Yong-Fan Zhang

List of Publications by Year
in descending order

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149 papers	6,891 citations	94269 37 h-index	66788 78 g-index
149 all docs	149 docs citations	149 times ranked	7788 citing authors

#	Article	IF	Citations
1	Tri-s-triazine-Based Crystalline Graphitic Carbon Nitrides for Highly Efficient Hydrogen Evolution Photocatalysis. ACS Catalysis, 2016, 6, 3921-3931.	5.5	756
2	Monolayered Bi2WO6 nanosheets mimicking heterojunction interface with open surfaces for photocatalysis. Nature Communications, 2015, 6, 8340.	5.8	578
3	Ionothermal Synthesis of Triazineâ€“Heptazineâ€Based Copolymers with Apparent Quantum Yields of 60â€‰% at 420â€…nm for Solar Hydrogen Production from â€œSea Waterâ€. Angewandte Chemie - International Edition, 2018, 57, 9372-9376.	7.2	369
4	Photocatalytic Oxygen Evolution from Functional Triazineâ€Based Polymers with Tunable Band Structures. Angewandte Chemie - International Edition, 2018, 57, 470-474.	7.2	278
5	Reducing the Exciton Binding Energy of Donorâ€“Acceptorâ€Based Conjugated Polymers to Promote Chargeâ€Induced Reactions. Angewandte Chemie - International Edition, 2019, 58, 10236-10240.	7.2	278
6	Ultrasmall MoO_x Clusters as a Novel Cocatalyst for Photocatalytic Hydrogen Evolution. Advanced Materials, 2019, 31, e1804883.	11.1	222
7	Insight into the effect of morphology on catalytic performance of porous CeO2 nanocrystals for H2S selective oxidation. Applied Catalysis B: Environmental, 2019, 252, 98-110.	10.8	213
8	Photocatalytic overall water splitting by conjugated semiconductors with crystalline poly(triazine) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	3.7	186
9	Acid and Base Resistant Zirconium Polyphenolateâ€Metalloporphyrin Scaffolds for Efficient CO₂ Photoreduction. Advanced Materials, 2018, 30, 1704388.	11.1	184
10	Direct probing of atomically dispersed Ru species over multi-edged TiO ₂ for highly efficient photocatalytic hydrogen evolution. Science Advances, 2020, 6, .	4.7	161
11	A Theoretical Study on the Electronic Structures of TiO2:Â Effect of Hartreeâ^Fock Exchange. Journal of Physical Chemistry B, 2005, 109, 19270-19277.	1.2	135
12	A Tumor-pH-Responsive Supramolecular Photosensitizer for Activatable Photodynamic Therapy with Minimal In Vivo Skin Phototoxicity. Theranostics, 2017, 7, 2746-2756.	4.6	117
13	Nanofibers with diameter below one nanometer from electrospinning. RSC Advances, 2018, 8, 4794-4802.	1.7	117
14	Role of Spacers and Substituents in the Self-Assembly Process:â€‰ Syntheses and Characterization of Three Novel Silver(I)/Iodine Polymers. Crystal Growth and Design, 2006, 6, 1813-1820.	1.4	115
15	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
16	A Fully Coplanar Donorâ€“Acceptor Polymeric Semiconductor with Promoted Charge Separation Kinetics for Photochemistry. Angewandte Chemie - International Edition, 2021, 60, 16355-16359.	7.2	94
17	Comparative density functional theory study on the electronic and optical properties of BiMO4 (M =) Tj ETQq1 1 0.784314 rgBT /Ove	5.2	78
18	Highly Efficient Porous Fe_xCe_{1â€“x}O_{2â^Î´} with Three-Dimensional Hierarchical Nanoflower Morphology for H₂S-Selective Oxidation. ACS Catalysis, 2020, 10, 3968-3983.	5.5	78

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19	Construction of Fe-doped TiO2â^'x ultrathin nanosheets with rich oxygen vacancies for highly efficient oxidation of H2S. Chemical Engineering Journal, 2022, 430, 132917.	6.6	77
20	Photocatalytic Oxygen Evolution from Functional Triazineâ€Based Polymers with Tunable Band Structures. Angewandte Chemie, 2018, 130, 479-483.	1.6	75
