Zhong-Fang Chen

List of Publications by Year
in descending order

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322 papers	33,528 citations	4103 90 h-index	5102 172 g-index
365 all docs	365 docs citations	365 times ranked	29077 citing authors

#	Article	IF	Citations
1	Revisiting catalytic performance of supported metal dimers for oxygen reduction reaction via magnetic coupling from first principles. , 2022, 1, 100031.		31
2	A novel 2D porous C₃N₂ framework as a promising anode material with ultra-high specific capacity for lithium-ion batteries. Journal of Materials Chemistry A, 2022, 10, 6551-6559.	5.2	22
3	Tailoring 2-electron oxygen reduction reaction selectivity on h-BN-based single-atom catalysts from superoxide dismutase: A DFT investigation. Applied Surface Science, 2022, 592, 153233.	3.1	18
4	Understanding the CH4 Conversion over Metal Dimers from First Principles. Nanomaterials, 2022, 12, 1518.	1.9	2
5	Atomically Dispersed Uranium Enables an Unprecedentedly High NH₃ Yield Rate. Nano Letters, 2022, 22, 4475-4481.	4.5	12
6	Constructing two-dimensional holey graphyne with unusual annulative Ï€-extension. Matter, 2022, 5, 2306-2318.	5.0	34
7	Particle Swarm Predictions of a SrB₈ Monolayer with 12-Fold Metal Coordination. Journal of the American Chemical Society, 2022, 144, 11120-11128.	6.6	12
8	Establishing a Theoretical Landscape for Identifying Basal Plane Active 2D Metal Borides (MBenes) toward Nitrogen Electroreduction. Advanced Functional Materials, 2021, 31, 2008056.	7.8	97
9	Doubleâ€sided surface functionalization: An effective approach to stabilize and modulate the electronic structure of grapheneâ€like borophene. InformaÄnÃ-MateriÃ¡ly, 2021, 3, 327-336.	8.5	18
10	In Situ Observation of Nonâ€Classical 2â€Norbornyl Cation in Confined Zeolites at Ambient Temperature. Angewandte Chemie - International Edition, 2021, 60, 4581-4587.	7.2	16
11	In Situ Observation of Nonâ€Classical 2â€Norbornyl Cation in Confined Zeolites at Ambient Temperature. Angewandte Chemie, 2021, 133, 4631-4637.	1.6	2
12	2D auxetic material with intrinsic ferromagnetism: a copper halide (CuCl₂) monolayer. Physical Chemistry Chemical Physics, 2021, 23, 22078-22085.	1.3	7
13	Predicting the adsorption of organic pollutants on boron nitride nanosheets via in silico techniques: DFT computations and QSAR modeling. Environmental Science: Nano, 2021, 8, 795-805.	2.2	13
14	Penta-MS₂ (M = Mn, Ni, Cu/Ag and Zn/Cd) monolayers with negative Poisson's ratios and tunable bandgaps as water-splitting photocatalysts. Journal of Materials Chemistry A, 2021, 9, 6993-7004.	5.2	42
15	Enhanced performance of Mo₂P monolayer as lithium-ion battery anode materials by carbon and nitrogen doping: a first principles study. Physical Chemistry Chemical Physics, 2021, 23, 4030-4038.	1.3	26
16	C₉N₄ and C₂N₆S₃ monolayers as promising anchoring materials for lithiumâ€“sulfur batteries: weakening the shuttle effect via optimizing lithium bonds. Physical Chemistry Chemical Physics, 2021, 23, 12958-12967.	1.3	9
17	Identifying the Activity Origin of a Cobalt Singleâ€Atom Catalyst for Hydrogen Evolution Using Supervised Learning. Advanced Functional Materials, 2021, 31, 2100547.	7.8	93
18	RÃ¼cktitelbild: In Situ Observation of Nonâ€Classical 2â€Norbornyl Cation in Confined Zeolites at Ambient Temperature (Angew. Chem. 9/2021). Angewandte Chemie, 2021, 133, 5004-5004.	1.6	0

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19	MX Anti-MXenes from Non-van der Waals Bulks for Electrochemical Applications: The Merit of Metallicity and Active Basal Plane. ACS Nano, 2021, 15, 6233-6242.	7.3	26
20	Enhancing Ferromagnetism and Tuning Electronic Properties of CrI₃ Monolayers by Adsorption of Transition-Metal Atoms. ACS Applied Materials & Interfaces, 2021, 13, 21593-21601.	4.0	30
