational exploration of two-dimensional silicon diarsenide and germanium arsenide for photovoltaic applications. <i>Beilstein Journal of Nanotechnology</i> , <b>2018</b> , 9, 1247-1253	3	11
94	A theoretical insight into a feasible strategy for the fabrication of borophane. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 16216-16221	3.6	11
93	B80 Fullerene: A Promising Metal-Free Photocatalyst for Efficient Conversion of CO <sub>2</sub> to HCOOH. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 24193-24199	3.8	10
92	The importance of atomic charge distributions of solid boron material in N <sub>2</sub> electrochemical reduction. <i>Applied Surface Science</i> , <b>2020</b> , 526, 146606	6.7	10
91	Role of Lithium Vacancies in Accelerating the Dehydrogenation Kinetics on a LiBH <sub>4</sub> (010) Surface: An Ab Initio Study. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 12124-12128	3.8	10
90	First-principles study of a Mn-doped In <sub>2</sub> Se <sub>3</sub> monolayer: Coexistence of ferromagnetism and ferroelectricity with robust half-metallicity and enhanced polarization. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	10
89	Prediction of a large-gap quantum-spin-Hall insulator: Diamond-like GaBi bilayer. <i>Nano Research</i> , <b>2015</b> , 8, 3823-3829	10	9
88	Tunable magnetic anisotropy in 2D magnets via molecular adsorption. <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 14948-14953	7.1	9
87	Calculations of helium separation via uniform pores of stanene-based membranes. <i>Beilstein Journal of Nanotechnology</i> , <b>2015</b> , 6, 2470-6	3	9
86	Impact induced chemisorption of C <sub>20</sub> isomers on diamond (001)(2x1) surface. <i>Chemical Physics Letters</i> , <b>2001</b> , 344, 270-276	2.5	9

85	Atomically Dispersed Heteronuclear Dual-Atom Catalysts: A New Rising Star in Atomic Catalysis.. <i>Small</i> , <b>2021</b> , e2106091	11	9
84	Tuning band alignment and optical properties of 2D van der Waals heterostructure via ferroelectric polarization switching. <i>Frontiers of Physics</i> , <b>2020</b> , 15, 1	3.7	9
83	First principles study of trirutile magnesium bismuth oxide: Ideal bandgap for photovoltaics, strain-mediated band-inversion and semiconductor-to-semimetal transition. <i>Computational Materials Science</i> , <b>2018</b> , 149, 158-161	3.2	8
82	First principle study of hydrogenation of MgB <sub>2</sub> : an important step toward reversible hydrogen storage in the coupled LiBH <sub>4</sub> /MgH <sub>2</sub> system. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2009</b> , 9, 4388-91 <sup>3</sup>		8
81	Controlling the Interfacial Charge Polarization of MOF-Derived 0D-2D vdW Architectures as a Unique Strategy for Bifunctional Oxygen Electrocatalysis.. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2022</b> ,	9.5	8
80	Intrinsic Ultrahigh Negative Poisson's Ratio in Two-Dimensional Ferroelectric ABP <sub>2</sub> X <sub>6</sub> Materials. <i>Wuli Huaxue Xuebao/Acta Physico-Chimica Sinica</i> , <b>2019</b> , 35, 1128-1133	3.8	8
79	Two-dimensional vanadium tetrafluoride with antiferromagnetic ferroelasticity and bidirectional negative Poisson's ratio. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 95-100	7.1	8
78	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> , <b>2020</b> , 8, 10402 <sup>13</sup> -1040 <sup>7</sup> 8		
77	Bandstructure engineering in 2D materials using Ferroelectric materials. <i>Applied Surface Science</i> , <b>2020</b> , 513, 145817	6.7	7
76	Metal-free graphene/boron nitride heterointerface for CO <sub>2</sub> reduction: Surface curvature controls catalytic activity and selectivity. <i>EcoMat</i> , <b>2020</b> , 2, e12013	9.4	7
75	Adina Rubella-Like Microsized SiO@N-Doped Carbon Grafted with N-Doped Carbon Nanotubes as Anodes for High-Performance Lithium Storage. <i>Small Science</i> , 2100105		7
74	Unravelling the Reaction Mechanisms of N Fixation on Molybdenum Nitride: A Full DFT Study from the Pristine Surface to Heteroatom Anchoring. <i>ChemSusChem</i> , <b>2021</b> , 14, 3257-3266	8.3	7
73	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> , <b>2021</b> , 536, 147779	6.7	7
72	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> , <b>2021</b> , 9, 13192-13199	13	7
