Zhong-Fang Chen

List of Publications by Year
in descending order

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324 papers	33,528 citations	3531 90 h-index	4432 172 g-index
365 all docs	365 docs citations	365 times ranked	25337 citing authors

#	Article	IF	Citations
1	Nucleus-Independent Chemical Shifts (NICS) as an Aromaticity Criterion. Chemical Reviews, 2005, 105, 3842-3888.	47.7	2,815
2	Atomically Thin Arsenene and Antimonene: Semimetalâ€“Semiconductor and Indirectâ€“Direct Bandâ€Gap Transitions. Angewandte Chemie - International Edition, 2015, 54, 3112-3115.	13.8	1,211
3	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.	30.8	1,078
4	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.	13.7	1,006
5	MoS₂ Nanoribbons: High Stability and Unusual Electronic and Magnetic Properties. Journal of the American Chemical Society, 2008, 130, 16739-16744.	13.7	876
6	Recent progress in 2D group-VA semiconductors: from theory to experiment. Chemical Society Reviews, 2018, 47, 982-1021.	38.1	697
7	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.	13.7	664
8	Semiconducting Groupâ€…15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. Angewandte Chemie - International Edition, 2016, 55, 1666-1669.	13.8	651
9	Graphene-related nanomaterials: tuning properties by functionalization. Nanoscale, 2013, 5, 4541.	5.6	614
10	Metallic VS₂ Monolayer: A Promising 2D Anode Material for Lithium Ion Batteries. Journal of Physical Chemistry C, 2013, 117, 25409-25413.	3.1	576
11	Curved Pi-Conjugation, Aromaticity, and the Related Chemistry of Small Fullerenes (<C60) and Single-Walled Carbon Nanotubes. Chemical Reviews, 2005, 105, 3643-3696.	47.7	517
12	Spin Gapless Semiconductorâ€”Metalâ€”Half-Metal Properties in Nitrogen-Doped Zigzag Graphene Nanoribbons. ACS Nano, 2009, 3, 1952-1958.	14.6	499
13	CO Catalytic Oxidation on Iron-Embedded Graphene: Computational Quest for Low-Cost Nanocatalysts. Journal of Physical Chemistry C, 2010, 114, 6250-6254.	3.1	454
14	Spherical Aromaticity:Â Recent Work on Fullerenes, Polyhedral Boranes, and Related Structuresâ€. Chemical Reviews, 2005, 105, 3613-3642.	47.7	436
15	Atomically Thin Arsenene and Antimonene: Semimetalâ€“Semiconductor and Indirectâ€“Direct Bandâ€Gap Transitions. Angewandte Chemie, 2015, 127, 3155-3158.	2.0	397
16	Enhanced Li Adsorption and Diffusion on MoS₂ Zigzag Nanoribbons by Edge Effects: A Computational Study. Journal of Physical Chemistry Letters, 2012, 3, 2221-2227.	4.6	390
17	Spherical Aromaticity inIh Symmetrical Fullerenes: The 2(N+1)2 Rule. Angewandte Chemie - International Edition, 2000, 39, 3915-3917.	13.8	382
18	Computational Screening of Efficient Singleâ€Atom Catalysts Based on Graphitic Carbon Nitride (gâ€C₃N₄) for Nitrogen Electroreduction. Small Methods, 2019, 3, 1800368.	8.6	347