21	MnSb₂S₄ Monolayer as an Anode Material for Metal-Ion Batteries. Chemistry of Materials, 2018, 30, 3208-3214.	3.2	74
22	Ionothermal Synthesis of Triazineâ€"Heptazineâ€Based Copolymers with Apparent Quantum Yields of 60â€‰% at 420â€…nm for Solar Hydrogen Production from â€œSea Waterâ€. Angewandte Chemie, 2018, 130, 9516-9520.	1.6	73
23	First-Principles Studies of Lithium Adsorption and Diffusion on Graphene with Grain Boundaries. Journal of Physical Chemistry C, 2014, 118, 28055-28062.	1.5	70
24	Computational design of inorganic nonlinear optical crystals based on a genetic algorithm. CrystEngComm, 2014, 16, 10569-10580.	1.3	67
25	Ionothermal Synthesis of Covalent Triazine Frameworks in a NaClâ€KClâ€ZnCl₂Eutectic Salt for the Hydrogen Evolution Reaction. Angewandte Chemie - International Edition, 2022, 61, .	7.2	67
26	1T-MoS2 monolayer as a promising anode material for (Li/Na/Mg)-ion batteries. Applied Surface Science, 2022, 584, 152537.	3.1	66
27	Defect engineering of metalâ€"oxide interface for proximity of photooxidation and photoreduction. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10232-10237.	3.3	63
28	Controllable P Doping of the LaCoO₃ Catalyst for Efficient Propane Oxidation: Optimized Surface Co Distribution and Enhanced Oxygen Vacancies. ACS Applied Materials & Interfaces, 2020, 12, 23789-23799.	4.0	61
29	Promoting effect of Cu-doping on catalytic activity and SO2 resistance of porous CeO2 nanorods for H2S selective oxidation. Journal of Catalysis, 2020, 389, 382-399.	3.1	59
30	Electronic properties and 4f â†' 5d transitions in Ce-doped Lu2SiO5: a theoretical investigation. Journal of Materials Chemistry, 2012, 22, 13723.	6.7	53
31	Density Functional Theory Study of Single-Atom V, Nb, and Ta Catalysts on Graphene and Carbon Nitride for Selective Nitrogen Reduction. ACS Applied Nano Materials, 2020, 3, 5149-5159.	2.4	51
32	Atomically Dispersed Ru Catalyst for Low-Temperature Nitrogen Activation to Ammonia via an Associative Mechanism. ACS Catalysis, 2020, 10, 9504-9514.	5.5	47
33	Whether Corrugated or Planar Vacancy Graphene-like Carbon Nitride (g-C₃N₄) Is More Effective for Nitrogen Reduction Reaction?. Journal of Physical Chemistry C, 2019, 123, 17296-17305.	1.5	46
34	Bond-Curvature Effect of Sidewall [2+1] Cycloadditions of Single-Walled Carbon Nanotubes:â€‰ A New Criterion To the Adduct Structures. Chemistry of Materials, 2006, 18, 3579-3584.	3.2	43
35	Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. Applied Surface Science, 2021, 563, 150269.	3.1	43
36	Highly Active and Sulfurâ€Resistant Feâ€"N₄ Sites in Porous Carbon Nitride for the Oxidation of H₂S into Elemental Sulfur. Small, 2020, 16, e2003904.	5.2	41

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37	A Theoretical Study on the Structural and Energy Spectral Properties of Ce³⁺ Ions Doped in Various Fluoride Compounds. Journal of Physical Chemistry C, 2012, 116, 20513-20521.	1.5	39
38	A comparative study of CO catalytic oxidation on Pd-anchored graphene oxide and Pd-embedded vacancy graphene. Journal of Nanoparticle Research, 2014, 16, 1.	0.8	38
39	First-principles investigation of the activation of CO2 molecule on TM/Cu (TM=Fe, Co and Ni) surface alloys. Applied Surface Science, 2015, 353, 902-912.	3.1	38
40	Facile fabrication of shape-controlled Co_xMn_yO_{Î²} nanocatalysts for benzene oxidation at low temperatures. Chemical Communications, 2018, 54, 2154-2157.	2.2	37
41	Effects of ligand functionalization on the photocatalytic properties of titanium-based MOF: A density functional theory study. AIP Advances, 2018, 8, .	0.6	35
