

Yan-Hui Chen

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88

papers

1,734

citations

22

h-index

38

g-index

90

ext. papers

1,989

ext. citations

4.3

avg, IF

4.59

L-index

#	Paper	IF	Citations
88	Graphitic carbon nitride as a metal-free catalyst for NO decomposition. <i>Chemical Communications</i> , 2010 , 46, 6965-7	5.8	157
87	Organic semiconductor for artificial photosynthesis: water splitting into hydrogen by a bioinspired C3N3S3 polymer under visible light irradiation. <i>Chemical Science</i> , 2011 , 2, 1826-1830	9.4	146
86	Bulk and surface properties of spinel Co3O4 by density functional calculations. <i>Surface Science</i> , 2009 , 603, 653-658	1.8	140
85	A DFT Study of CO Catalytic Oxidation by N2O or O2 on the Co3O4(110) Surface. <i>ChemCatChem</i> , 2009 , 1, 384-392	5.2	71
84	Interaction of photoactive catechol with TiO2 anatase (101) surface: A periodic density functional theory study. <i>Chemical Physics</i> , 2007 , 331, 275-282	2.3	67
83	A density functional theory study on the adsorption and dissociation of N2O on Cu2O(111) surface. <i>Applied Surface Science</i> , 2007 , 253, 7501-7505	6.7	58
82	Adsorption and dissociation of methanol on Au(1 1 1) surface: A first-principles periodic density functional study. <i>Computational and Theoretical Chemistry</i> , 2006 , 770, 87-91		57
81	Sn2+ dopant induced visible-light activity of SnO2 nanoparticles for H2 production. <i>Catalysis Communications</i> , 2011 , 16, 215-219	3.2	54
80	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. <i>Surface Science</i> , 2003 , 525, 13-23	1.8	51
79	Roles of oxygen vacancy in the adsorption properties of CO and NO on Cu2O(111) surface: Results of a first-principles study. <i>Applied Surface Science</i> , 2008 , 255, 3141-3148	6.7	48
78	A TD-DFT study on the electronic spectrum of Ru(II)L2 [L=bis(5?-methyl-2,2?-bipyridine-6-carboxylato)] in the gas phase and DMF solution. <i>Chemical Physics</i> , 2006 , 330, 204-211	2.3	42
77	Reaction mechanism of CO oxidation on Cu(2)O(111): A density functional study. <i>Journal of Chemical Physics</i> , 2010 , 133, 154502	3.9	38
76	A first-principles study of the chemi-adsorption of benzene on Au(100) surface. <i>Chemical Physics Letters</i> , 2006 , 417, 414-418	2.5	35
75	Structural and Electronic Properties of a W3O9 Cluster Supported on the TiO2(110) Surface. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 17509-17517	3.8	32
74	A comparative study of CO catalytic oxidation on Pd-anchored graphene oxide and Pd-embedded vacancy graphene. <i>Journal of Nanoparticle Research</i> , 2014 , 16, 1	2.3	31
73	Oxidation of Pd _n (n=1B) clusters on single vacancy graphene: A first-principles study. <i>Computational and Theoretical Chemistry</i> , 2013 , 1020, 91-99	2	26
72	Pt4 Clusters Supported on Monolayer Graphitic Carbon Nitride Sheets for Oxygen Adsorption: A First-Principles Study. <i>Wuli Huaxue Xuebao/Acta Physico-Chimica Sinica</i> , 2016 , 32, 1183-1190	3.8	26