21	Single-atom catalysts with anionic metal centers: Promising electrocatalysts for the oxygen reduction reaction and beyond. Journal of Energy Chemistry, 2021, 63, 285-293.	7.1	15
22	Molecular Crowding Effect in Aqueous Electrolytes to Suppress Hydrogen Reduction Reaction and Enhance Electrochemical Nitrogen Reduction. Advanced Energy Materials, 2021, 11, 2101699.	10.2	73
23	Controllable CO2 electrocatalytic reduction via ferroelectric switching on single atom anchored In2Se3 monolayer. Nature Communications, 2021, 12, 5128.	5.8	110
24	Tunable electronic properties and enhanced ferromagnetism in Cr₂Ge₂Te₆ monolayer by strain engineering. Nanotechnology, 2021, 32, 485408.	1.3	7
25	Coordination tailoring towards efficient single-atom catalysts for N2 fixation: A case study of iron-nitrogen-carbon (Fe@N-C) systems. Catalysis Today, 2020, 350, 91-99.	2.2	45
26	Semiconducting SN₂ monolayer with three-dimensional auxetic properties: a global minimum with tetracoordinated sulfurs. Nanoscale, 2020, 12, 85-92.	2.8	21
27	Relative Efficacy of Coâ^'X₄ Embedded Graphene (X=N, S, B, and P) Electrocatalysts towards Hydrogen Evolution Reaction: Is Nitrogen Really the Best Choice?. ChemCatChem, 2020, 12, 536-543.	1.8	32
28	N-heterocyclic carbene as a promising metal-free electrocatalyst with high efficiency for nitrogen reduction to ammonia. Journal of Energy Chemistry, 2020, 46, 78-86.	7.1	33
29	Machine-learning-assisted screening of pure-silica zeolites for effective removal of linear siloxanes and derivatives. Journal of Materials Chemistry A, 2020, 8, 3228-3237.	5.2	14
30	Scalable synthesis of 2D hydrogen-substituted graphdiyne on Zn substrate for high-yield N2 fixation. Nano Energy, 2020, 78, 105283.	8.2	38
31	Zeolite-templated carbons as effective sorbents to remove methylsiloxanes and derivatives: A computational screening. Green Energy and Environment, 2020, , .	4.7	0
32	Evaluation procedure of photocatalysts for VOCs degradation from the view of density functional theory calculations: g-C₃N₄ dots/graphene as an example. Journal of Materials Chemistry A, 2020, 8, 20363-20372.	5.2	54
33	Understanding activity origin for the oxygen reduction reaction on bi-atom catalysts by DFT studies and machine-learning. Journal of Materials Chemistry A, 2020, 8, 24563-24571.	5.2	71
34	Enhanced Ferromagnetism and Tunable Magnetism in Fe₃GeTe₂ Monolayer by Strain Engineering. ACS Applied Materials & Interfaces, 2020, 12, 26367-26373.	4.0	83
35	Rational Prediction of Single Metal Atom Supported on Two-Dimensional Metal Diborides for Electrocatalytic N₂ Reduction Reaction with Integrated Descriptor. Journal of Physical Chemistry Letters, 2020, 11, 5241-5247.	2.1	37
36	Polymorphism of low dimensional boron nanomaterials driven by electrostatic gating: a computational discovery. Nanoscale, 2020, 12, 10543-10549.	2.8	5

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37	Metallic FeSe monolayer as an anode material for Li and non-Li ion batteries: a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 8902-8912.	1.3	79
38	Planar Hypercoordinate Motifs in Two-Dimensional Materials. Accounts of Chemical Research, 2020, 53, 887-895.	7.6	54
39	Tackling the Activity and Selectivity Challenges of Electrocatalysts toward the Nitrogen Reduction Reaction via Atomically Dispersed Biatom Catalysts. Journal of the American Chemical Society, 2020, 142, 5709-5721.	6.6	664
40	Underlying mechanisms of reactive oxygen species and oxidative stress photoinduced by graphene and its surface-functionalized derivatives. Environmental Science: Nano, 2020, 7, 782-792.	2.2	21