42	Structural and Electronic Properties of a W₃O₉Cluster Supported on the TiO₂(110) Surface. Journal of Physical Chemistry C, 2009, 113, 17509-17517.	1.5	34
43	Energetic, Optical, and Electronic Properties of Intrinsic Electron-Trapping Defects in YAlO₃: A Hybrid DFT Study. Journal of Physical Chemistry C, 2014, 118, 19940-19947.	1.5	34
44	Iron-Based Metalâ€“Organic Frameworks as Platform for H₂S Selective Conversion: Structure-Dependent Desulfurization Activity. Inorganic Chemistry, 2020, 59, 4483-4492.	1.9	34
45	Electronic properties of red and black phosphorous and their potential application as photocatalysts. RSC Advances, 2016, 6, 80872-80884.	1.7	33
46	Preadsorption of O₂ on the Exposed (001) Facets of ZnO Nanostructures for Enhanced Sensing of Gaseous Acetone. ACS Applied Nano Materials, 2019, 2, 6144-6151.	2.4	33
47	Phthalocyanine and Metal Phthalocyanines Adsorbed on Graphene: A Density Functional Study. Journal of Physical Chemistry C, 2019, 123, 16614-16620.	1.5	33
48	Oxygen-vacancies-engaged efficient carrier utilization for the photocatalytic coupling reaction. Journal of Catalysis, 2019, 373, 116-125.	3.1	33
49	Screening novel candidates for mid-IR nonlinear optical materials from I₃â€“Vâ€“VI₄compounds. Journal of Materials Chemistry C, 2017, 5, 1963-1972.	2.7	32
50	Reducing the Exciton Binding Energy of Donorâ€“Acceptorâ€Based Conjugated Polymers to Promote Chargeâ€Induced Reactions. Angewandte Chemie, 2019, 131, 10342-10346.	1.6	32
51	What Is the Best Size of Subnanometer Copper Clusters for CO₂ Conversion to Methanol at Cu/TiO₂ Interfaces? A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 24118-24132.	1.5	32
52	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
53	Germanium and iron double-substituted ZnGa2O4 solid-solution photocatalysts with modulated band structure for boosting photocatalytic CO2 reduction with H2O. Applied Catalysis B: Environmental, 2020, 265, 118551.	10.8	31
54	Asymmetric Acceptorâ€“Donorâ€“Acceptor Polymers with Fast Charge Carrier Transfer for Solar Hydrogen Production. Chemistry - A European Journal, 2021, 27, 939-943.	1.7	31

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55	Unraveling the mechanisms of S-doped carbon nitride for photocatalytic oxygen reduction to H₂O₂. Physical Chemistry Chemical Physics, 2020, 22, 21099-21107.	1.3	29
56	Effects of doping high-valence transition metal (V, Nb and Zr) ions on the structure and electrochemical performance of LIB cathode material LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂. Physical Chemistry Chemical Physics, 2021, 23, 11528-11537.	1.3	29
57	Carbon Nanotubes Functionalized by NO2:Â Coexistence of Charge Transfer and Radical Transfer. Journal of Physical Chemistry B, 2006, 110, 22462-22470.	1.2	28
58	Structural and electronic properties of tungsten trioxides: from cluster to solid surface. Theoretical Chemistry Accounts, 2011, 130, 103-114.	0.5	28
59	Blue-AsP monolayer as a promising anode material for lithium- and sodium-ion batteries: a DFT study. Physical Chemistry Chemical Physics, 2021, 23, 5143-5151.	1.3	28
60	Electrocatalytic Nitrogen Reduction by Transition Metal Single-Atom Catalysts on Polymeric Carbon Nitride. Journal of Physical Chemistry C, 2021, 125, 13880-13888.	1.5	28
61	Single-Crystalline Covalent Organic Frameworks as High-Performance Liquid Chromatographic Stationary Phases for Positional Isomer Separation. ACS Applied Materials & Interfaces, 2022, 14, 9754-9762.	4.0	28
62	Subnanometer iron clusters confined in a porous carbon matrix for highly efficient zincâ€“air batteries. Nanoscale Horizons, 2020, 5, 359-365.	4.1	27
