Yong-Fan Zhang

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

142 papers	4,292 citations	30 h-index	62 g-index
149 ext. papers	5,534 ext. citations	6.1 avg, IF	6.01 L-index

#	Paper	IF	Citations
142	Single-phase proton- and electron-conducting Ag-organic coordination polymers for efficient CO2 electroreduction. *Journal of Materials Chemistry A*, **2022**, 10, 3216-3225	13	1
141	1T-MoS2 monolayer as a promising anode material for (Li/Na/Mg)-ion batteries. *Applied Surface Science*, **2022**, 584, 152537	6.7	7
140	Construction of Fe-doped TiO2 ultrathin nanosheets with rich oxygen vacancies for highly efficient oxidation of H2S. *Chemical Engineering Journal*, **2022**, 430, 132917	14.7	12
139	Potassium Storage Performance of UiO-66 Derivatives from First Principles Calculations. *Journal of Physical Chemistry C*, **2022**, 126, 4286-4295	3.8	1
138	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	3.8	0
137	Zn2SnxTi1O4 Continuous Solid-Solution Photocatalyst for Efficient Photocatalytic CO2 Conversion into Solar Fuels. *ACS Applied Energy Materials*, **2022**, 5, 3748-3756	6.1	1
136	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	3.8	0
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	4.4	1
134	Unveiling the Selectivity of CO2 Reduction on Cu2ZnSnS4: The Effect of Exposed Termination. *Journal of Physical Chemistry C*, **2021**, 125, 24967-24973	3.8	3
133	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO Activation. *ACS Omega*, **2021**, 6, 27259-27270	3.9	0
132	Energy Band Alignment and Redox-Active Sites in Metalloporphyrin-Spaced Metal-Catechol Frameworks for Enhanced CO Photoreduction. *Angewandte Chemie - International Edition*, **2021**,	16.4	4
131	A New Candidate in Polyanionic Compounds for a Potassium-Ion Battery Cathode: KTiOPO. *Journal of Physical Chemistry Letters*, **2021**, 12, 2721-2726	6.4	6
130	Defective BC2N as an Anode Material with Improved Performance for Lithium-Ion Batteries. *Journal of Physical Chemistry C*, **2021**, 125, 4946-4954	3.8	4
129	UiO-66 MetalOrganic Framework as an Anode for a Potassium-Ion Battery: Quantum Mechanical Analysis. *Journal of Physical Chemistry C*, **2021**, 125, 9679-9687	3.8	4
128	A Fully Coplanar Donor-Acceptor Polymeric Semiconductor with Promoted Charge Separation Kinetics for Photochemistry. *Angewandte Chemie - International Edition*, **2021**, 60, 16355-16359	16.4	22
127	Electrocatalytic Nitrogen Reduction by Transition Metal Single-Atom Catalysts on Polymeric Carbon Nitride. *Journal of Physical Chemistry C*, **2021**, 125, 13880-13888	3.8	7
126	A Fully Coplanar DonorAcceptor Polymeric Semiconductor with Promoted Charge Separation Kinetics for Photochemistry. *Angewandte Chemie*, **2021**, 133, 16491-16495	3.6	1

125	High efficiency and stable photoluminescence of CHNHPbBr@CsPbBr perovskite quantum dots. *Chemical Communications*, **2021**, 57, 1356-1359	5.8	3
124	Asymmetric Acceptor-Donor-Acceptor Polymers with Fast Charge Carrier Transfer for Solar Hydrogen Production. *Chemistry - A European Journal*, **2021**, 27, 939-943	4.8	11
123	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	3.6	7
122	Effects of doping high-valence transition metal (V, Nb and Zr) ions on the structure and electrochemical performance of LIB cathode material LiNiCoMnO. *Physical Chemistry Chemical Physics*, **2021**, 23, 11528-11537	3.6	7
121	Theoretical insights into the thermal reduction of N to NH over a single metal atom incorporated nitrogen-doped graphene. *Journal of Chemical Physics*, **2021**, 154, 054703	3.9	1