71	An Intrinsically Non-flammable Electrolyte for High-Performance Potassium Batteries. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 3667-3673	3.6	6
70	Adsorption and Dissociation of Ammonia Borane Outside and Inside Single-Walled Carbon Nanotubes: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 12580-12585	3.8	6
69	Formation energies of low-indexed surfaces of tin dioxide terminated by nonmetals. <i>Solid State Communications</i> , <b>2010</b> , 150, 957-960	1.6	6
68	GROWTH OF C <sub>36</sub> -FILMS ON DIAMOND SURFACE THROUGH MOLECULAR DYNAMICS SIMULATION. <i>International Journal of Modern Physics B</i> , <b>2002</b> , 16, 3971-3978	1.1	6

67	Computational screening of single-atom alloys TM@Ru(0001) for enhanced electrochemical nitrogen reduction reaction. <i>Journal of Materials Chemistry A</i> ,	13	6
66	Two-dimensional heterojunction SnS <sub>2</sub> /SnO <sub>2</sub> photoanode with excellent photoresponse up to near infrared region. <i>Solar Energy Materials and Solar Cells</i> , <b>2020</b> , 207, 110342	6.4	6
65	Solvent Effect on Supramolecular Self-Assembly of Chlorophylls a on Chemically Reduced Graphene Oxide. <i>Langmuir</i> , <b>2020</b> , 36, 13575-13582	4	6
64	PT-symmetry-protected Dirac states in strain-induced hidden MoS <sub>2</sub> monolayer. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	6
63	Free-radical gases on two-dimensional transition-metal disulfides (XS, X = Mo/W): robust half-metallicity for efficient nitrogen oxide sensors. <i>Beilstein Journal of Nanotechnology</i> , <b>2018</b> , 9, 1641-1646	16.46	6
62	Techniques enabling inorganic materials into wearable fiber/yarn and flexible lithium-ion batteries. <i>Energy Storage Materials</i> , <b>2021</b> , 43, 62-84	19.4	6
61	2D/2D Black Phosphorus/Nickel Hydroxide Heterostructures for Promoting Oxygen Evolution via Electronic Structure Modulation and Surface Reconstruction. <i>Advanced Energy Materials</i> , 2201141	21.8	6
60	Charging assisted structural phase transitions in monolayer InSe. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 22502-22508	3.6	5
59	Molecular dynamic investigation of the structure and stress in crystalline and amorphous silicon during lithiation. <i>Computational Materials Science</i> , <b>2020</b> , 183, 109811	3.2	5
58	Strain induced variation of PFOS adsorption on pristine and defected phosphorene: A DFT study. <i>Applied Surface Science</i> , <b>2020</b> , 532, 147452	6.7	5
57	Single Copper Atoms Supported on ZnS as an Efficient Catalyst for Electrochemical Reduction of CO to CH <sub>3</sub> OH. <i>ChemNanoMat</i> , <b>2020</b> , 6, 1806-1811	3.5	5
56	Sn <sup>2+</sup> -Regulated Synthesis of a Bone-like Fe <sub>3</sub> O <sub>4</sub> @N-Doped Carbon Composite as the Anode for High-Performance Lithium Storage. <i>ACS Applied Energy Materials</i> , <b>2021</b> , 4, 3785-3793	6.1	5
55	Unlocking the potential of ruthenium catalysts for nitrogen fixation with subsurface oxygen. <i>Journal of Materials Chemistry A</i> , <b>2021</b> , 9, 6575-6582	13	5
54	First-principles prediction of ferroelasticity tuned anisotropic auxeticity and carrier mobility in two-dimensional AgO. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 3155-3160	7.1	5
53	Nanostructure Shape-Effects in ZnO heterogeneous photocatalysis. <i>Journal of Colloid and Interface Science</i> , <b>2022</b> , 606, 588-599	9.3	5
52	DFT study of electronic and optical properties of anatase titanium dioxide tuned by nitrogen and lithium co-doping. <i>Solid State Communications</i> , <b>2016</b> , 228, 22-26	1.6	4
51	Structural and electronic properties of diazonium functionalized (4, 4) single walled carbon nanotube: an ab initio study. <i>Molecular Simulation</i> , <b>2006</b> , 32, 1213-1217	2	4
50	Structure character in small-carbon-cluster deposition on diamond surface. <i>European Physical Journal D</i> , <b>2003</b> , 23, 369-373	1.3	4

49	Energy dependence of methyl-radical adsorption on diamond (001)-(211) surface. <i>Surface and Coatings Technology</i> , <b>2001</b> , 141, 246-251	4.4	4
48	B-incorporated, N-doped hierarchically porous carbon nanosheets as anodes for boosted potassium storage capability. <i>Chinese Chemical Letters</i> , <b>2021</b> , 33, 480-480	8.1	4