63	Nitrogen fixation on metal-free SiC(111) polar surfaces. Journal of Materials Chemistry A, 2020, 8, 7412-7421.	5.2	26
64	High electrocatalytic performance of graphene nanoribbon supported PtAu nanoalloy for direct ethanol fuel cell and theoretical analysis of anti-CO poisoning. Electrochimica Acta, 2016, 187, 560-566.	2.6	23
65	Efficient ammonia synthesis over a coreâ€“shell Ru/CeO₂catalyst with a tunable CeO₂size: DFT calculations and XAS spectroscopy studies. Inorganic Chemistry Frontiers, 2019, 6, 396-406.	3.0	23
66	Germanium-substituted Zn2TiO4 solid solution photocatalyst for conversion of CO2 into fuels. Journal of Catalysis, 2019, 371, 144-152.	3.1	23
67	A New Candidate in Polyanionic Compounds for a Potassium-Ion Battery Cathode: KTiOPO₄. Journal of Physical Chemistry Letters, 2021, 12, 2721-2726.	2.1	23
68	Energy Band Alignment and Redoxâ€Active Sites in Metalloporphyrinâ€Spaced Metalâ€Catechol Frameworks for Enhanced CO₂ Photoreduction. Angewandte Chemie - International Edition, 2022, 61, .	7.2	23
69	First-Principles Study on Structural Properties and 4f â†’ 5d Transitions of Locally Charge-Compensated Ce³⁺ in CaF₂. Journal of Physical Chemistry C, 2012, 116, 18419-18426.	1.5	22
70	Toward improving CO2 dissociation and conversion to methanol via CO-hydrogenation on Cu(100) surface by introducing embedded Co nanoclusters as promoters: A DFT study. Applied Surface Science, 2018, 427, 837-847.	3.1	22
71	BC₂N/Graphene Heterostructure as a Promising Anode Material for Rechargeable Li-Ion Batteries by Density Functional Calculations. Journal of Physical Chemistry C, 2019, 123, 30809-30818.	1.5	22
72	Understanding the Linear and Second-Order Nonlinear Optical Properties of UiO-66-Derived Metalâ€“Organic Frameworks: A Comprehensive DFT Study. Journal of Physical Chemistry C, 2020, 124, 11595-11608.	1.5	22

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73	The effects of the introduction of Al atom into monoclinic BiVO4: a theoretical prediction. Theoretical Chemistry Accounts, 2010, 127, 751-757.	0.5	21
74	Probing the Smallest Molecular Model of MoS₂ Catalyst: S₂ Units in the MoS_n^{â€“/0} (n = 1â€“5) Clusters. Journal of Physical Chemistry A, 2013, 117, 5632-5641.	1.1	21
75	Different Atomic Terminations Affect the Photocatalytic Nitrogen Fixation of Bismuth Oxybromide: A First Principles Study. Chemistry - an Asian Journal, 2018, 13, 799-808.	1.7	21
76	UiO-66 Metalâ€“Organic Framework as an Anode for a Potassium-Ion Battery: Quantum Mechanical Analysis. Journal of Physical Chemistry C, 2021, 125, 9679-9687.	1.5	21
77	First-Principles Study on Electronic Properties and Optical Spectra of Ce-Doped La₂CaB₁₀O₁₉ Crystal. Journal of Physical Chemistry C, 2013, 117, 15241-15246.	1.5	20
78	Insight into the Mechanism of CO Oxidation on WO3(001) Surfaces for Gas Sensing: A DFT Study. Sensors, 2017, 17, 1898.	2.1	20
79	H₂ and CH₄ production from bio-alcohols using condensed poly(heptazine) Tj ETQq1 1 0.784314 rgBT /Ov	5.2	20
80	Molecular-level understanding of reaction path optimization as a function of shape concerning the metalâ€“support interaction effect of Co/CeO₂ on water-gas shift catalysis. Catalysis Science and Technology, 2019, 9, 4928-4937.	2.1	19
81	A boron-decorated melon-based carbon nitride as a metal-free photocatalyst for N₂ fixation: a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 21872-21880.	1.3	18
82	S Adsorption at Regular and Defect Sites of the MgO (001) Surface: Cluster Model Study at DFT Level. Surface Review and Letters, 2003, 10, 691-695.	0.5	17
