Yan-Hui Chen

List of Publications by Year
in descending order

90 papers	2,264 citations	236612 25 h-index	243296 44 g-index
90 all docs	90 docs citations	90 times ranked	3126 citing authors

#	Article	IF	Citations
1	Graphitic carbon nitride as a metal-free catalyst for NO decomposition. Chemical Communications, 2010, 46, 6965.	2.2	186
2	Organic semiconductor for artificial photosynthesis: water splitting into hydrogen by a bioinspired C₃N₃S₃polymer under visible light irradiation. Chemical Science, 2011, 2, 1826-1830.	3.7	167
3	Bulk and surface properties of spinel Co3O4 by density functional calculations. Surface Science, 2009, 603, 653-658.	0.8	156
4	A DFT Study of CO Catalytic Oxidation by N₂O or O₂ on the Co₃O₄(110) Surface. ChemCatChem, 2009, 1, 384-392.	1.8	75
5	Interaction of photoactive catechol with TiO2 anatase (101) surface: A periodic density functional theory study. Chemical Physics, 2007, 331, 275-282.	0.9	71
6	1T-MoS2 monolayer as a promising anode material for (Li/Na/Mg)-ion batteries. Applied Surface Science, 2022, 584, 152537.	3.1	66
7	A density functional theory study on the adsorption and dissociation of N2O on Cu2O(111) surface. Applied Surface Science, 2007, 253, 7501-7505.	3.1	64
8	Sn2+ dopant induced visible-light activity of SnO2 nanoparticles for H2 production. Catalysis Communications, 2011, 16, 215-219.	1.6	64
9	Adsorption and dissociation of methanol on Au(1 1 1) surface: A first-principles periodic density functional study. Computational and Theoretical Chemistry, 2006, 770, 87-91.	1.5	62
10	CO adsorption on MgO() surface with oxygen vacancy and its low-coordinated surface sites: embedded cluster model density functional study employing charge self-consistent technique. Surface Science, 2003, 525, 13-23.	0.8	54
11	Roles of oxygen vacancy in the adsorption properties of CO and NO on Cu2O(111) surface: Results of a first-principles study. Applied Surface Science, 2008, 255, 3141-3148.	3.1	54
12	A TD-DFT study on the electronic spectrum of Ru(II)L2 [L=bis(5â€²-methyl-2,2â€²-bipyridine-6-carboxylato)] in the gas phase and DMF solution. Chemical Physics, 2006, 330, 204-211.	0.9	46
13	Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. Applied Surface Science, 2021, 563, 150269.	3.1	43
14	Reaction mechanism of CO oxidation on Cu2O(111): A density functional study. Journal of Chemical Physics, 2010, 133, 154502.	1.2	42
15	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
16	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
17	A first-principles study of the chemi-adsorption of benzene on Au(100) surface. Chemical Physics Letters, 2006, 417, 414-418.	1.2	35
18	Pt₄ Clusters Supported on Monolayer Graphitic Carbon Nitride Sheets for Oxygen Adsorption: A First-Principles Study. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2016, 32, 1183-1190.	2.2	35

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19	Effects of ligand functionalization on the photocatalytic properties of titanium-based MOF: A density functional theory study. AIP Advances, 2018, 8, .	0.6	35
20	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
21	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
22	Oxidation of Pdn (n=1â€“5) clusters on single vacancy graphene: A first-principles study. Computational and Theoretical Chemistry, 2013, 1020, 91-99.	1.1	29
23	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
24	A molecular modeling study on small molecule gas transportation in poly (chloro-p-xylylene). Computational Materials Science, 2010, 49, S65-S69.	1.4	28
25	Structural and electronic properties of tungsten trioxides: from cluster to solid surface. Theoretical Chemistry Accounts, 2011, 130, 103-114.	0.5	28
26	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
27	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
28	Enhanced Oxidation Reactivity of WO3(001) Surface through the Formation of Oxygen Radical Centers. Journal of Physical Chemistry C, 2012, 116, 5067-5075.	1.5	27
29	Nitrogen fixation on metal-free SiC(111) polar surfaces. Journal of Materials Chemistry A, 2020, 8, 7412-7421.	5.2	26
30	On the coverage-dependent orientation of benzene adsorbed on Cu(100): A density functional theory study. Chemical Physics Letters, 2005, 407, 414-418.	1.2	25
31	Adsorption and dissociation of H2S on monometallic and monolayer bimetallic Ni/Pd(111) surfaces: A first-principles study. Applied Surface Science, 2016, 387, 301-307.	3.1	25
32	The adsorption and dissociation of Cl2 on the MgO (001) surface with vacancies: Embedded cluster model study. Journal of Chemical Physics, 2004, 120, 8753-8760.	1.2	24
33	Coadsorption of CO and NO on the Cu2O(111) surface: A periodic density functional theory study. Journal of Chemical Physics, 2009, 131, 174503.	1.2	23
34	Theoretical insights into the reaction mechanisms of NO oxidation catalyzed by Cu 2 O(1 1 1). Applied Surface Science, 2014, 316, 416-423.	3.1	23
35	A periodic density functional theory study of the dehydrogenation of methanol over CuCl(111) surface. Applied Surface Science, 2008, 254, 4421-4431.	3.1	22
36	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