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19	Graphene Oxide as an Ideal Substrate for Hydrogen Storage. ACS Nano, 2009, 3, 2995-3000.	14.6	342
20	Semiconducting Groupâ€…15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. Angewandte Chemie, 2016, 128, 1698-1701.	2.0	315
21	Simultaneously Achieving High Activity and Selectivity toward Two-Electron O₂ Electroreduction: The Power of Single-Atom Catalysts. ACS Catalysis, 2019, 9, 11042-11054.	11.2	314
22	Membraneless enzymatic biofuel cells based on graphene nanosheets. Biosensors and Bioelectronics, 2010, 25, 1829-1833.	10.1	299
23	Tuning Electronic Structure of Bilayer MoS₂ by Vertical Electric Field: A First-Principles Investigation. Journal of Physical Chemistry C, 2012, 116, 21556-21562.	3.1	297
24	Hydrogenation: A Simple Approach To Realize Semiconductorâ^'Half-Metalâ^'Metal Transition in Boron Nitride Nanoribbons. Journal of the American Chemical Society, 2010, 132, 1699-1705.	13.7	277
25	Graphene, inorganic graphene analogs and their composites for lithium ion batteries. Journal of Materials Chemistry A, 2014, 2, 12104.	10.3	251
26	Antimonene Oxides: Emerging Tunable Direct Bandgap Semiconductor and Novel Topological Insulator. Nano Letters, 2017, 17, 3434-3440.	9.1	250
27	Semi-metallic Be5C2 monolayer global minimum with quasi-planar pentacoordinate carbons and negative Poissonâ€™s ratio. Nature Communications, 2016, 7, 11488.	12.8	247
28	Be₂C Monolayer with Quasiâ€Planar Hexacoordinate Carbons: A Global Minimum Structure. Angewandte Chemie - International Edition, 2014, 53, 7248-7252.	13.8	223
29	Electronic structures of SiC nanoribbons. Journal of Chemical Physics, 2008, 129, 174114.	3.0	222
30	Graphene-like Two-Dimensional Ionic Boron with Double Dirac Cones at Ambient Condition. Nano Letters, 2016, 16, 3022-3028.	9.1	222
31	FeB₆ Monolayers: The Graphene-like Material with Hypercoordinate Transition Metal. Journal of the American Chemical Society, 2016, 138, 5644-5651.	13.7	219
32	Four Decades of the Chemistry of Planar Hypercoordinate Compounds. Angewandte Chemie - International Edition, 2015, 54, 9468-9501.	13.8	217
33	Exploration of High-Performance Single-Atom Catalysts on Support M₁/FeO_x for CO Oxidation via Computational Study. ACS Catalysis, 2015, 5, 544-552.	11.2	217
34	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.	13.7	216
35	Scalable Holey Graphene Synthesis and Dense Electrode Fabrication toward High-Performance Ultracapacitors. ACS Nano, 2014, 8, 8255-8265.	14.6	212
36	Innovation and discovery of grapheneâ€like materials via densityâ€functional theory computations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 360-379.	14.6	205

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37	Dirac State in the FeB₂ Monolayer with Graphene-Like Boron Sheet. Nano Letters, 2016, 16, 6124-6129.	9.1	200
38	Fe-Anchored Graphene Oxide: A Low-Cost and Easily Accessible Catalyst for Low-Temperature CO Oxidation. Journal of Physical Chemistry C, 2012, 116, 2507-2514.	3.1	189
39	Catalytic Activities of Subnanometer Gold Clusters (Au₁₆â€“Au₁₈,) Tj ETQq1 1 0.784314 rgBT /Overlock 1 7818-7829.	14.6	182
40	Reactivity of the Convex and Concave Surfaces of Single-Walled Carbon Nanotubes (SWCNTs) towards Addition Reactions: Dependence on the Carbon-Atom Pyramidalization. ChemPhysChem, 2003, 4, 93-97.	2.1	177
41	Two-dimensional polyphenylene: experimentally available porous graphene as a hydrogen purification membrane. Chemical Communications, 2010, 46, 3672.	4.1	176
42	SiC₂ Silagraphene and Its One-Dimensional Derivatives: Where Planar Tetracoordinate Silicon Happens. Journal of the American Chemical Society, 2011, 133, 900-908.	13.7	171
43	Spherical Aromaticity of Inorganic Cage Molecules. Angewandte Chemie - International Edition, 2001, 40, 2834-2838.	13.8	169
44	Extremely Stable Metal-EncapsulatedAlPb10+andAlPb12+Clusters: Mass-Spectrometric Discovery and Density Functional Theory Study. Physical Review Letters, 2004, 92, 163401.	7.8	169
45	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.	3.1	167
46	Ca-Coated Boron Fullerenes and Nanotubes as Superior Hydrogen Storage Materials. Nano Letters, 2009, 9, 1944-1948.	9.1	165
47	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.	5.6	164
48	Comparative Study of Hydrogen Adsorption on Carbon and BN Nanotubes. Journal of Physical Chemistry B, 2006, 110, 13363-13369.	2.6	157
49	Phosphorene as a promising anchoring material for lithiumâ€“sulfur batteries: a computational study. Journal of Materials Chemistry A, 2016, 4, 6124-6130.	10.3	156
50	Quantum spin hall insulators in strain-modified arsenene. Nanoscale, 2015, 7, 19152-19159.	5.6	151
51	B80 and B101â€“103 clusters: Remarkable stability of the core-shell structures established by validated density functionals. Journal of Chemical Physics, 2012, 136, 074302.	3.0	150
52	Boosting ORR/OER Activity of Graphdiyne by Simple Heteroatom Doping. Small Methods, 2019, 3, 1800550.	8.6	149
53	Open-Shell Singlet Character of Cyclacenes and Short Zigzag Nanotubes. Organic Letters, 2007, 9, 5449-5452.	4.6	147
54	Carbon-Doped Boron Nitride Nanosheet: An Efficient Metal-Free Electrocatalyst for the Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2015, 119, 26348-26354.	3.1	144