41	Ultrahigh capacity 2D anode materials for lithium/sodium-ion batteries: an entirely planar B₇P₂ monolayer with suitable pore size and distribution. Journal of Materials Chemistry A, 2020, 8, 10301-10309.	5.2	44
42	Directly predicting limiting potentials from easily obtainable physical properties of graphene-supported single-atom electrocatalysts by machine learning. Journal of Materials Chemistry A, 2020, 8, 5663-5670.	5.2	112
43	Identifying the Ground-State NP Sheet through a Global Structure Search in Two-Dimensional Space and Its Promising High-Efficiency Photovoltaic Properties. , 2019, 1, 375-382.		26
44	Highly porous, low band-gap Ni_xMn_{3â^'x}O₄(0.55 â‰¤xâ‰¤ 1.2) spinel nanoparticles within situcoated carbon as advanced cathode materials for zinc-ion batteries. Journal of Materials Chemistry A, 2019, 7, 17854-17866.	5.2	65
45	Oxygen Evolution Reaction on 2D Ferromagnetic Fe₃GeTe₂: Boosting the Reactivity by the Selfâ€Reduction of Surface Hydroxyl. Advanced Functional Materials, 2019, 29, 1904782.	7.8	42
46	Simultaneously Achieving High Activity and Selectivity toward Two-Electron O₂ Electroreduction: The Power of Single-Atom Catalysts. ACS Catalysis, 2019, 9, 11042-11054.	5.5	314
47	Defect-rich and ultrathin N doped carbon nanosheets as advanced trifunctional metal-free electrocatalysts for the ORR, OER and HER. Energy and Environmental Science, 2019, 12, 322-333.	15.6	1,078
48	Boosting ORR/OER Activity of Graphdiyne by Simple Heteroatom Doping. Small Methods, 2019, 3, 1800550.	4.6	149
49	Predicting Novel 2D MB₂ (M = Ti, Hf, V, Nb, Ta) Monolayers with Ultrafast Dirac Transport Channel and Electron-Orbital Controlled Negative Poissonâ€™s Ratio. Journal of Physical Chemistry Letters, 2019, 10, 2567-2573.	2.1	65
50	Nonvolatile Electrical Control and Heterointerfaceâ€Induced Halfâ€Metallicity of 2D Ferromagnets. Advanced Functional Materials, 2019, 29, 1901420.	7.8	109
51	1 + 1â€² > 2: Heteronuclear Biatom Catalyst Outperforms Its Homonuclear Counterparts for CO Oxidation. Small Methods, 2019, 3, 1800480.	4.6	92
52	Exohedral functionalization of endohedral metallofullerenes: Interplay between inside and outside. Coordination Chemistry Reviews, 2019, 388, 406-439.	9.5	54
53	B-terminated (111) polar surfaces of BP and BAs: promising metal-free electrocatalysts with large reaction regions for nitrogen fixation. Journal of Materials Chemistry A, 2019, 7, 13284-13292.	5.2	87
54	Two-dimensional Blue-AsP monolayers with tunable direct band gap and ultrahigh carrier mobility show promising high-performance photovoltaic properties. Nanoscale, 2019, 11, 8260-8269.	2.8	70

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55	Frustrated Lewis pairs photocatalyst for visible light-driven reduction of CO to multi-carbon chemicals. Nanoscale, 2019, 11, 20777-20784.	2.8	38
56	Computational Screening of Efficient Singleâ€Atom Catalysts Based on Graphitic Carbon Nitride (gâ€C₃N₄) for Nitrogen Electroreduction. Small Methods, 2019, 3, 1800368.	4.6	347
57	Computational Quest for High-Performance Electrocatalysts for Nitrogen Fixation. ECS Meeting Abstracts, 2019, , .	0.0	0
58	Computational Screening of Single-Atom Electrocatalysts for Oxygen Reduction Reaction By Machine Learning Algorithm. ECS Meeting Abstracts, 2019, , .	0.0	0
59	Towards High-Performancepgm-Free ORR Electrocatalysts: Interplay between Theory and Experiment. ECS Meeting Abstracts, 2019, , .	0.0	0
60	A two-dimensional CaSi monolayer with quasi-planar pentacoordinate silicon. Nanoscale Horizons, 2018, 3, 327-334.	4.1	51
61	Porous silaphosphorene, silaarsenene and silaantimonene: a sweet marriage of Si and P/As/Sb. Journal of Materials Chemistry A, 2018, 6, 3738-3746.	5.2	14
62	A non-innocent salen naphthalene ligand and its Co 2+ , Ni 2+ and Cu 2+ metal complexes: Structural, electrochemical, and spectroscopic characterization and computational studies. Inorganica Chimica Acta, 2018, 474, 118-127.	1.2	12