71	First-principles investigation of the activation of CO ₂ molecule on TM/Cu (TM = Fe, Co and Ni) surface alloys. <i>Applied Surface Science</i> , 2015 , 353, 902-912	6.7	24
70	Effects of ligand functionalization on the photocatalytic properties of titanium-based MOF: A density functional theory study. <i>AIP Advances</i> , 2018 , 8, 035012	1.5	24
69	On the coverage-dependent orientation of benzene adsorbed on Cu(1 0 0): A density functional theory study. <i>Chemical Physics Letters</i> , 2005 , 407, 414-418	2.5	24
68	The adsorption and dissociation of Cl ₂ on the MgO (001) surface with vacancies: embedded cluster model study. <i>Journal of Chemical Physics</i> , 2004 , 120, 8753-60	3.9	23
67	Structural and electronic properties of tungsten trioxides: from cluster to solid surface. <i>Theoretical Chemistry Accounts</i> , 2011 , 130, 103-114	1.9	22
66	Enhanced Oxidation Reactivity of WO ₃ (001) Surface through the Formation of Oxygen Radical Centers. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 5067-5075	3.8	21
65	A molecular modeling study on small molecule gas transportation in poly (chloro-p-xylylene). <i>Computational Materials Science</i> , 2010 , 49, S65-S69	3.2	21
64	Probing the smallest molecular model of MoS ₂ catalyst: S ₂ units in the MoS(-/0 (n = 1-5) clusters. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 5632-41	2.8	19
63	A periodic density functional theory study of the dehydrogenation of methanol over CuCl(1 1 1) surface. <i>Applied Surface Science</i> , 2008 , 254, 4421-4431	6.7	19
62	Adsorption and dissociation of H ₂ S on monometallic and monolayer bimetallic Ni/Pd(111) surfaces: A first-principles study. <i>Applied Surface Science</i> , 2016 , 387, 301-307	6.7	19
61	Facile electrochemical preparation of Ag nanothorns and their growth mechanism. <i>Chemistry - A European Journal</i> , 2010 , 16, 6766-70	4.8	18
60	Nitrogen fixation on metal-free SiC(111) polar surfaces. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 7412-7421	4.2	17
59	Theoretical insights into the reaction mechanisms of NO oxidation catalyzed by Cu ₂ O(1 1 1). <i>Applied Surface Science</i> , 2014 , 316, 416-423	6.7	17
58	Coadsorption of CO and NO on the Cu ₂ O(111) surface: A periodic density functional theory study. <i>Journal of Chemical Physics</i> , 2009 , 131, 174503	3.9	17
57	Toward improving CO ₂ dissociation and conversion to methanol via CO-hydrogenation on Cu(100) surface by introducing embedded Co nanoclusters as promoters: A DFT study. <i>Applied Surface Science</i> , 2018 , 427, 837-847	6.7	16
56	THE ROLE OF SURFACE OXYGEN VACANCY IN N ₂ O DECOMPOSITION ON Cu ₂ O(111) SURFACE: A DFT STUDY. <i>Journal of Theoretical and Computational Chemistry</i> , 2008 , 07, 263-276	1.8	16
55	Theoretical Studies of the Adsorption and Dissociation of Two NO Molecules on Cu ₂ O(111) Surface. <i>Acta Physico-chimica Sinica</i> , 2006 , 22, 1126-1131		16
54	Embedded Si/Graphene Composite Fabricated by Magnesium-Thermal Reduction as Anode Material for Lithium-Ion Batteries. <i>Nanoscale Research Letters</i> , 2017 , 12, 627	5	15