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55	Component Matters: Paving the Roadmap toward Enhanced Electrocatalytic Performance of Graphitic C₃N₄-Based Catalysts via Atomic Tuning. ACS Nano, 2017, 11, 6004-6014.	14.6	144
56	B₈₀ and Other Medium-Sized Boron Clusters: Coreâ^'Shell Structures, Not Hollow Cages. Journal of Physical Chemistry A, 2010, 114, 9969-9972.	2.5	143
57	Are Stoneâ^'Wales Defect Sites Always More Reactive Than Perfect Sites in the Sidewalls of Single-Wall Carbon Nanotubes?. Journal of the American Chemical Society, 2005, 127, 20-21.	13.7	135
58	Not your familiar two dimensional transition metal disulfide: structural and electronic properties of the PdS₂monolayer. Journal of Materials Chemistry C, 2015, 3, 9603-9608.	5.5	135
59	Properties of Fullerene[50] andD5hDecachlorofullerene[50]:Â A Computational Study. Journal of the American Chemical Society, 2004, 126, 14871-14878.	13.7	133
60	Do All-Metal Antiaromatic Clusters Exist?. Journal of the American Chemical Society, 2003, 125, 13930-13931.	13.7	131
61	Layer-by-Layer Hybrids of MoS2 and Reduced Graphene Oxide for Lithium Ion Batteries. Electrochimica Acta, 2014, 147, 392-400.	5.2	129
62	Electronic Structure and Reactivity of Boron Nitride Nanoribbons with Stone-Wales Defects. Journal of Chemical Theory and Computation, 2009, 5, 3088-3095.	5.3	127
63	CO Oxidation on TiO₂ (110) Supported Subnanometer Gold Clusters: Size and Shape Effects. Journal of the American Chemical Society, 2013, 135, 19336-19346.	13.7	127
64	Flexible structural and electronic properties of a pentagonal B₂C monolayer via external strain: a computational investigation. Physical Chemistry Chemical Physics, 2015, 17, 24151-24156.	2.8	127
65	Stability of graphene oxide phases from first-principles calculations. Physical Review B, 2010, 82, .	3.2	124
66	Structural and Electronic Properties of Graphane Nanoribbons. Journal of Physical Chemistry C, 2009, 113, 15043-15045.	3.1	118
67	Semiconductor-topological insulator transition of two-dimensional SbAs induced by biaxial tensile strain. Physical Review B, 2016, 93, .	3.2	118
68	Do Composite Single-Walled Nanotubes Have Enhanced Capability for Lithium Storage?. Chemistry of Materials, 2005, 17, 992-1000.	6.7	117
69	To Achieve Stable Spherical Clusters:Â General Principles and Experimental Confirmations. Journal of the American Chemical Society, 2006, 128, 12829-12834.	13.7	116
70	Amorphous structural models for graphene oxides. Carbon, 2012, 50, 1690-1698.	10.3	114
71	Versatile Electronic Properties of VSe₂ Bulk, Few-Layers, Monolayer, Nanoribbons, and Nanotubes: A Computational Exploration. Journal of Physical Chemistry C, 2014, 118, 21264-21274.	3.1	114
72	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.	10.3	112

