Qingfeng Ge

List of Publications by Year in Descending Order

175 papers	6,795 citations	47 h-index	75 g-index
188 ext. papers	7,789 ext. citations	5.3 avg, IF	6.15 L-index

#	Paper	IF	Citations
175	Effect of postsynthesis preparation methods on catalytic performance of Ti-Beta zeolite in ketonization of propionic acid. *Microporous and Mesoporous Materials*, **2022**, 330, 111625	5.3	1
174	CeO2 Facet-Dependent Surface Reactive Intermediates and Activity during Ketonization of Propionic Acid. *ACS Catalysis*, **2022**, 12, 2998-3012	13.1	0
173	Ultrafast Preparation of Nonequilibrium FeNi Spinels by Magnetic Induction Heating for Unprecedented Oxygen Evolution Electrocatalysis. *Research*, **2022**, 2022, 1-13	7.8	1
172	Mechanism of ozone adsorption and activation on B-, N-, P-, and Si-doped graphene: a DFT study. *Chemical Engineering Journal*, **2021**, 133114	14.7	2
171	Vapor phase hydrodeoxygenation of phenolic compounds on group 10 metal-based catalysts: Reaction mechanism and product selectivity control. *Catalysis Today*, **2021**, 365, 143-161	5.3	5
170	Multiple light scattering and nanotip effect of hierarchical sea urchin-like W18O49 boosting photocatalytic hydrolysis of ammonia borane. *International Journal of Hydrogen Energy*, **2021**, 46, 18964-18976	6.7	1
169	Enhanced Ethylene Formation from Carbon Dioxide Reduction through Sequential Catalysis on Au Decorated Cubic Cu2O Electrocatalyst. *European Journal of Inorganic Chemistry*, **2021**, 2021, 2353-2364	2.3	1
168	Ketonization of Propionic Acid on Lewis Acidic Zr-Beta Zeolite with Improved Stability and Selectivity. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 7982-7992	8.3	6
167	Highly efficient electrochemical hydrogenation of acetonitrile to ethylamine for primary amine synthesis and promising hydrogen storage. *Chem Catalysis*, **2021**, 1, 393-406		4
166	A DFT study of methane conversion on Mo-terminated Mo2C carbides: Carburization vs C□ coupling. *Catalysis Today*, **2021**, 368, 140-147	5.3	6
165	Promoting carbon dioxide electroreduction toward ethanol through loading Au nanoparticles on hollow Cu2O nanospheres. *Catalysis Today*, **2021**, 365, 348-356	5.3	2
164	Electrochemical reduction of CO to CO and HCOO using metal-cyclam complex catalysts: predicting selectivity and limiting potential from DFT. *Dalton Transactions*, **2021**, 50, 11446-11457	4.3	1
163	Elucidating the Structure of Bimetallic NiW/SiO2 Catalysts and Its Consequences on Selective Deoxygenation of m-Cresol to Toluene. *ACS Catalysis*, **2021**, 11, 2935-2948	13.1	6
162	Tuning reverse water gas shift and methanation reactions during CO2 reduction on Ni catalysts via surface modification by MoOx. *Journal of CO2 Utilization*, **2021**, 52, 101678	7.6	5
161	Visible-Light-Driven Multichannel Regulation of Local Electron Density to Accelerate Activation of O□ and B□ Bonds for Ammonia Borane Hydrolysis. *ACS Catalysis*, **2020**, 10, 14903-14915	13.1	19
160	Ce□iO-66 Derived CeO2 Octahedron Catalysts for Efficient Ketonization of Propionic Acid. *Industrial & Engineering Chemistry Research*, **2020**, 59, 17269-17278	3.9	12
159	A highly active Pt/In2O3 catalyst for CO2 hydrogenation to methanol with enhanced stability. *Green Chemistry*, **2020**, 22, 5059-5066	10	46

158	A density functional theory study on reduction-induced structural transformation of copper-oxide-based oxygen carrier. *Journal of Chemical Physics*, **2020**, 152, 054709	3.9	3
157	Catalytic Reduction of CO2 to CO via Reverse Water Gas Shift Reaction: Recent Advances in the Design of Active and Selective Supported Metal Catalysts. *Transactions of Tianjin University*, **2020**, 26, 172-187	2.9	37