120	Understanding the Role of Various Dopant Metals (Sb, Sn, Ga, Ge, and V) in the Structural and Electrochemical Performances of LiNi0.5Co0.2Mn0.3O2. *Journal of Physical Chemistry C*, **2021**, 125, 19600-19608	3.8	3
119	Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. *Applied Surface Science*, **2021**, 563, 150269	6.7	11
118	Anionic Oxygen Redox in the High-Lithium Material Li8SnO6. *Chemistry of Materials*, **2021**, 33, 834-844	9.6	5
117	Growth, structure and defects of (La,Sr)(Al,Ta)O crystals for preparing BiFeO thin films. *Dalton Transactions*, **2021**, 50, 13306-13311	4.3	
116	Structural design of cubic Sr,V:CeFeO thin films with a strong magneto-optical effect and high compatibility with a Si substrate. *Dalton Transactions*, **2020**, 49, 7713-7721	4.3	2
115	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	5.6	25
114	Exploring the Reaction Mechanism of HS Decomposition with MS (M = Mo, W) Clusters. *ACS Omega*, **2020**, 5, 13324-13332	3.9	4
113	Understanding the Linear and Second-Order Nonlinear Optical Properties of UiO-66-Derived Metal□Organic Frameworks: A Comprehensive DFT Study. *Journal of Physical Chemistry C*, **2020**, 124, 11595-11608	3.8	9
112	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	7.3	23
111	Iron-Based Metal-Organic Frameworks as Platform for HS Selective Conversion: Structure-Dependent Desulfurization Activity. *Inorganic Chemistry*, **2020**, 59, 4483-4492	5.1	15
110	Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. *Journal of Physical Chemistry C* , **2020**, 124, 7031-7038	3.8	11
109	Visible-light-driven selective alcohol dehydrogenation and hydrogenolysis via the Mott Schottky effect. *Journal of Materials Chemistry A*, **2020**, 8, 6854-6862	13	12
108	Nitrogen fixation on metal-free SiC(111) polar surfaces. *Journal of Materials Chemistry A*, **2020**, 8, 7412-7421	13	17

107	Highly Efficient Porous FexCe1−xO2−δ with Three-Dimensional Hierarchical Nanoflower Morphology for H2S-Selective Oxidation. *ACS Catalysis*, **2020**, 10, 3968-3983	13.1	36
106	Controllable P Doping of the LaCoO Catalyst for Efficient Propane Oxidation: Optimized Surface Co Distribution and Enhanced Oxygen Vacancies. *ACS Applied Materials & Interfaces*, **2020**, 12, 23789-23799	9.5	24
105	A boron-decorated melon-based carbon nitride as a metal-free photocatalyst for N fixation: a DFT study. *Physical Chemistry Chemical Physics*, **2020**, 22, 21872-21880	3.6	9
104	Subnanometer iron clusters confined in a porous carbon matrix for highly efficient zinc–air batteries. *Nanoscale Horizons*, **2020**, 5, 359-365	10.8	18
103	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	21.8	19
102	Highly Active and Sulfur-Resistant Fe-N Sites in Porous Carbon Nitride for the Oxidation of H S into Elemental Sulfur. *Small*, **2020**, 16, e2003904	11	13
101	Understanding the Efficiency and Selectivity of Two-Electron Production of Metalloporphyrin-Embedded Zirconium-Pyrogallol Scaffolds in Electrochemical CO Reduction. *ACS Applied Materials & Interfaces*, **2020**, 12, 52588-52594	9.5	2
100	Atomically Dispersed Ru Catalyst for Low-Temperature Nitrogen Activation to Ammonia via an Associative Mechanism. *ACS Catalysis*, **2020**, 10, 9504-9514	13.1	20
99	The mechanism for CO reduction over Fe-modified Cu(100) surfaces with thermodynamics and kinetics: a DFT study.. *RSC Advances*, **2020**, 10, 32569-32580	3.7	2
98	Direct probing of atomically dispersed Ru species over multi-edged TiO for highly efficient photocatalytic hydrogen evolution. *Science Advances*, **2020**, 6,	14.3	62