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73	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.	10.3	112
74	Appropriate description of intermolecular interactions in the methane hydrates: An assessment of DFT methods. Journal of Computational Chemistry, 2013, 34, 121-131.	3.3	111
75	Controllable CO2 electrocatalytic reduction via ferroelectric switching on single atom anchored In2Se3 monolayer. Nature Communications, 2021, 12, 5128.	12.8	110
76	Nonvolatile Electrical Control and Heterointerfaceâ€Induced Halfâ€Metallicity of 2D Ferromagnets. Advanced Functional Materials, 2019, 29, 1901420.	14.9	109
77	Molecular Charge Transfer: A Simple and Effective Route To Engineer the Band Structures of BN Nanosheets and Nanoribbons. Journal of Physical Chemistry C, 2011, 115, 18531-18537.	3.1	107
78	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.	5.2	106
79	Side-Wall Opening of Single-Walled Carbon Nanotubes (SWCNTs) by Chemical Modification: A Critical Theoretical Study. Angewandte Chemie - International Edition, 2004, 43, 1552-1554.	13.8	105
80	Stoneâ^'Wales Defects in Single-Walled Boron Nitride Nanotubes:â€‰ Formation Energies, Electronic Structures, and Reactivity. Journal of Physical Chemistry C, 2008, 112, 1365-1370.	3.1	105
81	Graphane/Fluorographene Bilayer: Considerable Câ€“HÂ·Â·Â·Fâ€“C Hydrogen Bonding and Effective Band Structure Engineering. Journal of the American Chemical Society, 2012, 134, 11269-11275.	13.7	105
82	Hollow Cages versus Space-Filling Structures for Medium-Sized Gold Clusters:â€‰ The Spherical Aromaticity of the Au50 Cage. Journal of Physical Chemistry A, 2005, 109, 9265-9269.	2.5	101
83	Aromatic Boron Wheels with More than One Carbon Atom in the Center: C 2 B 8 , C 3 B 9 3+ , and C 5 B 11 +. Angewandte Chemie - International Edition, 2005, 44, 1078-1082.	13.8	100
84	Investigation of a Putative MÃ¶bius Aromatic Hydrocarbon. The Effect of Benzannelation on MÃ¶bius [4n]Annulene Aromaticity. Journal of the American Chemical Society, 2005, 127, 2425-2432.	13.7	100
85	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.	2.8	99
86	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.	10.3	99
87	Selectivity trend of gas separation through nanoporous graphene. Journal of Solid State Chemistry, 2015, 224, 2-6.	2.9	97
88	Establishing a Theoretical Landscape for Identifying Basal Plane Active 2D Metal Borides (MBenes) toward Nitrogen Electroreduction. Advanced Functional Materials, 2021, 31, 2008056.	14.9	97
89	Identifying the Activity Origin of a Cobalt Singleâ€Atom Catalyst for Hydrogen Evolution Using Supervised Learning. Advanced Functional Materials, 2021, 31, 2100547.	14.9	93
90	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.	3.1	92

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91	1 + 1â€² > 2: Heteronuclear Biatom Catalyst Outperforms Its Homonuclear Counterparts for CO Oxidation. Small Methods, 2019, 3, 1800480.	8.6	92
92	Theoretical Studies on the Smallest Fullerene: from Monomer to Oligomers and Solid States. Chemistry - A European Journal, 2004, 10, 963-970.	3.3	90
93	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.	10.3	87
94	Magnetic properties of atomic clusters and endohedral metallofullerenes. Coordination Chemistry Reviews, 2015, 289-290, 315-340.	18.8	86
95	Holey graphene: a unique structural derivative of graphene. Materials Research Letters, 2017, 5, 209-234.	8.7	85
96	Enhanced Ferromagnetism and Tunable Magnetism in Fe₃GeTe₂ Monolayer by Strain Engineering. ACS Applied Materials & Interfaces, 2020, 12, 26367-26373.	8.0	83
97	The 2(N+1)2 rule for spherical aromaticity: further validation. Journal of Molecular Modeling, 2001, 7, 161-163.	1.8	82
98	What Protects the Core When the Thiolated Au Cluster is Extremely Small?. Journal of Physical Chemistry C, 2009, 113, 16983-16987.	3.1	82
99	XH/Ï€ (X = C, Si) Interactions in Graphene and Silicene: Weak in Strength, Strong in Tuning Band Structures. Journal of Physical Chemistry Letters, 2013, 4, 269-275.	4.6	82
100	Al₂C monolayer: the planar tetracoordinate carbon global minimum. Nanoscale, 2014, 6, 10784.	5.6	82
101	An Improbable Monometallic Cluster Entrapped in a Popular Fullerene Cage: YCN@Cs(6)-C82. Scientific Reports, 2013, 3, 1487.	3.3	81
102	Two-Dimensional Y₂C Electride: A Promising Anode Material for Na-Ion Batteries. Journal of Physical Chemistry C, 2016, 120, 18473-18478.	3.1	81
103	Dirac Nodal Lines and Tilted Semi-Dirac Cones Coexisting in a Striped Boron Sheet. Journal of Physical Chemistry Letters, 2017, 8, 1707-1713.	4.6	81
104	Highly Efficient Photocatalytic Degradation of Dyes by a Copperâ€“Triazolate Metalâ€“Organic Framework. Chemistry - A European Journal, 2018, 24, 16804-16813.	3.3	81
105	Myriad Planar Hexacoordinate Carbon Molecules Inviting Synthesis. Journal of the American Chemical Society, 2007, 129, 1510-1511.	13.7	80
106	Why the photocatalytic activity of Mo-doped BiVO4 is enhanced: a comprehensive density functional study. Physical Chemistry Chemical Physics, 2014, 16, 13465.	2.8	80
107	Tuning Electronic and Magnetic Properties of Wurtzite ZnO Nanosheets by Surface Hydrogenation. ACS Applied Materials & Interfaces, 2010, 2, 2442-2447.	8.0	79
108	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.	2.8	79