47	Predicting ultrafast Dirac transport channel at the one-dimensional interface of the two-dimensional coplanar ZnO/MoS <sub>2</sub> heterostructure. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	4
46	Functionalized boron nitride monolayers as promising materials for uranyl ion capture: A first-principles study. <i>Journal of Molecular Structure</i> , <b>2020</b> , 1200, 127080	3.4	4
45	Atypical Defect Motions in Brittle Layered Sodium Titanate Nanowires. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 6052-6059	6.4	4
44	Boron-rich boron nitride nanomaterials as efficient metal-free catalysts for converting CO <sub>2</sub> into valuable fuel. <i>Applied Surface Science</i> , <b>2021</b> , 555, 149652	6.7	4
43	Coupling Fe <sub>3</sub> O <sub>4</sub> /Fe <sub>1-x</sub> S@Carbon with carbon-coated MoS <sub>2</sub> nanosheets as a superior anode for sodium-ion batteries. <i>Chemical Engineering Journal</i> , <b>2022</b> , 427, 131652	14.7	4
42	Carbon-coated MoS <sub>2</sub> nanosheets@CNTs-Ti <sub>3</sub> C <sub>2</sub> MXene quaternary composite with the superior rate performance for sodium-ion batteries. <i>Journal of Materials Science and Technology</i> , <b>2022</b> , 100, 101-109	9.1	4
41	Anomalous Enhancement of Mechanical Properties in the Ammonia Adsorbed Defective Graphene. <i>Scientific Reports</i> , <b>2016</b> , 6, 33810	4.9	3
40	A remarkable two-dimensional membrane for multifunctional gas separation: halogenated metal-free fused-ring polyphthalocyanine. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 18931-18937	3.6	3
39	Mechanism of ferromagnetism in non-magnetic ion-doped zinc oxides. <i>Physica Scripta</i> , <b>2014</b> , 89, 015807	2.6	3
38	Half metallicity in a zigzag double-walled nanotube nanodot: An ab initio prediction. <i>Chemical Physics Letters</i> , <b>2009</b> , 468, 257-259	2.5	3
37	Impact energy dependence of Al <sub>13</sub> cluster deposition on Ni(0 0 1) surface. <i>Surface Science</i> , <b>2002</b> , 512, 128-134	1.8	3
36	Adatom CCV Auger rates via the local density of states. <i>Surface Science</i> , <b>2003</b> , 545, L753-L760	1.8	3
35	Wavelength-Specific Product Desorption as a Key to Raising Nitrile Yield of Primary Alcohol Ammoxidation over Illuminated Pd Nanoparticles. <i>ACS Catalysis</i> , 2280-2289	13.1	3
34	Regulating the interfacial behavior of carbon nanotubes for fast lithium storage. <i>Electrochimica Acta</i> , <b>2021</b> , 388, 138591	6.7	3
33	First principles studies of mononuclear and dinuclear Pacman complexes for electrocatalytic reduction of CO <sub>2</sub> . <i>Catalysis Science and Technology</i> , <b>2021</b> , 11, 637-645	5.5	3
32	In-situ conversion growth of carbon-coated MoS <sub>2</sub> /N-doped carbon nanotubes as anodes with superior capacity retention for sodium-ion batteries. <i>Journal of Materials Science and Technology</i> , <b>2022</b> , 102, 8-15	9.1	3

31	Polymorphism of low dimensional boron nanomaterials driven by electrostatic gating: a computational discovery. <i>Nanoscale</i> , <b>2020</b> , 12, 10543-10549	7.7	2
30	Water Splitting: In Situ Formation of Oxygen Vacancies Achieving Near-Complete Charge Separation in Planar BiVO <sub>4</sub> Photoanodes (Adv. Mater. 26/2020). <i>Advanced Materials</i> , <b>2020</b> , 32, 2070198	24	2
29	Reversible Intercalation of Multivalent Al <sup>3+</sup> Ions into Potassium-Rich Cryptomelane Nanowires for Aqueous Rechargeable Al-Ion Batteries. <i>ChemSusChem</i> , <b>2019</b> , 12, 3670-3670	8.3	2
28	The location of Ti atom in sodium alanate: an ab initio spin-polarised study. <i>International Journal of Nanotechnology</i> , <b>2007</b> , 4, 564	1.5	2
27	Co Nanoparticles Encapsulated in N-Doped Carbon Nanotubes Grafted CNTs as Electrocatalysts for Enhanced Oxygen Reduction Reaction. <i>Advanced Materials Interfaces</i> , 2101877	4.6	2
26	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> , <b>2021</b> , 9, 12046-12050	7.1	2
25	Prediction of two-dimensional ferroelectric metal Mxenes. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 11343-11348	7.1	2
24	Predicting the strain-mediated topological phase transition in 3D cubic ThTaN. <i>Beilstein Journal of Nanotechnology</i> , <b>2018</b> , 9, 1399-1404	3	2