97	Unraveling the mechanisms of S-doped carbon nitride for photocatalytic oxygen reduction to HO. *Physical Chemistry Chemical Physics*, **2020**, 22, 21099-21107	3.6	7
96	Relative Efficacy of CoX4 Embedded Graphene (X=N, S, B, and P) Electrocatalysts towards Hydrogen Evolution Reaction: Is Nitrogen Really the Best Choice?. *ChemCatChem*, **2020**, 12, 536-543	5.2	17
95	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	3.8	13
94	Efficient ammonia synthesis over a core–shell Ru/CeO2 catalyst with a tunable CeO2 size: DFT calculations and XAS spectroscopy studies. *Inorganic Chemistry Frontiers*, **2019**, 6, 396-406	6.8	17
93	A chemical-bond-driven edge reconstruction of Sb nanoribbons and their thermoelectric properties from first-principles calculations.. *RSC Advances*, **2019**, 9, 1047-1054	3.7	1
92	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	3.5	1
91	Phthalocyanine and Metal Phthalocyanines Adsorbed on Graphene: A Density Functional Study. *Journal of Physical Chemistry C*, **2019**, 123, 16614-16620	3.8	19
90	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	3.8	27

89	Reducing the Exciton Binding Energy of Donor-Acceptor-Based Conjugated Polymers to Promote Charge-Induced Reactions. *Angewandte Chemie - International Edition*, **2019**, 58, 10236-10240	16.4	132
88	High magneto-optical performance of GdFeO3 thin film with high orientation and heavy Ce3+ doping. *Ceramics International*, **2019**, 45, 14928-14933	5.1	3
87	Defect engineering of metal-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	11.5	47
86	First-principles calculations of photoluminescence and defect states of Ce3+-doped (Ca/Sr)2B5O9Cl. *Physical Review B*, **2019**, 99,	3.3	10
85	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	21.8	118
84	Oxygen-vacancies-engaged efficient carrier utilization for the photocatalytic coupling reaction. *Journal of Catalysis*, **2019**, 373, 116-125	7.3	15
83	Germanium-substituted Zn2TiO4 solid solution photocatalyst for conversion of CO2 into fuels. *Journal of Catalysis*, **2019**, 371, 144-152	7.3	14
82	Molecular-level understanding of reaction path optimization as a function of shape concerning the metal–support interaction effect of Co/CeO2 on water-gas shift catalysis. *Catalysis Science and Technology*, **2019**, 9, 4928-4937	5.5	11
81	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	5.6	20
80	Reducing the Exciton Binding Energy of Donor–Acceptor-Based Conjugated Polymers to Promote Charge-Induced Reactions. *Angewandte Chemie*, **2019**, 131, 10342-10346	3.6	20
79	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	3.8	11
78	Exploring the potentials of TiN and TiNX (X = O, F, OH) monolayers as anodes for Li or non-Li ion batteries from first-principles calculations.. *RSC Advances*, **2019**, 9, 40340-40347	3.7	7
77	Tailoring the Linear and Second-Order Nonlinear Optical Responses of the Titanium-MIL-125 Metal–Organic Framework through Ligand Functionalization: A First Principles Study. *Journal of Physical Chemistry C*, **2019**, 123, 653-664	3.8	7
76	Ultrasmall MoO Clusters as a Novel Cocatalyst for Photocatalytic Hydrogen Evolution. *Advanced Materials*, **2019**, 31, e1804883	24	82
75	Hybrid Density Functional Study of the Local Structures and Energy Levels of CaAlO:Ce. *Journal of Physical Chemistry A*, **2018**, 122, 4306-4312	2.8	4
74	MnSb2S4 Monolayer as an Anode Material for Metal-Ion Batteries. *Chemistry of Materials*, **2018**, 30, 3208-3214	9.6	38
73	Nanofibers with diameter below one nanometer from electrospinning.. *RSC Advances*, **2018**, 8, 4794-4802	3.7	87