53	Density functional theory for adsorption of HCHO on the FeO(100) surface. <i>Journal of Natural Gas Chemistry</i> , 2010 , 19, 21-24		15
52	What Is the Best Size of Subnanometer Copper Clusters for CO ₂ Conversion to Methanol at Cu/TiO ₂ Interfaces? A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 24118-24132	3.8	13
51	First-principles study of O ₂ adsorption and dissociation on the CuCr ₂ O ₄ (100) surface. <i>Computational and Theoretical Chemistry</i> , 2008 , 860, 18-23		13
50	Adsorption of Methanol and Methoxy on Cu(111) Surface: A First-principles Periodic Density Functional Theory Study. <i>Chinese Journal of Chemistry</i> , 2006 , 24, 872-876	4.9	12
49	Insight into the mechanism for the methanol synthesis via the hydrogenation of CO over a Co-modified Cu(100) surface: A DFT study. <i>Journal of Chemical Physics</i> , 2016 , 145, 134701	3.9	12
48	Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 7031-7038	3.8	11
47	First-principles study of Na _{2+x} Ti ₇ O ₁₅ as anode materials for sodium-ion batteries. <i>Journal of Alloys and Compounds</i> , 2016 , 689, 805-811	5.7	11
46	BC ₂ N/Graphene Heterostructure as a Promising Anode Material for Rechargeable Li-Ion Batteries by Density Functional Calculations. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 30809-30818	3.8	11
45	Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. <i>Applied Surface Science</i> , 2021 , 563, 150269	6.7	11
44	Interaction of CO and NO with the spinel CuCr ₂ O ₄ (100) surface: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2008 , 108, 1435-1443	2.1	10
43	First-principles study of MoS ₂ /graphene heterostructures as anode for Li-ion batteries. <i>Chemical Physics</i> , 2020 , 529, 110583	2.3	10
42	Pressure-tuning the nonlinear-optical properties of AgGaS ₂ crystal: a first-principle study. <i>Optical Materials Express</i> , 2015 , 5, 1738	2.6	9
41	A boron-decorated melon-based carbon nitride as a metal-free photocatalyst for N fixation: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 21872-21880	3.6	9
40	Growth mechanism of palladium clusters on rutile TiO ₂ (110) surface. <i>Journal of Natural Gas Chemistry</i> , 2012 , 21, 544-555		8
39	Deposition of (WO ₃) ₃ nanoclusters on the MgO(001) surface: a possible way to identify the charge states of the defect centers. <i>Journal of Chemical Physics</i> , 2013 , 138, 034711	3.9	8
38	Deposition of Nonstoichiometric Tungsten Oxides on the TiO ₂ (110) Surface: A Possible Way to Stabilize the Unstable Clusters in the Gas Phase. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 15335-15344	3.8	8
37	Why does F-doping enhance the photocatalytic water-splitting performance of mBiVO ₄ ? A density functional theory study. <i>New Journal of Chemistry</i> , 2017 , 41, 1094-1102	3.6	7
36	Density functional theory and surface enhanced Raman spectroscopy studies of tautomeric hypoxanthine and its adsorption behaviors in electrochemical processes. <i>Electrochimica Acta</i> , 2015 , 164, 132-138	6.7	7

35	Effects of N-doping concentration on graphene structures and properties. <i>Chemical Physics Letters</i> , 2013 , 581, 74-79	2.5	7
34	Theoretical Comparison of Oxygen Adsorption on Cu(100) Surface. <i>Chinese Journal of Chemical Physics</i> , 2006 , 19, 54-58	0.9	7
33	1T-MoS ₂ monolayer as a promising anode material for (Li/Na/Mg)-ion batteries. <i>Applied Surface Science</i> , 2022 , 584, 152537	6.7	7
32	Electrocatalytic Nitrogen Reduction by Transition Metal Single-Atom Catalysts on Polymeric Carbon Nitride. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 13880-13888	3.8	7
31	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.. <i>RSC Advances</i> , 2019 , 9, 40340-40347	3.7	7
30	Blue-AsP monolayer as a promising anode material for lithium- and sodium-ion batteries: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 5143-5151	3.6	7
29	Effects of doping high-valence transition metal (V, Nb and Zr) ions on the structure and electrochemical performance of LIB cathode material LiNiCoMnO. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 11528-11537	3.6	7
28	Study of CO adsorption on perfect and defective pyrite(100) surfaces by density functional theory. <i>Journal of Natural Gas Chemistry</i> , 2011 , 20, 60-64		6
27	Effects of Ti doping at the reduced SnO ₂ (110) surface with different oxygen vacancies: a first principles study. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	5
26	Coverage-Dependent Behavior on Organic Functionalization of the Semiconductor X(100)-2 × 1 Surface (X = C, Si, and Ge) by Carbene, Silylene, Germylene, and Nitrene: A Periodic DFT Study. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 6543-6552	3.8	5
25	A DFT investigation of the effects of doped Pb atoms on Pdn clusters (13?n?116). <i>Computational and Theoretical Chemistry</i> , 2011 , 966, 375-382	2	5
24	A theoretical study on the dissociation of Cl ₂ on MgO(0 0 1) surface: Prompted by silver atoms supported on surface. <i>Chemical Physics</i> , 2006 , 328, 236-242	2.3	5
23	STRUCTURES AND ELECTRONIC PROPERTIES OF A Co ₂ P CLUSTER DEPOSITED ON THE RUTILE TiO ₂ (110) SURFACE BY FIRST-PRINCIPLES CALCULATIONS. <i>Journal of Theoretical and Computational Chemistry</i> , 2013 , 12, 1250102	1.8	4
22	Defective BC ₂ N as an Anode Material with Improved Performance for Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 4946-4954	3.8	4
21	Influence of denticity and combined soft-hard strategy on the interaction of picolinic-type ligands with NpO ₂ ⁺ . <i>RSC Advances</i> , 2017 , 7, 12236-12246	3.7	3
20	Density functional theory study of CO catalytic oxidation on Co ₂ B ₂ /TiO ₂ (110) surface. <i>Journal of Natural Gas Chemistry</i> , 2010 , 19, 300-306		3
19	First-principles Periodic Density Functional Study of CO Adsorption on Spinel-type CuCr ₂ O ₄ (100) Surface. <i>Chinese Journal of Chemical Physics</i> , 2007 , 20, 557-562	0.9	3
18	Structural and Spectral Properties of a Nonclassical C Isomer with Its Hydrogenated Derivative CH in Theory. <i>ACS Omega</i> , 2021 , 6, 27101-27111	3.9	3