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37	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
38	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
39	Facile Electrochemical Preparation of Ag Nanothorns and Their Growth Mechanism. Chemistry - A European Journal, 2010, 16, 6766-6770.	1.7	20
40	Embedded Si/Graphene Composite Fabricated by Magnesium-Thermal Reduction as Anode Material for Lithium-Ion Batteries. Nanoscale Research Letters, 2017, 12, 627.	3.1	20
41	Kinetic and mechanistic analysis of NH₃decomposition on Ru(0001), Ru(111) and Ir(111) surfaces. Nanoscale Advances, 2021, 3, 1624-1632.	2.2	19
42	Theoretical Studies of the Adsorption and Dissociation of Two NO Molecules on Cu2O(111) Surface. Acta Physico-chimica Sinica, 2006, 22, 1126-1131.	0.6	18
43	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
44	THE ROLE OF SURFACE OXYGEN VACANCY INN₂ODECOMPOSITION ONCu₂O(111) SURFACE: A DFT STUDY. Journal of Theoretical and Computational Chemistry, 2008, 07, 263-276.	1.8	17
45	Density functional theory for adsorption of HCHO on the FeO(100) surface. Journal of Natural Gas Chemistry, 2010, 19, 21-24.	1.8	15
46	Exploring the potentials of Ti₃N₂ and Ti₃N₂X₂ (X = O, F, OH) monolayers as anodes for Li or non-Li ion batteries from first-principles calculations. RSC Advances, 2019, 9, 40340-40347.	1.7	15
47	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
48	First-principles study of O2 adsorption and dissociation on the CuCr2O4 (100) surface. Computational and Theoretical Chemistry, 2008, 860, 18-23.	1.5	14
49	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
50	First-principles study of MoSSe_graphene heterostructures as anode for Li-ion batteries. Chemical Physics, 2020, 529, 110583.	0.9	14
51	Adsorption of Methanol and Methoxy on Cu(111) Surface: A First-principles Periodic Density Functional Theory Study. Chinese Journal of Chemistry, 2006, 24, 872-876.	2.6	13
52	Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 7031-7038.	1.5	13
53	Investigating the potentials of TiVC MXenes as anode materials for Li-ion batteries by DFT calculations. Applied Surface Science, 2021, 569, 151002.	3.1	13
54	First-principles study of Na2+xTi7O15 as anode materials for sodium-ion batteries. Journal of Alloys and Compounds, 2016, 689, 805-811.	2.8	12