156	Gas Surface Interaction and Surface Reactions. *Springer Handbooks*, **2020**, 905-928	1.3	
155	Oxygen Reduction Reaction Catalyzed by Pt3M (M = 3d Transition Metals) Supported on O-doped Graphene. *Catalysts*, **2020**, 10, 156	4	7
154	Anisotropic N-Modification of the Mo4 Ensemble for Efficient Ammonia Synthesis on Molybdenum Nitrides. *Journal of Physical Chemistry C*, **2020**, 124, 616-624	3.8	2
153	Facile synthesis of hierarchical flower-like Ag/Cu2O and Au/Cu2O nanostructures and enhanced catalytic performance in electrochemical reduction of CO2. *Frontiers of Chemical Science and Engineering*, **2020**, 14, 813-823	4.5	3
152	Aqueous Phase Aldol Condensation of Formaldehyde and Acetone on Anatase TiO2(101) Surface: A Theoretical Investigation. *ChemCatChem*, **2020**, 12, 1220-1229	5.2	7
151	Surface-Mediated Interconnections of Nanoparticles in Cellulosic Fibrous Materials toward 3D Sensors. *Advanced Materials*, **2020**, 32, e2002171	24	9
150	Construction of Highly Active and Selective Polydopamine Modified Hollow ZnO/Co3O4 p-n Heterojunction Catalyst for Photocatalytic CO2 Reduction. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 11465-11476	8.3	38
149	Balancing the Activity and Selectivity of Propane Oxidative Dehydrogenation on NiOOH (001) and (010). *Transactions of Tianjin University*, **2020**, 26, 341-351	2.9	2
148	DFT Study of Methane Activation and Coupling on the (0001) and (112 0) Surfaces of □WC. *Journal of Physical Chemistry C*, **2020**, 124, 26722-26729	3.8	5
147	Effect of acid-metal balance of bifunctional Pt/Beta catalysts on vapor phase hydrodeoxygenation of m-cresol. *Catalysis Today*, **2020**, 355, 43-50	5.3	10
146	CH4 dissociation and CC coupling on Mo-terminated MoC surfaces: A DFT study. *Catalysis Today*, **2020**, 339, 54-61	5.3	12
145	Influence of Re addition to Ni/SiO2 catalyst on the reaction network and deactivation during hydrodeoxygenation of m-cresol. *Catalysis Today*, **2020**, 347, 79-86	5.3	14
144	Tuning Sn-Cu Catalysis for Electrochemical Reduction of CO2 on Partially Reduced Oxides SnOx-CuOx-Modified Cu Electrodes. *Catalysts*, **2019**, 9, 476	4	18
143	Conversion of C2□4 Carboxylic Acids to Hydrocarbons on HZSM-5: Effect of Carbon Chain Length. *Industrial & Engineering Chemistry Research*, **2019**, 58, 10307-10316	3.9	11
142	Hollow Au-ZnO/CN Nanocages Derived from ZIF-8 for Efficient Visible-Light-Driven Hydrogen Evolution from Formaldehyde Alkaline Solution. *European Journal of Inorganic Chemistry*, **2019**, 2019, 2761-2767	2.3	6
141	Metal-free amino-incorporated organosilica nanotubes for cooperative catalysis in the cycloaddition of CO2 to epoxides. *Catalysis Today*, **2019**, 324, 59-65	5.3	16

140	Surface chemistry and reactivity of □-MoO toward methane: A SCAN-functional based DFT study. *Journal of Chemical Physics*, **2019**, 151, 044708	3.9	8
139	Simultaneous Activation of CH4 and CO2 for Concerted C□□ Coupling at Oxide□Oxide Interfaces. *ACS Catalysis*, **2019**, 9, 3187-3197	13.1	25
138	Ti3+ Defective SnS2/TiO2 Heterojunction Photocatalyst for Visible-Light Driven Reduction of CO2 to CO with High Selectivity. *Catalysts*, **2019**, 9, 927	4	18
137	Insights into the Mechanism of Ammonia Decomposition on Molybdenum Nitrides Based on DFT Studies. *Journal of Physical Chemistry C*, **2019**, 123, 554-564	3.8	16
136	Polydopamine and Barbituric Acid Co-Modified Carbon Nitride Nanospheres for Highly Active and Selective Photocatalytic CO2 Reduction. *European Journal of Inorganic Chemistry*, **2019**, 2019, 2058-2064	2.3	10