17	Density Functional Theory Study of CO and O ₂ Adsorption on NiFeB ₂ /TiO ₂ Surface. <i>Chinese Journal of Catalysis</i> , 2010 , 31, 423-428	11.3	3
16	The sources of hydrogen affect the productivity and selectivity of CO ₂ photoreduction on SiC. <i>Applied Surface Science</i> , 2021 , 538, 148010	6.7	3
15	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} O ₂ . <i>Journal of Physical Chemistry C</i> , 2021 , 125, 19600-19608	3.8	3
14	First-principles investigation of H ₂ O on HfO ₂ (110) surface. <i>Applied Surface Science</i> , 2013 , 264, 424-432	6.7	2
13	Adsorption of H ₂ O, OH, and O on CuCl(111) Surface: A Density Functional Theory Study. <i>Chinese Journal of Chemical Physics</i> , 2008 , 21, 39-44	0.9	2
12	Density Functional Study on Adsorption of NO on AuSe (010) Surface. <i>Chinese Journal of Chemistry</i> , 2008 , 26, 107-112	4.9	2
11	Density Functional Theory and Surface Enhanced Raman Spectroscopy Studies of Dicyandiamide Adsorbed on Au Clusters. <i>Wuli Huaxue Xuebao/Acta Physico - Chimica Sinica</i> , 2015 , 31, 1872-1879	3.8	2
10	Adsorption and Decomposition of N ₂ O on Cu/t-ZrO ₂ (101) Surfaces. <i>Chinese Journal of Catalysis</i> , 2013 , 33, 1850-1856	11.3	2
9	Investigating the potentials of TiVC MXenes as anode materials for Li-ion batteries by DFT calculations. <i>Applied Surface Science</i> , 2021 , 569, 151002	6.7	2
8	Kinetic and mechanistic analysis of NH ₃ decomposition on Ru(0001), Ru(111) and Ir(111) surfaces. <i>Nanoscale Advances</i> , 2021 , 3, 1624-1632	5.1	2
7	The oxo exchange reaction mechanism of americyl(VI): a density functional theory study. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2020 , 324, 857-868	1.5	1
6	Computational Investigation of Coverage-Dependent Behavior on Functionalization of the Semiconductor X (100)-2 × 1 Surface (X = C, Si, and Ge) by Cycloaddition of Transition Metal Oxides. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 5800-5808	3.8	1
5	Density Functional Theory Study of IB Metals Binding to Perfect and N-Doped Graphene. <i>Chinese Journal of Catalysis</i> , 2013 , 33, 1578-1585	11.3	1
4	Theoretical insights into the thermal reduction of N to NH over a single metal atom incorporated nitrogen-doped graphene. <i>Journal of Chemical Physics</i> , 2021 , 154, 054703	3.9	1
3	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO Activation. <i>ACS Omega</i> , 2021 , 6, 27259-27270	3.9	0
2	How does the defect ZnO@Au surface activate the methane via the precursor-mediated mechanism?. <i>Applied Surface Science</i> , 2021 , 555, 149728	6.7	0
1	Investigation of Ordered TiMC and TiMCT ₂ (M = Cr and Mo; T = O and S) MXenes as High-Performance Anode Materials for Lithium-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2022 , 126, 5283-5291	3.8	0