63	Recent progress in 2D group-VA semiconductors: from theory to experiment. Chemical Society Reviews, 2018, 47, 982-1021.	18.7	697
64	Penta-P2X (X=C, Si) monolayers as wide-bandgap semiconductors: A first principles prediction. Frontiers of Physics, 2018, 13, 1.	2.4	60
65	A Coâ€“N₄ moiety embedded into graphene as an efficient single-atom-catalyst for NO electrochemical reduction: a computational study. Journal of Materials Chemistry A, 2018, 6, 7547-7556.	5.2	99
66	Photophysical and photochemical insights into the photodegradation of sulfapyridine in water: A joint experimental and theoretical study. Chemosphere, 2018, 191, 1021-1027.	4.2	21
67	Extraordinary Magnetoresistance in Janus Monolayer MoTeB₂: A Theoretical Prediction. Journal of Physical Chemistry C, 2018, 122, 28423-28430.	1.5	6
68	To Be or Not To Be Protonated: cyclo-N₅^{â€“} in Crystal and Solvent. Journal of Physical Chemistry Letters, 2018, 9, 7137-7145.	2.1	12
69	Modulating the electronic properties of perovskite via Ïƒâ€“Ï€ interfacial interactions: A computational study. APL Materials, 2018, 6, .	2.2	6
70	The dimensional and hydrogenating effect on the electronic properties of ZnSe nanomaterials: a computational investigation. Physical Chemistry Chemical Physics, 2018, 20, 24453-24464.	1.3	4
71	PdSeO₃ Monolayer: Promising Inorganic 2D Photocatalyst for Direct Overall Water Splitting Without Using Sacrificial Reagents and Cocatalysts. Journal of the American Chemical Society, 2018, 140, 12256-12262.	6.6	216
72	Porous hexagonal boron oxide monolayer with robust wide band gap: A computational study. FlatChem, 2018, 9, 27-32.	2.8	29

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73	Aromaticity and Antiaromaticity in Zintl Clusters. Chemistry - A European Journal, 2018, 24, 14583-14597.	1.7	52
74	1T phase as an efficient hole injection layer to TMDs transistors: a universal approach to achieve p-type contacts. 2D Materials, 2018, 5, 031012.	2.0	27
75	Direct-gap semiconducting tri-layer silicene with 29% photovoltaic efficiency. Nano Energy, 2018, 51, 489-495.	8.2	46
76	Cu dimer anchored on C₂N monolayer: low-cost and efficient Bi-atom catalyst for CO oxidation. Nanoscale, 2018, 10, 15696-15705.	2.8	68
77	A hidden symmetry-broken phase of MoS₂ revealed as a superior photovoltaic material. Journal of Materials Chemistry A, 2018, 6, 16087-16093.	5.2	16
78	Exploring adsorption of neutral aromatic pollutants onto graphene nanomaterials via molecular dynamics simulations and theoretical linear solvation energy relationships. Environmental Science: Nano, 2018, 5, 2117-2128.	2.2	22
79	Thiol-maleimide poly(ethylene glycol) crosslinking of L-asparaginase subunits at recombinant cysteine residues introduced by mutagenesis. PLoS ONE, 2018, 13, e0197643.	1.1	11
80	Recent Advances in Aromatic Antimony Clusters. Chinese Journal of Chemistry, 2018, 36, 955-960.	2.6	8
81	Two-dimensional aluminum monoxide nanosheets: A computational study. Frontiers of Physics, 2018, 13, 1.	2.4	3
82	Spindle nodal chain in three-dimensional Î±â€² boron. Physical Chemistry Chemical Physics, 2018, 20, 23500-23506.	1.3	21
83	Copper Dimer Supported on a C₂N Layer as an Efficient Electrocatalyst for CO₂ Reduction Reaction: A Computational Study. Journal of Physical Chemistry C, 2018, 122, 19712-19721.	1.5	167
84	Highly Efficient Photocatalytic Degradation of Dyes by a Copperâ€“Triazolate Metalâ€“Organic Framework. Chemistry - A European Journal, 2018, 24, 16804-16813.	1.7	81
85	Two-Dimensional C₄N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. Journal of Physical Chemistry C, 2017, 121, 2669-2674.	1.5	49