135	Enhanced selective deoxygenation of m-cresol to toluene on Ni/SiO2 catalysts derived from nickel phyllosilicate. *Catalysis Today*, **2019**, 330, 149-156	5.3	18
134	Active Site Ensembles Enabled C□□ Coupling of CO2 and CH4 for Acetone Production. *Journal of Physical Chemistry C*, **2018**, 122, 9570-9577	3.8	10
133	Size Dependence of Vapor Phase Hydrodeoxygenation of m-Cresol on Ni/SiO2 Catalysts. *ACS Catalysis*, **2018**, 8, 1672-1682	13.1	94
132	Role of CO2 in the oxy-dehydrogenation of ethylbenzene to styrene on the CeO2(111) surface. *Applied Surface Science*, **2018**, 427, 973-980	6.7	10
131	Synergy between Cu and Br□sted acid sites in carbonylation of dimethyl ether over Cu/H-MOR. *Journal of Catalysis*, **2018**, 365, 440-449	7.3	25
130	Rhenium-promoted selective CO2 methanation on Ni-based catalyst. *Journal of CO2 Utilization*, **2018**, 26, 8-18	7.6	37
129	Cooperative cobinding of synthetic and natural ligands to the nuclear receptor PPAR□ *ELife*, **2018**, 7,	8.9	32
128	Ketonization of Propionic Acid to 3-Pentanone over CexZr1□xO2 Catalysts: The Importance of Acid□Base Balance. *Industrial & Engineering Chemistry Research*, **2018**, 57, 17086-17096	3.9	20
127	Effect of Strong Metal-Support Interaction of Pt/TiO2 on Hydrodeoxygenation of m-Cresol. *ChemistrySelect*, **2018**, 3, 10364-10370	1.8	14
126	Competition and Cooperation of Hydrogenation and Deoxygenation Reactions during Hydrodeoxygenation of Phenol on Pt(111). *Journal of Physical Chemistry C*, **2017**, 121, 12249-12260	3.8	40
125	Mesoporous silica-based nanotubes loaded Pd nanoparticles: Effect of framework compositions on the performance in heterogeneous catalysis. *Microporous and Mesoporous Materials*, **2017**, 247, 1-8	5.3	10
124	Geometric and electronic effects of bimetallic Ni□Re catalysts for selective deoxygenation of m-cresol to toluene. *Journal of Catalysis*, **2017**, 349, 84-97	7.3	80
123	Mechanistic understanding on oxygen evolution reaction on □-FeOOH (010) under alkaline condition based on DFT computational study. *Chinese Journal of Catalysis*, **2017**, 38, 1621-1628	11.3	11

122	Conversion of propionic acid and 3-pentanone to hydrocarbons on ZSM-5 catalysts: Reaction pathway and active site. *Applied Catalysis A: General*, **2017**, 545, 79-89	5.1	19
121	CO2 hydrogenation to methanol over Pd/In2O3: effects of Pd and oxygen vacancy. *Applied Catalysis B: Environmental*, **2017**, 218, 488-497	21.8	265
120	Titania-Modified Silver Electrocatalyst for Selective CO2 Reduction to CH3OH and CH4 from DFT Study. *Journal of Physical Chemistry C*, **2017**, 121, 16275-16282	3.8	29
119	Research Progress in Ketonization of Biomass-derived Carboxylic Acids over Metal Oxides. *Acta Chimica Sinica*, **2017**, 75, 439	3.3	7
118	Reverse water gas shift over In2O3□CeO2 catalysts. *Catalysis Today*, **2016**, 259, 402-408	5.3	57
117	Direct C-C Coupling of CO2 and the Methyl Group from CH4 Activation through Facile Insertion of CO2 into Zn-CH3 □Bond. *Journal of the American Chemical Society*, **2016**, 138, 10191-8	16.4	54
116	Insights into the Major Reaction Pathways of Vapor-Phase Hydrodeoxygenation of m-Cresol on a Pt/HBeta Catalyst. *ChemCatChem*, **2016**, 8, 551-561	5.2	26
115	Enhanced CO selectivity and stability for electrocatalytic reduction of CO 2 on electrodeposited nanostructured porous Ag electrode. *Journal of CO2 Utilization*, **2016**, 15, 41-49	7.6	36
114	Promotional effect of surface hydroxyls on electrochemical reduction of CO2 over SnO /Sn electrode. *Journal of Catalysis*, **2016**, 343, 257-265	7.3	83