72	Facile fabrication of shape-controlled CoMnO nanocatalysts for benzene oxidation at low temperatures. *Chemical Communications*, **2018**, 54, 2154-2157	5.8	33

71	Different Atomic Terminations Affect the Photocatalytic Nitrogen Fixation of Bismuth Oxybromide: A First Principles Study. *Chemistry - an Asian Journal*, **2018**, 13, 799-808	4.5	16
70	Structural Evolution and Chemical Bonding of Diniobium Boride Clusters Nb2Bx− (x = 1–8): Hexagonal-Bipyramidal Nb2B6− Species. *European Journal of Inorganic Chemistry*, **2018**, 2018, 940-950	2.3	5
69	Effects of ligand functionalization on the photocatalytic properties of titanium-based MOF: A density functional theory study. *AIP Advances*, **2018**, 8, 035012	1.5	24
68	Indium selenide monolayer: a two-dimensional material with strong second harmonic generation. *CrystEngComm*, **2018**, 20, 2573-2582	3.3	14
67	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	6.7	16
66	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	1.7	
65	Mononuclear thorium halide clusters ThX (X = F, Cl): gas-phase hydrolysis reactions. *Physical Chemistry Chemical Physics*, **2018**, 20, 21184-21193	3.6	3
64	Ionothermal Synthesis of Triazine–Heptazine-Based Copolymers with Apparent Quantum Yields of 60 % at 420 nm for Solar Hydrogen Production from "Sea Water". *Angewandte Chemie*, **2018**, 130, 9516-9520	3.6	49
63	Photocatalytic Oxygen Evolution from Functional Triazine-Based Polymers with Tunable Band Structures. *Angewandte Chemie*, **2018**, 130, 479-483	3.6	54
62	Photocatalytic Oxygen Evolution from Functional Triazine-Based Polymers with Tunable Band Structures. *Angewandte Chemie - International Edition*, **2018**, 57, 470-474	16.4	191
61	Ionothermal Synthesis of Triazine-Heptazine-Based Copolymers with Apparent Quantum Yields of 60 % at 420 nm for Solar Hydrogen Production from "Sea Water". *Angewandte Chemie - International Edition*, **2018**, 57, 9372-9376	16.4	259
60	Acid and Base Resistant Zirconium Polyphenolate-Metalloporphyrin Scaffolds for Efficient CO Photoreduction. *Advanced Materials*, **2018**, 30, 1704388	24	131
59	A promising lead-free fluoride carbonate SHG material designed from a theoretical perspective. *Dalton Transactions*, **2017**, 46, 2635-2642	4.3	11
58	Screening novel candidates for mid-IR nonlinear optical materials from I3VVI4 compounds. *Journal of Materials Chemistry C*, **2017**, 5, 1963-1972	7.1	18
57	Photocatalytic overall water splitting by conjugated semiconductors with crystalline poly(triazine imide) frameworks. *Chemical Science*, **2017**, 8, 5506-5511	9.4	134
56	Why does F-doping enhance the photocatalytic water-splitting performance of mBiVO4? A density functional theory study. *New Journal of Chemistry*, **2017**, 41, 1094-1102	3.6	7
55	Insight into the Mechanism of CO Oxidation on WO(001) Surfaces for Gas Sensing: A DFT Study. *Sensors*, **2017**, 17,	3.8	16
54	The structural, electronic and catalytic properties of Aun (n = 1–4) nanoclusters on monolayer MoS2. *RSC Advances*, **2017**, 7, 42529-42540	3.7	2

53	A DFT study of (WO3)3 nanoclusters adsorption on defective MgO ultrathin films on Ag(001). *RSC Advances*, **2017**, 7, 54091-54099	3.7	3
52	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	7.1	2
51	A Tumor-pH-Responsive Supramolecular Photosensitizer for Activatable Photodynamic Therapy with Minimal Skin Phototoxicity. *Theranostics*, **2017**, 7, 2746-2756	12.1	83
50	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, 19217-26	3.6	78