83	Visible-light-driven selective alcohol dehydrogenation and hydrogenolysis via the Mott Schottky effect. Journal of Materials Chemistry A, 2020, 8, 6854-6862.	5.2	17
84	Indium selenide monolayer: a two-dimensional material with strong second harmonic generation. CrystEngComm, 2018, 20, 2573-2582.	1.3	16
85	First-principles calculations of photoluminescence and defect states of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msup><mml:mrow><mml:mi mathvariant="normal">e</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup> -doped <mml:math		

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91	Defective BC₂N as an Anode Material with Improved Performance for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2021, 125, 4946-4954.	1.5	15
92	Insight into the mechanism for the methanol synthesis via the hydrogenation of CO2 over a Co-modified Cu(100) surface: A DFT study. Journal of Chemical Physics, 2016, 145, 134701.	1.2	14
93	Exploring the Reaction Mechanism of H₂S Decomposition with MS₃ (M = Mo,) Tj ETQq1 1 0.784314 rgBT /	1.6	14
94	Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 7031-7038.	1.5	13
95	Catalytic oxidation of CO by N₂O on neutral Y₂MO₅ (M = Y, Al) clusters: a density functional theory study. RSC Advances, 2015, 5, 76651-76659.	1.7	12
96	Predicting the electronic and optical properties of IB metals doped monoclinic BiVO₄: First principle calculations. International Journal of Quantum Chemistry, 2016, 116, 388-395.	1.0	12
97	Why does F-doping enhance the photocatalytic water-splitting performance of mBiVO₄? â€“ a density functional theory study. New Journal of Chemistry, 2017, 41, 1094-1102.	1.4	12
98	Structure, Composition, and Electronic Properties of TiOx/Mo(112) Thin Films. Journal of Physical Chemistry C, 2007, 111, 7437-7445.	1.5	11
99	High magneto-optical performance of GdFeO3 thin film with high orientation and heavy Ce3+ doping. Ceramics International, 2019, 45, 14928-14933.	2.3	11
100	Conversion of N₂O to N₂ on MgO (001) surface with vacancy: A DFT study. Chinese Journal of Chemistry, 2003, 21, 1123-1129.	2.6	10
101	Pressure-tuning the nonlinear-optical properties of AgGaS_2 crystal: a first-principle study. Optical Materials Express, 2015, 5, 1738.	1.6	10
102	The structural, electronic and catalytic properties of Au_n (n = 1â€“4) nanoclusters on monolayer MoS₂. RSC Advances, 2017, 7, 42529-42540.	1.7	10
103	Anionic Oxygen Redox in the High-Lithium Material Li₈SnO₆. Chemistry of Materials, 2021, 33, 834-844.	3.2	10
104	Tailoring the Linear and Second-Order Nonlinear Optical Responses of the Titanium-MIL-125 Metalâ€“Organic Framework through Ligand Functionalization: A First Principles Study. Journal of Physical Chemistry C, 2019, 123, 653-664.	1.5	9
105	Investigation of Ordered TiMC and TiMCT₂ (M = Cr and Mo; T = O and S) MXenes as High-Performance Anode Materials for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2022, 126, 5283-5291.	1.5	9
106	Deposition of Nonstoichiometric Tritungsten Oxides on the TiO₂(110) Surface: A Possible Way to Stabilize the Unstable Clusters in the Gas Phase. Journal of Physical Chemistry C, 2011, 115, 15335-15344.	1.5	8
107	On the structural and electronic properties of hexanuclear vanadium oxide clusters V6Onâ¯/0 (n=12â€“15): Is V6O12 cluster planar or cage-like?. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 131, 446-454.	2.0	8
108	Structural Evolution and Chemical Bonding of Diniobium Boride Clusters Nb₂B_x^{â€“/0} (x= 1â€“6): HexagonalâEBipyramidal Nb₂B₆^{â€“/0} Species. European Journal of Inorganic Chemistry, 2018, 2018, 940-950.	1.0	8