113	A DFT-based study of surface chemistries of rutile TiO2 and SnO2(110) toward formaldehyde and formic acid. *Catalysis Today*, **2016**, 274, 103-108	5.3	15
112	Enhancing tungsten oxide/SBA-15 catalysts for hydrolysis of cellobiose through doping ZrO2. *Applied Catalysis A: General*, **2016**, 523, 182-192	5.1	17
111	Interaction of Formaldehyde with the Rutile TiO2(110) Surface: A Combined Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2016**, 120, 12626-12636	3.8	40
110	Effect of calcination and metal loading on the characteristics of Co/NaY catalyst for liquid-phase hydrogenation of ethyl lactate to 1,2-propanediol. *Microporous and Mesoporous Materials*, **2016**, 233, 184-193	5.3	5
109	A Comparative Study of Methanol Adsorption and Dissociation over WO3(001) and ReO3(001). *Topics in Catalysis*, **2015**, 58, 655-664	2.3	5
108	Low-Temperature Reductive Coupling of Formaldehyde on Rutile TiO2(110). *Journal of Physical Chemistry C*, **2015**, 119, 18452-18457	3.8	19
107	Vapor phase hydrodeoxygenation and hydrogenation of m-cresol on silica supported Ni, Pd and Pt catalysts. *Chemical Engineering Science*, **2015**, 135, 145-154	4.4	80
106	Imaging of Formaldehyde Adsorption and Diffusion on TiO2(110). *Topics in Catalysis*, **2015**, 58, 103-113	2.3	25
105	A DFT study of oxygen reduction reaction mechanism over O-doped graphene-supported Pt4, Pt3Fe and Pt3V alloy catalysts. *International Journal of Hydrogen Energy*, **2015**, 40, 5126-5134	6.7	28

104	Hydrogenation of CO2 to methanol over In2O3 catalyst. *Journal of CO2 Utilization*, **2015**, 12, 1-6	7.6	161
103	Effect of PdIn bimetallic particle formation on CO 2 reduction over the Pd□n/SiO 2 catalyst. *Chemical Engineering Science*, **2015**, 135, 193-201	4.4	59
102	Tracking Site-Specific C□ Coupling of Formaldehyde Molecules on Rutile TiO2(110). *Journal of Physical Chemistry C*, **2015**, 119, 14267-14272	3.8	21
101	Efficient Hydrolytic Hydrogenation of Cellulose on Mesoporous HZSM-5 Supported Ru Catalysts. *Topics in Catalysis*, **2015**, 58, 623-632	2.3	13
100	A DFT study of CO2 electrochemical reduction on Pb(211) and Sn(112). *Science China Chemistry*, **2015**, 58, 607-613	7.9	18
99	Role of Dissociation of Phenol in Its Selective Hydrogenation on Pt(111) and Pd(111). *ACS Catalysis*, **2015**, 5, 2009-2016	13.1	108
98	Selective conversion of microcrystalline cellulose into hexitols over a Ru/[Bmim]3PW12O40 catalyst under mild conditions. *Catalysis Today*, **2014**, 233, 70-76	5.3	27
97	Methanol synthesis from CO2 hydrogenation over a Pd4/In2O3 model catalyst: A combined DFT and kinetic study. *Journal of Catalysis*, **2014**, 317, 44-53	7.3	149
96	In2O3 as a promising catalyst for CO2 utilization: A case study with reverse water gas shift over In2O3 **2014**, 4, 140-144		43
95	Ru supported on zirconia-modified SBA-15 for selective conversion of cellobiose to hexitols. *Microporous and Mesoporous Materials*, **2014**, 198, 215-222	5.3	18
94	Mechanistic Understanding of Catalytic CO2 Activation from First Principles Theory **2013**, 49-79		6
93	Effect of defects and dopants in graphene on hydrogen interaction in graphene-supported NaAlH4. *International Journal of Hydrogen Energy*, **2013**, 38, 3670-3680	6.7	19
92	Imaging reactions of acetone with oxygen adatoms on partially oxidized TiO2(110). *Physical Chemistry Chemical Physics*, **2013**, 15, 13897-901	3.6	7
91	Active Oxygen Vacancy Site for Methanol Synthesis from CO2 Hydrogenation on In2O3(110): A DFT Study. *ACS Catalysis*, **2013**, 3, 1296-1306	13.1	355