86	Predicting a graphene-like WB4 nanosheet with a double Dirac cone, an ultra-high Fermi velocity and significant gap opening by spinâ€“orbit coupling. Physical Chemistry Chemical Physics, 2017, 19, 5449-5453.	1.3	40
87	Holey graphene: a unique structural derivative of graphene. Materials Research Letters, 2017, 5, 209-234.	4.1	85
88	Tetra-silicene: A Semiconducting Allotrope of Silicene with Negative Poissonâ€™s Ratios. Journal of Physical Chemistry C, 2017, 121, 9627-9633.	1.5	57
89	Antimonene Oxides: Emerging Tunable Direct Bandgap Semiconductor and Novel Topological Insulator. Nano Letters, 2017, 17, 3434-3440.	4.5	250
90	Guidelines for rational design of high-performance absorbents: A case study of zeolite adsorbents for emerging pollutants in water. Green Energy and Environment, 2017, 2, 363-369.	4.7	13

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91	Component Matters: Paving the Roadmap toward Enhanced Electrocatalytic Performance of Graphitic C₃N₄-Based Catalysts via Atomic Tuning. ACS Nano, 2017, 11, 6004-6014.	7.3	144
92	Dirac Nodal Lines and Tilted Semi-Dirac Cones Coexisting in a Striped Boron Sheet. Journal of Physical Chemistry Letters, 2017, 8, 1707-1713.	2.1	81
93	Dielsâ€“Alder reactions of graphene oxides: greatly enhanced chemical reactivity by oxygen-containing groups. Physical Chemistry Chemical Physics, 2017, 19, 11142-11151.	1.3	10
94	Frustrated Lewis Pair Catalysts in Two Dimensions: B/Al-Doped Phosphorenes as Promising Catalysts for Hydrogenation of Small Unsaturated Molecules. ACS Catalysis, 2017, 7, 766-771.	5.5	45
95	Small Dopants Make Big Differences: Enhanced Electrocatalytic Performance of MoS2 Monolayer for Oxygen Reduction Reaction (ORR) by Nâ€“ and Pâ€“Doping. Electrochimica Acta, 2017, 225, 543-550.	2.6	106
96	A two-dimensional TiB₄monolayer exhibits planar octacoordinate Ti. Nanoscale, 2017, 9, 17983-17990.	2.8	50
97	Unveiling Adsorption Mechanisms of Organic Pollutants onto Carbon Nanomaterials by Density Functional Theory Computations and Linear Free Energy Relationship Modeling. Environmental Science & Technology, 2017, 51, 11820-11828.	4.6	38
98	Single Mo Atom Supported on Defective Boron Nitride Monolayer as an Efficient Electrocatalyst for Nitrogen Fixation: A Computational Study. Journal of the American Chemical Society, 2017, 139, 12480-12487.	6.6	1,006
99	Synthesis, characterization and electronic properties of an endohedral plumbaspherene [Au@Pb₁₂]^{3â^’}. Inorganic Chemistry Frontiers, 2017, 4, 1393-1396.	3.0	26
100	Hexagonal honeycomb silicon: Silicene. Series in Materials Science and Engineering, 2017, , 171-188.	0.1	0
101	Semiconducting Groupâ€…15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. Angewandte Chemie, 2016, 128, 1698-1701.	1.6	315
102	Toward enhanced activity of a graphitic carbon nitride-based electrocatalyst in oxygen reduction and hydrogen evolution reactions via atomic sulfur doping. Journal of Materials Chemistry A, 2016, 4, 12205-12211.	5.2	112
103	FeB₆ Monolayers: The Graphene-like Material with Hypercoordinate Transition Metal. Journal of the American Chemical Society, 2016, 138, 5644-5651.	6.6	219
104	Enhanced lithium adsorption/diffusion and improved Li capacity on SnS₂ nanoribbons: A computational investigation. Journal of Materials Research, 2016, 31, 878-885.	1.2	31
105	Graphene-like Two-Dimensional Ionic Boron with Double Dirac Cones at Ambient Condition. Nano Letters, 2016, 16, 3022-3028.	4.5	222
106	Insight into the Origin of Boosted Photosensitive Efficiency of Graphene from the Cooperative Experiment and Theory Study. Journal of Physical Chemistry C, 2016, 120, 27091-27103.	1.5	37
107	Two-Dimensional Y₂C Electride: A Promising Anode Material for Na-Ion Batteries. Journal of Physical Chemistry C, 2016, 120, 18473-18478.	1.5	81