49	Structures and Chemical Bonding in NbS 2[0]n (n = 3[5]) Clusters: Effects of Sulfur Content and Charge States. *Journal of Cluster Science*, **2016**, 27, 387-401	3	2
48	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	6.7	19
47	Predicting the electronic and optical properties of IB metals doped monoclinic BiVO4: First principle calculations. *International Journal of Quantum Chemistry*, **2016**, 116, 388-395	2.1	11
46	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	3.9	3
45	Insight into the mechanism for the methanol synthesis via the hydrogenation of CO over a Co-modified Cu(100) surface: A DFT study. *Journal of Chemical Physics*, **2016**, 145, 134701	3.9	12
44	Tri-s-triazine-Based Crystalline Graphitic Carbon Nitrides for Highly Efficient Hydrogen Evolution Photocatalysis. *ACS Catalysis*, **2016**, 6, 3921-3931	13.1	531
43	Electronic properties of red and black phosphorous and their potential application as photocatalysts. *RSC Advances*, **2016**, 6, 80872-80884	3.7	27
42	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	6.7	24
41	Catalytic oxidation of CO by N2O on neutral Y2MO5 (M = Y, Al) clusters: a density functional theory study. *RSC Advances*, **2015**, 5, 76651-76659	3.7	9
40	Pressure-tuning the nonlinear-optical properties of AgGaS_2 crystal: a first-principle study. *Optical Materials Express*, **2015**, 5, 1738	2.6	9
39	Monolayered Bi2WO6 nanosheets mimicking heterojunction interface with open surfaces for photocatalysis. *Nature Communications*, **2015**, 6, 8340	17.4	430
38	The reactivity of stoichiometric tungsten oxide clusters towards carbon monoxide: the effects of cluster sizes and charge states. *Physical Chemistry Chemical Physics*, **2015**, 17, 11499-508	3.6	7
37	Curvature effect of vacancies in single-walled carbon nanotubes. *Surface Science*, **2015**, 633, 29-37	1.8	2
36	A comparative study of CO catalytic oxidation on Pd-anchored graphene oxide and Pd-embedded vacancy graphene. *Journal of Nanoparticle Research*, **2014**, 16, 1	2.3	31

35	Group VB transition metal oxide clusters M4O10 n (M = Nb, Ta; n = 8–11): structural evolution and chemical bonding. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	2
34	Structural evolution, sequential oxidation and chemical bonding in tri-yttrium oxide clusters: Y3Ox and Y3Ox (x = 0–8). *RSC Advances*, **2014**, 4, 60270-60279	3.7	4
33	Computational design of inorganic nonlinear optical crystals based on a genetic algorithm. *CrystEngComm*, **2014**, 16, 10569-10580	3.3	49
32	First-Principles Studies of Lithium Adsorption and Diffusion on Graphene with Grain Boundaries. *Journal of Physical Chemistry C*, **2014**, 118, 28055-28062	3.8	62
31	Original Investigation of a Novel Photocatalyst Driven by Visible Light: ZnIn2S4. *Journal of the Physical Society of Japan*, **2014**, 83, 074301	1.5	12
30	Comparative density functional theory study on the electronic and optical properties of BiMO4 (M = V, Nb, Ta). *Journal of Materials Chemistry A*, **2014**, 2, 8294	13	65
29	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	3.8	30
28	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	13	7
27	On the structural and electronic properties of hexanuclear vanadium oxide clusters V6On(-/0) (n=12-15): is V6O12 cluster planar or cage-like?. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 131, 446-54	4.4	6
26	Probing the smallest molecular model of MoS2 catalyst: S2 units in the MoS(-/0 (n = 1-5) clusters. *Journal of Physical Chemistry A*, **2013**, 117, 5632-41	2.8	19
25	First-Principles Study on Electronic Properties and Optical Spectra of Ce-Doped La2CaB10O19 Crystal. *Journal of Physical Chemistry C*, **2013**, 117, 15241-15246	3.8	19