23	Purely one-dimensional ferroelectricity and antiferroelectricity from van der Waals niobium oxide trihalides. <i>Npj Computational Materials</i> , <b>2021</b> , 7,	10.9	2
22	Graphynes as emerging 2D-platforms for electronic and energy applications: a computational perspective. <i>Materials Chemistry Frontiers</i> , <b>2021</b> , 5, 6392-6412	7.8	2
21	Two-Dimensional CuTe <sub>2</sub> X (X = Cl, Br, and I): Potential Photocatalysts for Water Splitting under the Visible/Infrared Light. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 25543-25548	3.8	1
20	Porous Graphene and Nanomeshes <b>2013</b> , 129-151		1
19	Hydrogen trapping in MAX phase Ti <sub>3</sub> SiC <sub>2</sub> : Insight from chemical bonding by density functional theory. <i>Europhysics Letters</i> , <b>2017</b> , 118, 47002	1.6	1
18	hcp-phased Ni nanoparticles with generic catalytic hydrogenation activities toward different functional groups. <i>Science China Materials</i> , <b>2022</b> , 65, 1252	7.1	1
17	Vacancy engineering of oxidized Nb <sub>2</sub> CT <sub>x</sub> MXenes for a biased nitrogen fixation. <i>Green Energy and Environment</i> , <b>2022</b> ,	5.7	1
16	Two-Dimensional Janus Antimony Selenium Telluride with Large Rashba Spin Splitting and High Electron Mobility. <i>ACS Omega</i> , <b>2021</b> , 6, 31919-31925	3.9	1
15	Understanding the roles of carbon in carbon/g-C <sub>3</sub> N <sub>4</sub> based photocatalysts for H <sub>2</sub> evolution. <i>Nano Research</i> , 1	10	1
14	2D Nanomaterials: Molecule-Induced Conformational Change in Boron Nitride Nanosheets with Enhanced Surface Adsorption (Adv. Funct. Mater. 45/2016). <i>Advanced Functional Materials</i> , <b>2016</b> , 26, 8356-8356	15.6	1

13	N <sub>2</sub> electrochemical reduction on two dimensional transition metal monoborides: A density functional theory study. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26548	2.1	1
12	Exploring Aluminum-Ion Insertion into Magnesium-Doped Manjiroite (MnO <sub>2</sub> ) Nanorods in Aqueous Solution. <i>ChemElectroChem</i> , <b>2021</b> , 8, 1048-1054	4.3	1
11	Rhodium-molybdenum oxide electrocatalyst with dual active sites for electrochemical ammonia synthesis under neutral pH condition. <i>Journal of Electroanalytical Chemistry</i> , <b>2021</b> , 896, 115157	4.1	1
10	CO Capture, Separation and Reduction on Boron-Doped MoS <sub>2</sub> , MoSe <sub>2</sub> and Heterostructures with Different Doping Densities: A Theoretical Study. <i>ChemPhysChem</i> , <b>2021</b> , 22, 2392-2400	3.2	1
9	Predicting MnB <sub>6</sub> monolayer with room temperature ferromagnetism and high magnetic anisotropy. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2021</b> , 134, 114930	3	1
8	Interfacing 2D VS <sub>2</sub> with Janus MoSSe: Antiferromagnetic electric polarization and charge transfer driven Half-metallicity. <i>Applied Surface Science</i> , <b>2021</b> , 570, 151129	6.7	1
7	Controllable Acceleration and Deceleration of Charge Carrier Transport in Metal-Halide Perovskite Single-Crystal by Cs-Cation Induced Bandgap Engineering.. <i>Small</i> , <b>2022</b> , e2107680	11	1
6	A Highly Efficient Conjoined-twin Porphyrin-based Complex for the Electrochemical Reduction of CO to Ethanol. <i>ChemNanoMat</i> , <b>2021</b> , 7, 935-941	3.5	0
5	K-Functionalized Carbon Quantum Dots-Induced Interface Assembly of Carbon Nanocages for Ultrastable Potassium Storage Performance.. <i>Small Methods</i> , <b>2022</b> , e2101627	12.8	0
4	N/P-Doped MoS <sub>2</sub> Monolayers as Promising Materials for Controllable CO <sub>2</sub> Capture and Separation under Reduced Electric Fields: A Theoretical Modeling. <i>Journal of Physical Chemistry C</i> , <b>2022</b> , 126, 203-211	3.8	0
3	Versatile Gold Telluride Iodide Monolayer as a Potential Photocatalyst for Water Splitting. <i>Nanomaterials</i> , <b>2022</b> , 12, 1915	5.4	0
2	Exploring Aluminum-Ion Insertion into Magnesium-Doped Manjiroite (MnO <sub>2</sub> ) Nanorods in Aqueous Solution. <i>ChemElectroChem</i> , <b>2021</b> , 8, 995-995	4.3	
1	Numerical investigation of microstructure and failure of lithiated silicon under biaxial tension. <i>Computational Materials Science</i> , <b>2021</b> , 200, 110764	3.2	