108	Dirac State in the FeB₂ Monolayer with Graphene-Like Boron Sheet. Nano Letters, 2016, 16, 6124-6129.	4.5	200

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109	A Cr₂CO₂ monolayer as a promising cathode for lithium and non-lithium ion batteries: a computational exploration. RSC Advances, 2016, 6, 81591-81596.	1.7	29
110	Semiconductor-topological insulator transition of two-dimensional SbAs induced by biaxial tensile strain. Physical Review B, 2016, 93, .	1.1	118
111	Computational investigation on MB n (Mâ€‰=â€‰Li-Cs, Be-Ba, Sc-La and Ti; nâ€‰=â€‰28 and 38). Journal of Molecular Modeling, 2016, 22, 184.	0.8	12
112	Highâ€Performance Ru₁/CeO₂ Singleâ€Atom Catalyst for CO Oxidation: A Computational Exploration. ChemPhysChem, 2016, 17, 3170-3175.	1.0	47
113	Evolution of MoirÃ© Profiles from van der Waals Superstructures of Boron Nitride Nanosheets. Scientific Reports, 2016, 6, 26084.	1.6	19
114	Anomalous Enhancement of Mechanical Properties in the Ammonia Adsorbed Defective Graphene. Scientific Reports, 2016, 6, 33810.	1.6	3
115	Semi-metallic Be5C2 monolayer global minimum with quasi-planar pentacoordinate carbons and negative Poissonâ€™s ratio. Nature Communications, 2016, 7, 11488.	5.8	247
116	How does the B,F-monodoping and B/F-codoping affect the photocatalytic water-splitting performance of g-C₃N₄?. Physical Chemistry Chemical Physics, 2016, 18, 19217-19226.	1.3	99
117	Scandium carbides/cyanides in the boron cage: computational prediction of X@B₈₀(X =) Tj ETQq1 1 0.784314 rgBT /Ov	1.3	8
118	Semiconducting Groupâ€…15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. Angewandte Chemie - International Edition, 2016, 55, 1666-1669.	7.2	651
119	Singleâ^'sided fluorineâ€“functionalized graphene: A metalâ€“free electrocatalyst with high efficiency for oxygen reduction reaction. Carbon, 2016, 104, 56-63.	5.4	51
120	Phosphorene as a promising anchoring material for lithiumâ€“sulfur batteries: a computational study. Journal of Materials Chemistry A, 2016, 4, 6124-6130.	5.2	156
121	Predicting a new phase (Tâ€²â€²) of two-dimensional transition metal di-chalcogenides and strain-controlled topological phase transition. Nanoscale, 2016, 8, 4969-4975.	2.8	50
122	Single Layer Bismuth Iodide: Computational Exploration of Structural, Electrical, Mechanical and Optical Properties. Scientific Reports, 2015, 5, 17558.	1.6	67
123	Oxidative Etching of Hexagonal Boron Nitride Toward Nanosheets with Defined Edges and Holes. Scientific Reports, 2015, 5, 14510.	1.6	58
124	Four Decades of the Chemistry of Planar Hypercoordinate Compounds. Angewandte Chemie - International Edition, 2015, 54, 9468-9501.	7.2	217
125	Innovation and discovery of grapheneâ€like materials via densityâ€functional theory computations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 360-379.	6.2	205
126	A Density Functional Theory Study of the Mechanical Properties of Graphane With van der Waals Corrections. Mechanics of Advanced Materials and Structures, 2015, 22, 717-721.	1.5	32

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127	Computational investigation on the endohedral borofullerenes M@B40 (MÂ=ÂSc, Y, La). Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	61
128	Mechanical properties and stabilities of g-ZnS monolayers. RSC Advances, 2015, 5, 11240-11247.	1.7	49
129	Atomically Thin Arsenene and Antimonene: Semimetalâ€“Semiconductor and Indirectâ€“Direct Bandâ€Gap Transitions. Angewandte Chemie - International Edition, 2015, 54, 3112-3115.	7.2	1,211
130	Atomically Thin Arsenene and Antimonene: Semimetalâ€“Semiconductor and Indirectâ€“Direct Bandâ€Gap Transitions. Angewandte Chemie, 2015, 127, 3155-3158.	1.6	397