90	Understanding electronic and optical properties of anatase TiO2 photocatalysts co-doped with nitrogen and transition metals. *Physical Chemistry Chemical Physics*, **2013**, 15, 9549-61	3.6	76
89	First-Principles Studies on Hydrogen Desorption Mechanism of MgnH2n (n = 3, 4). *Journal of Physical Chemistry C*, **2013**, 117, 8099-8104	3.8	6
88	DFT Study of CO2 Adsorption and Hydrogenation on the In2O3 Surface. *Journal of Physical Chemistry C*, **2012**, 116, 7817-7825	3.8	202
87	A DFT study of methanol dehydrogenation on the PdIn(110) surface. *Physical Chemistry Chemical Physics*, **2012**, 14, 16660-7	3.6	26

86	Selective CO2 hydrogenation on the Al2O3 supported bimetallic CoCu catalyst. *Catalysis Today*, **2012**, 194, 30-37	5.3	15
85	Acetone-Assisted Oxygen Vacancy Diffusion on TiO2(110). *Journal of Physical Chemistry Letters*, **2012**, 3, 2970-4	6.4	16
84	Coverage-dependent molecular tilt of carbon monoxide chemisorbed on Pt{110}: A combined LEED and DFT structural analysis. *Surface Science*, **2012**, 606, 383-393	1.8	10
83	A DFT+U study of structure and reducibility of CenO2n (n?4, 0?x?n) nanoclusters. *Computational and Theoretical Chemistry*, **2012**, 987, 25-31	2	8
82	Tunability of band gaps in metal-organic frameworks. *Inorganic Chemistry*, **2012**, 51, 9039-44	5.1	123
81	Computational Nanostructure Design for Hydrogen Storage. *Green Energy and Technology*, **2011**, 761-790	0.6	
80	Hydrogen Adsorption on Ga2O3 Surface: A Combined Experimental and Computational Study. *Journal of Physical Chemistry C*, **2011**, 115, 10140-10146	3.8	45
79	Hydride-Assisted Hydrogenation of Ti-Doped NaH/Al: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2011**, 115, 2522-2528	3.8	10
78	Using first-principles metadynamics simulation to predict new phases and probe the phase transition of NaAlH4. *Journal of Physics Condensed Matter*, **2011**, 23, 345401	1.8	2
77	Adsorption and activation of CO2 over the CuCo catalyst supported on partially hydroxylated Al2O3. *Catalysis Today*, **2011**, 165, 10-18	5.3	33
76	Transition-metal-doped aluminum hydrides as building blocks for supramolecular assemblies. *Journal of Physical Chemistry A*, **2010**, 114, 12318-22	2.8	4
75	Promotion effects of Ga2O3 on CO2 adsorption and conversion over a SiO2-supported Ni catalyst. *Energy and Environmental Science*, **2010**, 3, 1322	35.4	70
74	Effects of hydration and oxygen vacancy on CO2 adsorption and activation on beta-Ga2O3(100). *Langmuir*, **2010**, 26, 5551-8	4	104
73	A DFT Investigation of the Al2O3 Supported Fe3Zn and Fe4 Clusters as Catalysts for CO2 Adsorption and Activation. *ACS Symposium Series*, **2010**, 197-208	0.4	2
72	Layered atomic structures of double oxides for low shear strength at high temperatures. *Scripta Materialia*, **2010**, 62, 735-738	5.6	106
71	Effect of surface hydroxyls on selective CO2 hydrogenation over Ni4/Al2O3: A density functional theory study. *Journal of Catalysis*, **2010**, 272, 227-234	7.3	141
70	Catalyst size and morphological effects on the interaction of NO2 with BaO/Al2O3 materials. *Catalysis Today*, **2010**, 151, 304-313	5.3	8
69	Effect of doped transition metal on reversible hydrogen release/uptake from NaAlH4. *Chemistry - A European Journal*, **2009**, 15, 1685-95	4.8	31

68	Probing the properties of the (1 1 1) and (1 0 0) surfaces of LaB6 through infrared spectroscopy of adsorbed CO. *Surface Science*, **2009**, 603, 3011-3020	1.8	14
67	Tribological investigation of adaptive Mo2N/MoS2/Ag coatings with high sulfur content. *Surface and Coatings Technology*, **2009**, 203, 1304-1309	4.4	140
