Yan-Hui Chen

List of Publications by Year in Descending Order

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	1T-MoS2 monolayer as a promising anode material for (Li/Na/Mg)-ion batteries. *Applied Surface Science*, **2022**, 584, 152537	6.7	7
87	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
86	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO Activation. *ACS Omega*, **2021**, 6, 27259-27270	3.9	0
85	Structural and Spectral Properties of a Nonclassical C Isomer with Its Hydrogenated Derivative CH in Theory. *ACS Omega*, **2021**, 6, 27101-27111	3.9	3
84	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
83	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
82	The sources of hydrogen affect the productivity and selectivity of CO2 photoreduction on SiC. *Applied Surface Science*, **2021**, 538, 148010	6.7	3
81	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
80	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
79	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
78	How does the defect ZnO@Au surface activate the methane via the precursor-mediated mechanism?. *Applied Surface Science*, **2021**, 555, 149728	6.7	0
77	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
76	Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. *Applied Surface Science*, **2021**, 563, 150269	6.7	11
75	Investigating the potentials of TiVC MXenes as anode materials for Li-ion batteries by DFT calculations. *Applied Surface Science*, **2021**, 569, 151002	6.7	2
74	Kinetic and mechanistic analysis of NH3 decomposition on Ru(0001), Ru(111) and Ir(111) surfaces. *Nanoscale Advances*, **2021**, 3, 1624-1632	5.1	2
73	The oxo exchange reaction mechanism of americyl(VI): a density functional theory study. *Journal of Radioanalytical and Nuclear Chemistry*, **2020**, 324, 857-868	1.5	1
72	Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. *Journal of Physical Chemistry C* , **2020**, 124, 7031-7038	3.8	11

71	Nitrogen fixation on metal-free SiC(111) polar surfaces. *Journal of Materials Chemistry A*, **2020**, 8, 7412-7421	11	17
70	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
69	First-principles study of MoSSe_graphene heterostructures as anode for Li-ion batteries. *Chemical Physics*, **2020**, 529, 110583	2.3	10
68	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
67	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
66	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
65	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
64	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
63	Influence of denticity and combined soft□hard strategy on the interaction of picolinic-type ligands with NpO2+. *RSC Advances*, **2017**, 7, 12236-12246	3.7	3
62	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
61	Embedded Si/Graphene Composite Fabricated by Magnesium-Thermal Reduction as Anode Material for Lithium-Ion Batteries. *Nanoscale Research Letters*, **2017**, 12, 627	5	15
60	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	3.8	26
59	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	6.7	19
58	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
57	First-principles study of Na2+xTi7O15 as anode materials for sodium-ion batteries. *Journal of Alloys and Compounds*, **2016**, 689, 805-811	5.7	11
56	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	6.7	7
55	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
54	Pressure-tuning the nonlinear-optical properties of AgGaS_2 crystal: a first-principle study. *Optical Materials Express*, **2015**, 5, 1738	2.6	9

53	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	3.8	2
52	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
51	Theoretical insights into the reaction mechanisms of NO oxidation catalyzed by Cu2O(1 1 1). *Applied Surface Science*, **2014**, 316, 416-423	6.7	17
50	Effects of N-doping concentration on graphene structures and properties. *Chemical Physics Letters*, **2013**, 581, 74-79	2.5	7
49	Oxidation of Pdn (n=1□5) clusters on single vacancy graphene: A first-principles study. *Computational and Theoretical Chemistry*, **2013**, 1020, 91-99	2	26
48	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
47	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	3.9	8
46	First-principles investigation of H2O on HfO2 (110) surface. *Applied Surface Science*, **2013**, 264, 424-432	6.7	2
45	STRUCTURES AND ELECTRONIC PROPERTIES OF A Co2P CLUSTER DEPOSITED ON THE RUTILE TiO2(110) SURFACE BY FIRST□PRINCIPLES CALCULATIONS. *Journal of Theoretical and Computational Chemistry*, **2013**, 12, 1250102	1.8	4
44	Adsorption and Decomposition of N2O on Cu/t-ZrO2(101) Surfaces. *Chinese Journal of Catalysis*, **2013**, 33, 1850-1856	11.3	2
43	Density Functional Theory Study of IB Metals Binding to Perfect and N-Doped Graphene. *Chinese Journal of Catalysis*, **2013**, 33, 1578-1585	11.3	1
42	Growth mechanism of palladium clusters on rutile TiO2(110) surface. *Journal of Natural Gas Chemistry*, **2012**, 21, 544-555		8
41	Enhanced Oxidation Reactivity of WO3(001) Surface through the Formation of Oxygen Radical Centers. *Journal of Physical Chemistry C*, **2012**, 116, 5067-5075	3.8	21
40	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
39	Organic semiconductor for artificial photosynthesis: water splitting into hydrogen by a bioinspired C3N3S3polymer under visible light irradiation. *Chemical Science*, **2011**, 2, 1826-1830	9.4	146
38	Study of CO adsorption on perfect and defective pyrite(100) surfaces by density functional theory. *Journal of Natural Gas Chemistry*, **2011**, 20, 60-64		6
37	Sn2+ dopant induced visible-light activity of SnO2 nanoparticles for H2 production. *Catalysis Communications*, **2011**, 16, 215-219	3.2	54
36	Structural and electronic properties of tungsten trioxides: from cluster to solid surface. *Theoretical Chemistry Accounts*, **2011**, 130, 103-114	1.9	22