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109	First-principles studies of the TE properties of [110]-Ge/Si core/shell nanowires with different surface structures. Journal of Materials Chemistry A, 2014, 2, 2538.	5.2	7
110	The reactivity of stoichiometric tungsten oxide clusters towards carbon monoxide: the effects of cluster sizes and charge states. Physical Chemistry Chemical Physics, 2015, 17, 11499-11508.	1.3	7
111	The mechanism for CO2 reduction over Fe-modified Cu(100) surfaces with thermodynamics and kinetics: a DFT study. RSC Advances, 2020, 10, 32569-32580.	1.7	7
112	Single-phase proton- and electron-conducting Ag-organic coordination polymers for efficient CO₂electroreduction. Journal of Materials Chemistry A, 2022, 10, 3216-3225.	5.2	7
113	Ionothermal Synthesis of Covalent Triazine Frameworks in a NaClâ€KClâ€ZnCl₂Eutectic Salt for the Hydrogen Evolution Reaction. Angewandte Chemie, 2022, 134, .	1.6	7
114	Theoretical study on Y-doped Na₂ZrO₃ as a high-capacity Na-rich cathode material based on anionic redox. Physical Chemistry Chemical Physics, 2022, 24, 16183-16192.	1.3	7
115	Effects of Ti doping at the reduced SnO2(110) surface with different oxygen vacancies: a first principles study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	6
116	Mononuclear thorium halide clusters ThX₄ (X = F, Cl): gas-phase hydrolysis reactions. Physical Chemistry Chemical Physics, 2018, 20, 21184-21193.	1.3	6
117	Theoretical insights into the thermal reduction of N2 to NH3 over a single metal atom incorporated nitrogen-doped graphene. Journal of Chemical Physics, 2021, 154, 054703.	1.2	6
118	A Fully Coplanar Donorâ€“Acceptor Polymeric Semiconductor with Promoted Charge Separation Kinetics for Photochemistry. Angewandte Chemie, 2021, 133, 16491-16495.	1.6	6
119	Unveiling the Selectivity of CO₂ Reduction on Cu₂ZnSnS₄: The Effect of Exposed Termination. Journal of Physical Chemistry C, 2021, 125, 24967-24973.	1.5	6
120	Validation of Density Functional Theory Methods for Predicting the Optical Properties of Cu-Based Multinary Chalcogenide Semiconductors. Journal of Physical Chemistry C, 2022, 126, 4684-4697.	1.5	6
121	DFT investigations of KTiOPO4Mx (M = K, Na, and Li) anodes for alkali-ion battery. Journal of Chemical Physics, 2022, 156, .	1.2	6
122	Microscopic functionality of FeN4 sites in polymeric carbon nitride for efficient H2S oxidation. Applied Surface Science, 2022, 600, 154011.	3.1	6
123	Hybrid Density Functional Study of the Local Structures and Energy Levels of CaAl₂O₄:Ce³⁺. Journal of Physical Chemistry A, 2018, 122, 4306-4312.	1.1	5
124	Structural design of cubic Sr,V:CeFeO3 thin films with a strong magneto-optical effect and high compatibility with a Si substrate. Dalton Transactions, 2020, 49, 7713-7721.	1.6	5
125	High efficiency and stable photoluminescence of CH₃NH₃PbBr₃@CsPbBr₃ perovskite quantum dots. Chemical Communications, 2021, 57, 1356-1359.	2.2	5
126	Understanding the Role of Various Dopant Metals (Sb, Sn, Ga, Ge, and V) in the Structural and Electrochemical Performances of LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂. Journal of Physical Chemistry C, 2021, 125, 19600-19608.	1.5	5

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127	Potassium Storage Performance of UiO-66 Derivatives from First Principles Calculations. Journal of Physical Chemistry C, 2022, 126, 4286-4295.	1.5	5
128	Density Functional Study on Structures and Relative Stability of Gd(H2O)n3+ (n= 8,9). Chinese Journal of Chemical Physics, 2009, 22, 395-400.	0.6	4
129	A reasonable criterion of reactivities at the defective region of singleâ€walled carbon nanotubes. International Journal of Quantum Chemistry, 2009, 109, 668-678.	1.0	4