66	CO2 adsorption and activation over γ-Al2O3-supported transition metal dimers: A density functional study. *Catalysis Today*, **2009**, 147, 68-76	5.3	87
65	Hydrogen Spillover Enhanced Hydriding Kinetics of Palladium-Doped Lithium Nitride to Lithium Imide. *Journal of Physical Chemistry C*, **2009**, 113, 8513-8517	3.8	15
64	Hydrogen Interaction in Ti-Doped LiBH4 for Hydrogen Storage: A Density Functional Analysis. *Journal of Chemical Theory and Computation*, **2009**, 5, 3079-87	6.4	18
63	Origin of Support Effects on the Reactivity of a Ceria Cluster. *Journal of Physical Chemistry C*, **2009**, 113, 18296-18303	3.8	7
62	First-Principles Analysis of NOx Adsorption on Anhydrous γ-Al2O3 Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 7779-7789	3.8	25
61	Characterization of surface and bulk nitrates of gamma-Al2O3-supported alkaline earth oxides using density functional theory. *Physical Chemistry Chemical Physics*, **2009**, 11, 3380-9	3.6	9
60	Effect of Pt Clusters on Methanol Adsorption and Dissociation over Perfect and Defective Anatase TiO2(101) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 20674-20682	3.8	22
59	Adsorption and protonation of CO2 on partially hydroxylated gamma-Al2O3 surfaces: a density functional theory study. *Langmuir*, **2008**, 24, 12410-9	4	95
58	Density Functional Theory Study of Methanol Decomposition on the CeO2(110) Surface. *Journal of Physical Chemistry C*, **2008**, 112, 4257-4266	3.8	37
57	Adsorption and Formation of BaO Overlayers on γ-Al2O3 Surfaces. *Journal of Physical Chemistry C*, **2008**, 112, 18050-18060	3.8	26
56	Effect of BaO Morphology on NOx Abatement: NO2 Interaction with Unsupported and γ-Al2O3-Supported BaO. *Journal of Physical Chemistry C*, **2008**, 112, 16924-16931	3.8	19
55	Vacancy-assisted diffusion of alkoxy species on rutile TiO2(110). *Physical Review Letters*, **2008**, 101, 156103	7.4	30
54	Effect of Surface Oxygen Vacancy on Pt Cluster Adsorption and Growth on the Defective Anatase TiO2(101) Surface. *Journal of Physical Chemistry C*, **2007**, 111, 16397-16404	3.8	49
53	Methanol Adsorption on the Clean CeO2(111) Surface: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2007**, 111, 10514-10522	3.8	51
52	An ab initio analysis of adsorption and diffusion of silver atoms on alumina surfaces. *Surface Science* , **2007**, 601, 134-145	1.8	53
51	Effect of γ-Al2O3 substrate on NO2 interaction with supported BaO clusters. *Surface Science*, **2007**, 601, L65-L68	1.8	20

50	Imaging intrinsic diffusion of bridge-bonded oxygen vacancies on TiO2(110). *Physical Review Letters*, **2007**, 99, 126105	7.4	83
49	A first-principles study of Sc-doped NaAlH4 for reversible hydrogen storage. *Journal of Alloys and Compounds*, **2007**, 446-447, 267-270	5.7	17
48	Grain boundary sliding mechanisms in ZrN-Ag, ZrN-Au, and ZrN-Pd nanocomposite films. *Applied Physics Letters*, **2006**, 88, 021902	3.4	20
47	Adsorption and activation of CO over flat and stepped Co surfaces: a first principles analysis. *Journal of Physical Chemistry B*, **2006**, 110, 15368-80	3.4	136
46	Interaction of Pt clusters with the anatase TiO(2)(101) surface: a first principles study. *Journal of Physical Chemistry B*, **2006**, 110, 7463-72	3.4	78
45	A precursor state for formation of TiAl3 complex in reversible hydrogen desorption/adsorption from Ti-doped NaAlH4. *Chemical Communications*, **2006**, 1822-4	5.8	37
44	A first-principles analysis of hydrogen interaction in Ti-doped NaAlH4 surfaces: structure and energetics. *Journal of Physical Chemistry B*, **2006**, 110, 25863-8	3.4	45