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109	Comparative density functional theory study on the electronic and optical properties of BiMO4 (M =) Tj ETQq1 1 0.784314 rgBT /Ove	10.3	78
110	Theoretical investigation into structures and magnetic properties of smaller fullerenes and their heteroanalogues. Theoretical Chemistry Accounts, 2001, 106, 352-363.	1.4	76
111	Energetics and electronic structures of AlN nanotubes/wires and their potential application as ammonia sensors. Nanotechnology, 2007, 18, 424023.	2.6	76
112	Performance of semiempirical methods in fullerene chemistry: relative energies and nucleus-independent chemical shifts. Chemical Physics Letters, 2003, 367, 15-25.	2.6	74
113	Carbon atoms trapped in cages: Metal carbide clusterfullerenes. Coordination Chemistry Reviews, 2014, 270-271, 89-111.	18.8	73
114	Molecular Crowding Effect in Aqueous Electrolytes to Suppress Hydrogen Reduction Reaction and Enhance Electrochemical Nitrogen Reduction. Advanced Energy Materials, 2021, 11, 2101699.	19.5	73
115	Engineering the Electronic Structure of Single-Walled Carbon Nanotubes by Chemical Functionalization. ChemPhysChem, 2005, 6, 598-601.	2.1	71
116	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.	10.3	71
117	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.	5.6	70
118	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.	10.3	68
119	Cu dimer anchored on C₂N monolayer: low-cost and efficient Bi-atom catalyst for CO oxidation. Nanoscale, 2018, 10, 15696-15705.	5.6	68
120	Endohedral chemical shifts in higher fullerenes with 72-86 carbon atoms. Theoretical Chemistry Accounts, 2001, 106, 364-368.	1.4	67
121	Atomic and Electronic Structures of Fluorinated BN Nanotubes:Â Computational Study. Journal of Physical Chemistry B, 2006, 110, 25678-25685.	2.6	67
122	Size- and Surface-dependent Stability, Electronic Properties, and Potential as Chemical Sensors: Computational Studies on One-dimensional ZnO Nanostructures. Journal of Physical Chemistry C, 2008, 112, 13926-13931.	3.1	67
123	Chemical Sharpening, Shortening, and Unzipping of Boron Nitride Nanotubes. Advanced Functional Materials, 2014, 24, 4497-4506.	14.9	67
124	Single Layer Bismuth Iodide: Computational Exploration of Structural, Electrical, Mechanical and Optical Properties. Scientific Reports, 2015, 5, 17558.	3.3	67
125	Comparative Study of Carbon and BN Nanographenes: Ground Electronic States and Energy Gap Engineering. Journal of Physical Chemistry C, 2008, 112, 12677-12682.	3.1	66
126	Boron fullerenes with 32â€“56 atoms: Irregular cage configurations and electronic properties. Chemical Physics Letters, 2010, 501, 16-19.	2.6	65