131	Magnetic properties of atomic clusters and endohedral metallofullerenes. Coordination Chemistry Reviews, 2015, 289-290, 315-340.	9.5	86
132	Mechanical degradation of graphene by epoxidation: insights from first-principles calculations. Physical Chemistry Chemical Physics, 2015, 17, 19484-19490.	1.3	25
133	Two-dimensional iron-phthalocyanine (Fe-Pc) monolayer as a promising single-atom-catalyst for oxygen reduction reaction: a computational study. Nanoscale, 2015, 7, 11633-11641.	2.8	164
134	Dynamic motion of an Lu pair inside a C₇₆(T_d) cage. RSC Advances, 2015, 5, 34383-34389.	1.7	4
135	Carbon-Doped Boron Nitride Nanosheet: An Efficient Metal-Free Electrocatalyst for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2015, 119, 26348-26354.	1.5	144
136	Designing high-voltage carbonyl-containing polycyclic aromatic hydrocarbon cathode materials for Li-ion batteries guided by Clar's theory. Journal of Materials Chemistry A, 2015, 3, 19137-19143.	5.2	68
137	Quantum spin hall insulators in strain-modified arsenene. Nanoscale, 2015, 7, 19152-19159.	2.8	151
138	Flexible structural and electronic properties of a pentagonal B₂C monolayer via external strain: a computational investigation. Physical Chemistry Chemical Physics, 2015, 17, 24151-24156.	1.3	127
139	Not your familiar two dimensional transition metal disulfide: structural and electronic properties of the PdS₂monolayer. Journal of Materials Chemistry C, 2015, 3, 9603-9608.	2.7	135
140	Exploration of High-Performance Single-Atom Catalysts on Support M₁/FeO_x for CO Oxidation via Computational Study. ACS Catalysis, 2015, 5, 544-552.	5.5	217
141	Mechanical properties and stabilities of Î±-boron monolayers. Physical Chemistry Chemical Physics, 2015, 17, 2160-2168.	1.3	37
142	Selectivity trend of gas separation through nanoporous graphene. Journal of Solid State Chemistry, 2015, 224, 2-6.	1.4	97
143	Reducing Band Gap and Enhancing Carrier Mobility of Boron Nitride Nanoribbons by Conjugated Ï€ Edge States. Journal of Physical Chemistry C, 2014, 118, 25051-25056.	1.5	25
144	Nanotubes: Chemical Sharpening, Shortening, and Unzipping of Boron Nitride Nanotubes (Adv. Funct.) Tj ETQq0 0 0 rgBT /Overlock 10 T	7.8	1

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145	Computational quest for spherical C12B68 fullerenes with â€œmagicâ€Ï€-electrons and quasi-planar tetra-coordinated carbon. Journal of Molecular Modeling, 2014, 20, 2085.	0.8	6
146	Chemical Sharpening, Shortening, and Unzipping of Boron Nitride Nanotubes. Advanced Functional Materials, 2014, 24, 4497-4506.	7.8	67
147	Be₂C Monolayer with Quasiâ€Planar Hexacoordinate Carbons: A Global Minimum Structure. Angewandte Chemie - International Edition, 2014, 53, 7248-7252.	7.2	223
148	Carbon atoms trapped in cages: Metal carbide clusterfullerenes. Coordination Chemistry Reviews, 2014, 270-271, 89-111.	9.5	73
149	Tuning Electronic Properties of Germanane Layers by External Electric Field and Biaxial Tensile Strain: A Computational Study. Journal of Physical Chemistry C, 2014, 118, 1148-1154.	1.5	92
150	Theoretical design of MoO₃-based high-rate lithium ion battery electrodes: the effect of dimensionality reduction. Journal of Materials Chemistry A, 2014, 2, 19180-19188.	5.2	32
151	Metallic BSi₃ Silicene and Its One-Dimensional Derivatives: Unusual Nanomaterials with Planar Aromatic D_{6h} Six-Membered Silicon Rings. Journal of Physical Chemistry C, 2014, 118, 25825-25835.	1.5	37
152	Metallic BSi₃ Silicene: A Promising High Capacity Anode Material for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2014, 118, 25836-25843.	1.5	62
153	With the same Clar formulas, do the two-dimensional sandwich nanostructures Xâ€“Crâ€“X (X = C4H,) Tj ETQq1 1 0.784314 rgBT /Ov	1.3	13
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