130	Structural evolution, sequential oxidation and chemical bonding in tri-yttrium oxide clusters: Y₃O_x^{â^'} and Y₃O_x (x = 0â€“6). RSC Advances, 2014, 4, 60270-60279.	1.7	4
131	Tuning the charge states of CrW2O9 clusters deposited on perfect and defective MgO(001) surfaces with different color centers: A comprehensive DFT study. Journal of Chemical Physics, 2016, 144, 174706.	1.2	4
132	Mild preparation and high fluorescence emission efficiency of europium-doped gallium nitride nanocrystals and first-principles density functional theoretical analysis of optical properties. Journal of Materials Chemistry C, 2017, 5, 7904-7910.	2.7	4
133	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO2 Activation. ACS Omega, 2021, 6, 27259-27270.	1.6	4
134	Zn₂Sn_xTi_{1â€“x}O₄ Continuous Solid-Solution Photocatalyst for Efficient Photocatalytic CO₂ Conversion into Solar Fuels. ACS Applied Energy Materials, 2022, 5, 3748-3756.	2.5	4
135	Highly fluorescent carbon nitride oligomer with aggregation-induced emission characteristic for plastic staining. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 276, 121238.	2.0	4
136	Group VB transition metal oxide clusters M4O n â^'/0 (MÂ=ÂNb, Ta; nÂ=Â8â€“11): structural evolution and chemical bonding. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	3
137	Curvature effect of vacancies in single-walled carbon nanotubes. Surface Science, 2015, 633, 29-37.	0.8	3
138	Structures and Chemical Bonding in NbS n 2â^'/â^'/0 (nÂ=Â3â€“5) Clusters: Effects of Sulfur Content and Charge States. Journal of Cluster Science, 2016, 27, 387-401.	1.7	3
139	A DFT study of (WO3)3 nanoclusters adsorption on defective MgO ultrathin films on Ag(001). RSC Advances, 2017, 7, 54091-54099.	1.7	3
140	Understanding the Efficiency and Selectivity of Two-Electron Production of Metalloporphyrin-Embedded Zirconiumâ€“Pyrogallol Scaffolds in Electrochemical CO2 Reduction. ACS Applied Materials & Interfaces, 2020, 12, 52588-52594.	4.0	3
141	Energy Band Alignment and Redoxâ€Active Sites in Metalloporphyrinâ€Spaced Metalâ€Catechol Frameworks for Enhanced CO₂ Photoreduction. Angewandte Chemie, 2022, 134, .	1.6	3
142	Bisimidazolium Tungstate Ionic Liquids: Highly Efficient Catalysts for the Synthesis of Linear Organic Carbonates by the Reaction of Ethylene Carbonate with Alcohols. Catalysis Letters, 2023, 153, 62-73.	1.4	3
143	A chemical-bond-driven edge reconstruction of Sb nanoribbons and their thermoelectric properties from first-principles calculations. RSC Advances, 2019, 9, 1047-1054.	1.7	2
144	Title is missing!. Journal of Cluster Science, 1999, 10, 459-473.	1.7	1

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145	Density Functional Study on Relative Energies, Structures, and Bonding of Low-lying Electronic States of Lutetium Dimer. Chinese Journal of Chemical Physics, 2009, 22, 371-379.	0.6	1
146	Electronic Properties and Chemical Bonding of O-Rich Clusters MMâ€²O7 â^' (M, Mâ€²Â=ÂV, Nb, Ta). Journal of Cluster Science, 2011, 22, 397-404.	1.7	1
147	Theoretical Design of Layered AlGaS3 as a New Nonlinear Optical Material with a Strong Second Harmonic Generation Response. Crystal Growth and Design, 2019, 19, 1632-1639.	1.4	1
148	Tailoring nonlinear optical crystal borophosphate through the introduction of transition metal d orbitals for improving optical anisotropy and SHG response: a first-principles investigation. Materials Research Express, 2018, 5, 096204.	0.8	0
149	Growth, structure and defects of (La,Sr)(Al,Ta)O3 crystals for preparing BiFeO3 thin films. Dalton Transactions, 2021, 50, 13306-13311.	1.6	0