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127	Tuning electronic and magnetic properties of MoO3 sheets by cutting, hydrogenation, and external strain: a computational investigation. Nanoscale, 2013, 5, 5321.	5.6	65
128	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.	10.3	65
129	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.	4.6	65
130	Tuning band gaps of BN nanosheets and nanoribbons via interfacial dihalogen bonding and external electric field. Nanoscale, 2014, 6, 8624-8634.	5.6	64
131	Metallic BSi₃ Silicene: A Promising High Capacity Anode Material for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2014, 118, 25836-25843.	3.1	62
132	Computational investigation on the endohedral borofullerenes M@B40 (MÂ=ÂSc, Y, La). Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	61
133	Theoretical Studies of the Substitution Patterns in Heterofullerenes C60-xNxand C60-xBx(x= 2â^'8). Journal of Physical Chemistry A, 1999, 103, 10961-10968.	2.5	60
134	Penta-P2X (X=C, Si) monolayers as wide-bandgap semiconductors: A first principles prediction. Frontiers of Physics, 2018, 13, 1.	5.0	60
135	Is C60 buckminsterfullerene aromatic?. Physical Chemistry Chemical Physics, 2012, 14, 14886.	2.8	58
136	Oxidative Etching of Hexagonal Boron Nitride Toward Nanosheets with Defined Edges and Holes. Scientific Reports, 2015, 5, 14510.	3.3	58
137	La2@C72and Sc2@C72:Â Computational Characterizations. Journal of Physical Chemistry A, 2006, 110, 2231-2234.	2.5	57
138	Tetra-silicene: A Semiconducting Allotrope of Silicene with Negative Poissonâ€™s Ratios. Journal of Physical Chemistry C, 2017, 121, 9627-9633.	3.1	57
139	Structure and Bonding in the Omnicapped Truncated Tetrahedral Au20Cluster:Â Analogies between Gold and Carbon Cluster Chemistry. Inorganic Chemistry, 2004, 43, 4564-4566.	4.0	54
140	Exohedral functionalization of endohedral metallofullerenes: Interplay between inside and outside. Coordination Chemistry Reviews, 2019, 388, 406-439.	18.8	54
141	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.	10.3	54
142	Planar Hypercoordinate Motifs in Two-Dimensional Materials. Accounts of Chemical Research, 2020, 53, 887-895.	15.6	54
143	Aromaticity and Antiaromaticity in Zintl Clusters. Chemistry - A European Journal, 2018, 24, 14583-14597.	3.3	52
144	Singleâ^'sided fluorineâ€“functionalized graphene: A metalâ€“free electrocatalyst with high efficiency for oxygen reduction reaction. Carbon, 2016, 104, 56-63.	10.3	51

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145	A two-dimensional CaSi monolayer with quasi-planar pentacoordinate silicon. Nanoscale Horizons, 2018, 3, 327-334.	8.0	51
146	Firstâ€principles study of molecular hydrogen dissociation on doped Al₁₂X (X = B, Al, C, Si,) Tj ETQq0 0 0 rgBT /Overlock 10	3.3	50
147	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.	5.6	50
148	A two-dimensional TiB₄monolayer exhibits planar octacoordinate Ti. Nanoscale, 2017, 9, 17983-17990.	5.6	50
149	Mechanical properties and stabilities of g-ZnS monolayers. RSC Advances, 2015, 5, 11240-11247.	3.6	49
150	Two-Dimensional C₄N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. Journal of Physical Chemistry C, 2017, 121, 2669-2674.	3.1	49
151	BN-Doped Fullerenes:Â An NICS Characterization. Journal of Organic Chemistry, 2001, 66, 3380-3383.	3.2	47
152	Highâ€Performance Ru₁/CeO₂ Singleâ€Atom Catalyst for CO Oxidation: A Computational Exploration. ChemPhysChem, 2016, 17, 3170-3175.	2.1	47
153	Spherical Homoaromaticity. Angewandte Chemie - International Edition, 2002, 41, 4309-4312.	13.8	46
154	Oxidation Unzipping of Stable Nanographenes into Joint Spin-Rich Fragments. Journal of the American Chemical Society, 2009, 131, 9663-9669.	13.7	46
155	What is the best density functional to describe water clusters: evaluation of widely used density functionals with various basis sets for (H2O) n (nÂ=Â1â€“10). Theoretical Chemistry Accounts, 2011, 130, 341-352.	1.4	46
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