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55	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
56	Interaction of CO and NO with the spinel CuCr₂O₄ (100) surface: A DFT study. International Journal of Quantum Chemistry, 2008, 108, 1435-1443.	1.0	11
57	Growth mechanism of palladium clusters on rutile TiO2(110) surface. Journal of Natural Gas Chemistry, 2012, 21, 544-555.	1.8	10
58	Density functional theory and surface enhanced Raman spectroscopy studies of tautomeric hypoxanthine and its adsorption behaviors in electrochemical processes. Electrochimica Acta, 2015, 164, 132-138.	2.6	10
59	Pressure-tuning the nonlinear-optical properties of AgGaS_2 crystal: a first-principle study. Optical Materials Express, 2015, 5, 1738.	1.6	10
60	Deposition of (WO3)3 nanoclusters on the MgO(001) surface: A possible way to identify the charge states of the defect centers. Journal of Chemical Physics, 2013, 138, 034711.	1.2	9
61	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
62	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
63	Study of CO adsorption on perfect and defective pyrite(100) surfaces by density functional theory. Journal of Natural Gas Chemistry, 2011, 20, 60-64.	1.8	8
64	Effects of N-doping concentration on graphene structures and properties. Chemical Physics Letters, 2013, 581, 74-79.	1.2	8
65	Theoretical Comparison of Oxygen Adsorption on Cu(100) Surface. Chinese Journal of Chemical Physics, 2006, 19, 54-58.	0.6	7
66	A DFT investigation of the effects of doped Pb atoms on Pdn clusters (13â©½nâ©½116). Computational and Theoretical Chemistry, 2011, 966, 375-382.	1.1	7
67	A theoretical study on the dissociation of Cl2 on MgO(001) surface: Prompted by silver atoms supported on surface. Chemical Physics, 2006, 328, 236-242.	0.9	6
68	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
69	The sources of hydrogen affect the productivity and selectivity of CO2 photoreduction on SiC. Applied Surface Science, 2021, 538, 148010.	3.1	6
70	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
71	Coverage-Dependent Behavior on Organic Functionalization of the Semiconductor X(100)-2 Ã— 1 Surface (X = C, Si, and Ge) by Carbene, Silylene, Germylene, and Nitrene: A Periodic DFT Study. Journal of Physical Chemistry C, 2010, 114, 6543-6552.	1.5	5
72	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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73	First-principles Periodic Density Functional Study of CO Adsorption on Spinel-type CuCr2O4 (100) Surface. Chinese Journal of Chemical Physics, 2007, 20, 557-562.	0.6	4
74	STRUCTURES AND ELECTRONIC PROPERTIES OF A Co₂P CLUSTER DEPOSITED ON THE RUTILE TiO₂(110) SURFACE BY FIRSTâ€“PRINCIPLES CALCULATIONS. Journal of Theoretical and Computational Chemistry, 2013, 12, 1250102.	1.8	4
75	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO2 Activation. ACS Omega, 2021, 6, 27259-27270.	1.6	4
76	Structural and Spectral Properties of a Nonclassical C₆₆ Isomer with Its Hydrogenated Derivative C₆₆H₄ in Theory. ACS Omega, 2021, 6, 27101-27111.	1.6	4
77	Density Functional Study on Adsorption of NO on AuSe (010) Surface. Chinese Journal of Chemistry, 2008, 26, 107-112.	2.6	3
78	Adsorption of H2O, OH, and O on CuCl(111) Surface: A Density Functional Theory Study. Chinese Journal of Chemical Physics, 2008, 21, 39-44.	0.6	3
79	Density functional theory study of CO catalytic oxidation on Co2B2/TiO2 (110) surface. Journal of Natural Gas Chemistry, 2010, 19, 300-306.	1.8	3
80	First-principles investigation of H2O on HfO2 (110) surface. Applied Surface Science, 2013, 264, 424-432.	3.1	3
81	Influence of denticity and combined softâ€“hard strategy on the interaction of picolinic-type ligands with NpO₂⁺. RSC Advances, 2017, 7, 12236-12246.	1.7	3
82	How does the defect ZnO@Au surface activate the methane via the precursor-mediated mechanism?. Applied Surface Science, 2021, 555, 149728.	3.1	3
83	Density Functional Theory Study of CO and O₂ Adsorption on NiFeB₂/TiO₂ Surface. Chinese Journal of Catalysis, 2010, 31, 423-428.	6.9	3
84	Density Functional Theory and Surface Enhanced Raman Spectroscopy Studies of Dicyandiamide Adsorbed on Au Clusters. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2015, 31, 1872-1879.	2.2	2
85	Adsorption and Decomposition of N₂O on Cu/t-ZrO₂(101) Surfaces. Chinese Journal of Catalysis, 2013, 33, 1850-1856.	6.9	2
86	Computational Investigation of Coverage-Dependent Behavior on Functionalization of the Semiconductor X (100)-2 Ã— 1 Surface (X = C, Si, and Ge) by Cycloaddition of Transition Metal Oxides. Journal of Physical Chemistry C, 2011, 115, 5800-5808.	1.5	1
87	The oxo exchange reaction mechanism of americyl(VI): a density functional theory study. Journal of Radioanalytical and Nuclear Chemistry, 2020, 324, 857-868.	0.7	1
88	Density Functional Theory Study of IB Metals Binding to Perfect and N-Doped Graphene. Chinese Journal of Catalysis, 2013, 33, 1578-1585.	6.9	1
89	Electronic Structure and Mechanical Properties of Zircaloy-2 and Zircaloy-4: A First Principle Study. , 2013, , .		0
90	Theoretical Study of the Adsorption of Formaldehyde on Perfect and S-Deficient FeS2(100) Surfaces. Chinese Journal of Catalysis, 2014, 32, 1046-1050.	6.9	0