35	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. *Journal of Physical Chemistry C*, **2011**, 115, 5800-5808	3.8	1
34	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
33	A DFT investigation of the effects of doped Pb atoms on Pdn clusters (13?n?116). *Computational and Theoretical Chemistry*, **2011**, 966, 375-382	2	5
32	Reaction mechanism of CO oxidation on Cu(2)O(111): A density functional study. *Journal of Chemical Physics*, **2010**, 133, 154502	3.9	38
31	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. *Journal of Physical Chemistry C*, **2010**, 114, 6543-6552	3.8	5
30	Graphitic carbon nitride as a metal-free catalyst for NO decomposition. *Chemical Communications*, **2010**, 46, 6965-7	5.8	157
29	A molecular modeling study on small molecule gas transportation in poly (chloro-p-xylylene). *Computational Materials Science*, **2010**, 49, S65-S69	3.2	21
28	Density functional theory for adsorption of HCHO on the FeO(100) surface. *Journal of Natural Gas Chemistry*, **2010**, 19, 21-24		15
27	Density functional theory study of CO catalytic oxidation on Co2B2/TiO2 (110) surface. *Journal of Natural Gas Chemistry*, **2010**, 19, 300-306		3
26	Facile electrochemical preparation of Ag nanothorns and their growth mechanism. *Chemistry - A European Journal*, **2010**, 16, 6766-70	4.8	18
25	Density Functional Theory Study of CO and O2 Adsorption on NiFeB2/TiO2 Surface. *Chinese Journal of Catalysis*, **2010**, 31, 423-428	11.3	3
24	Coadsorption of CO and NO on the Cu(2)O(111) surface: A periodic density functional theory study. *Journal of Chemical Physics*, **2009**, 131, 174503	3.9	17
23	Bulk and surface properties of spinel Co3O4 by density functional calculations. *Surface Science*, **2009**, 603, 653-658	1.8	140
22	A DFT Study of CO Catalytic Oxidation by N2O or O2 on the Co3O4(110) Surface. *ChemCatChem*, **2009**, 1, 384-392	5.2	71
21	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
20	THE ROLE OF SURFACE OXYGEN VACANCY IN N2O DECOMPOSITION ON Cu2O(111) SURFACE: A DFT STUDY. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 263-276	1.8	16
19	Adsorption of H2O, OH, and O on CuCl(111) Surface: A Density Functional Theory Study. *Chinese Journal of Chemical Physics*, **2008**, 21, 39-44	0.9	2
18	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	6.7	48

17	Interaction of CO and NO with the spinel CuCr2O4 (100) surface: A DFT study. *International Journal of Quantum Chemistry*, **2008**, 108, 1435-1443	2.1	10
16	Density Functional Study on Adsorption of NO on AuSe (010) Surface. *Chinese Journal of Chemistry*, **2008**, 26, 107-112	4.9	2
15	A periodic density functional theory study of the dehydrogenation of methanol over CuCl(1 1 1) surface. *Applied Surface Science*, **2008**, 254, 4421-4431	6.7	19
14	First-principles study of O2 adsorption and dissociation on the CuCr2O4 (100) surface. *Computational and Theoretical Chemistry*, **2008**, 860, 18-23		13
13	A density functional theory study on the adsorption and dissociation of N2O on Cu2O(111) surface. *Applied Surface Science*, **2007**, 253, 7501-7505	6.7	58
12	Interaction of photoactive catechol with TiO2 anatase (101) surface: A periodic density functional theory study. *Chemical Physics*, **2007**, 331, 275-282	2.3	67
11	First-principles Periodic Density Functional Study of CO Adsorption on Spinel-type CuCr2O4 (100) Surface. *Chinese Journal of Chemical Physics*, **2007**, 20, 557-562	0.9	3
10	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. *Chemical Physics*, **2006**, 330, 204-211	2.3	42
9	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	4.9	12
8	Theoretical Comparison of Oxygen Adsorption on Cu(100) Surface. *Chinese Journal of Chemical Physics*, **2006**, 19, 54-58	0.9	7
7	Theoretical Studies of the Adsorption and Dissociation of Two NO Molecules on Cu2O(111) Surface. *Acta Physico-chimica Sinica*, **2006**, 22, 1126-1131		16
6	A theoretical study on the dissociation of Cl2 on MgO(0 0 1) surface: Prompted by silver atoms supported on surface. *Chemical Physics*, **2006**, 328, 236-242	2.3	5
5	A first-principles study of the chemi-adsorption of benzene on Au(100) surface. *Chemical Physics Letters*, **2006**, 417, 414-418	2.5	35
4	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		57
3	On the coverage-dependent orientation of benzene adsorbed on Cu(1 0 0): A density functional theory study. *Chemical Physics Letters*, **2005**, 407, 414-418	2.5	24
2	The adsorption and dissociation of Cl2 on the MgO (001) surface with vacancies: embedded cluster model study. *Journal of Chemical Physics*, **2004**, 120, 8753-60	3.9	23
1	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	1.8	51