24	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	3.8	35
23	Electronic properties and 4f -5d transitions in Ce-doped Lu2SiO5: a theoretical investigation. *Journal of Materials Chemistry*, **2012**, 22, 13723		48
22	First-Principles Study on Structural Properties and 4f -5d Transitions of Locally Charge-Compensated Ce3+ in CaF2. *Journal of Physical Chemistry C*, **2012**, 116, 18419-18426	3.8	22
21	Effects of Ti doping at the reduced SnO2(110) surface with different oxygen vacancies: a first principles study. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	5
20	Electronic Properties and Chemical Bonding of O-Rich Clusters MM?O7 (M, M? = V, Nb, Ta). *Journal of Cluster Science*, **2011**, 22, 397-404	3	1
19	Structural and electronic properties of tungsten trioxides: from cluster to solid surface. *Theoretical Chemistry Accounts*, **2011**, 130, 103-114	1.9	22
18	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	3.8	8

17	The effects of the introduction of Al atom into monoclinic BiVO4: a theoretical prediction. *Theoretical Chemistry Accounts*, **2010**, 127, 751-757	1.9	19
16	Conversion of N2O to N2 on MgO (001) surface with vacancy: A DFT study. *Chinese Journal of Chemistry*, **2010**, 21, 1123-1129	4.9	10
15	Density Functional Study on Structures and Relative Stability of Gd(H2O)n3+ (n = 8,9). *Chinese Journal of Chemical Physics*, **2009**, 22, 395-400	0.9	4
14	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	0.9	1
13	A reasonable criterion of reactivities at the defective region of single-walled carbon nanotubes. *International Journal of Quantum Chemistry*, **2009**, 109, 668-678	2.1	4
12	Structural and Electronic Properties of a W3O9 Cluster Supported on the TiO2(110) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 17509-17517	3.8	32
11	Gold Nanostructures on TiOx/Mo(112) Thin Films. *Journal of Physical Chemistry C*, **2008**, 112, 191-200	3.8	14
10	Structure, Composition, and Electronic Properties of TiOx/Mo(112) Thin Films. *Journal of Physical Chemistry C*, **2007**, 111, 7437-7445	3.8	11
9	Bond-Curvature Effect of Sidewall [2+1] Cycloadditions of Single-Walled Carbon Nanotubes: A New Criterion To the Adduct Structures. *Chemistry of Materials*, **2006**, 18, 3579-3584	9.6	41
8	Carbon nanotubes functionalized by NO2: coexistence of charge transfer and radical transfer. *Journal of Physical Chemistry B*, **2006**, 110, 22462-70	3.4	26
7	Role of Spacers and Substituents in the Self-Assembly Process: Syntheses and Characterization of Three Novel Silver(I)/Iodine Polymers. *Crystal Growth and Design*, **2006**, 6, 1813-1820	3.5	112
6	A theoretical study on the electronic structures of TiO2: Effect of Hartree-Fock exchange. *Journal of Physical Chemistry B*, **2005**, 109, 19270-7	3.4	120
5	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	1.1	17
4	Theoretical predictions of the structure, gas-phase acidity, and aromaticity of tetrathiosquaric acid. *International Journal of Quantum Chemistry*, **2000**, 78, 443-449	2.1	14
3	An ab Initio Study on the Chemical Bond and Reactivity of Molybdenum−Sulfur Clusters with a Mo2O n S4− (n=1−) Core. *Journal of Cluster Science*, **1999**, 10, 459-473	3	1
2	H2 and CH4 production from bio-alcohols using condensed poly(heptazine imide) with visible light. *Journal of Materials Chemistry A*,	13	2
1	Bisimidazolium Tungstate Ionic Liquids: Highly Efficient Catalysts for the Synthesis of Linear Organic Carbonates by the Reaction of Ethylene Carbonate with Alcohols. *Catalysis Letters*,1	2.8	1