43	A density functional theory study of CO adsorption on Pt□Au nanoparticles. *Computational Materials Science*, **2006**, 35, 247-253	3.2	54
42	DFT studies of Pt/Au bimetallic clusters and their interactions with the CO molecule. *Journal of Physical Chemistry B*, **2005**, 109, 22341-50	3.4	117
41	Correlation between interfacial electronic structure and mechanical properties of ZrN□Me (Me?Ag, Au, or Pd) nanocomposite films. *Applied Physics Letters*, **2005**, 87, 041902	3.4	12
40	Adsorption of CO2 on Model Surfaces of Cesium Oxides Determined from First Principles. *Journal of Physical Chemistry B*, **2004**, 108, 16798-16805	3.4	24
39	First-principles-based kinetic Monte Carlo simulation of nitric oxide decomposition over Pt and Rh surfaces under lean-burn conditions. *Molecular Physics*, **2004**, 102, 361-369	1.7	42
38	Structure dependence of NO adsorption and dissociation on platinum surfaces. *Journal of the American Chemical Society*, **2004**, 126, 1551-9	16.4	104
37	Structure and Energetics of LiBH4 and Its Surfaces: A First-Principles Study□*Journal of Physical Chemistry A*, **2004**, 108, 8682-8690	2.8	63
36	Structure effects on the energetic, electronic, and magnetic properties of palladium nanoparticles. *Journal of Chemical Physics*, **2003**, 118, 5793-5801	3.9	65
35	Steric Effects on the Adsorption of Alkylthiolate Self-Assembled Monolayers on Au (111)□*Journal of Physical Chemistry B*, **2003**, 107, 3803-3807	3.4	70
34	Correlation of adsorption energy with surface structure: ethylene adsorption on Pd surfaces. *Chemical Physics Letters*, **2002**, 358, 377-382	2.5	58
33	Studies of rhodium nanoparticles using the first principles density functional theory calculations. *Chemical Physics Letters*, **2002**, 366, 368-376	2.5	51

32	Mechanisms for Chain Growth in Fischer–Tropsch Synthesis over Ru(0001). *Journal of Catalysis*, **2002**, 212, 136-144	7.3	106
31	A First Principles Study of Carbon–Carbon Coupling over the {0001} Surfaces of Co and Ru. *Journal of Physical Chemistry B*, **2002**, 106, 2826-2829	3.4	64
30	Structure, bonding, and anharmonic librational motion of CO on Ir{100}. *Journal of Chemical Physics*, **2002**, 116, 8097-8105	3.9	15
29	Response to "Comment on 'Surface diffusion potential energy surfaces from first principles' [J. Chem. Phys. 114, 1051 (2001)]. *Journal of Chemical Physics*, **2001**, 114, 1053	3.9	29
28	Facile H/D exchange in adsorbed methylidyne on Pt{110}-(1×2) and deuteration to gaseous methane. *Journal of Chemical Physics*, **2001**, 115, 11306-11316	3.9	8
27	The structure of carbon adsorbed on Ir{100}: LEED I/V analysis and benchmarking of DFT. *Surface Science*, **2001**, 478, 49-56	1.8	12
26	CO Adsorption on Pt–Ru Surface Alloys and on the Surface of Pt–Ru Bulk Alloy. *Journal of Physical Chemistry B*, **2001**, 105, 9533-9536	3.4	77
25	Localisation of adsorbate-induced demagnetisation: CO chemisorbed on Ni{110}. *Chemical Physics Letters*, **2000**, 327, 125-130	2.5	96
24	Unusual bridged site for adsorbed oxygen adatoms: Theory and experiment for Ir{100}-(1×2)-O. *Journal of Chemical Physics*, **2000**, 112, 10460-10466	3.9	61
23	Adsorption energetics and bonding from femtomole calorimetry and from first principles theory. *Advances in Catalysis*, **2000**, 45, 207-259	2.4	37
22	Surface diffusion potential energy surfaces from first principles: CO chemisorbed on Pt{110}. *Journal of Chemical Physics*, **1999**, 111, 9461-9464	3.9	42
21	NO monomer and (NO)x polymeric chain chemisorption on Pt{110}: Structure and energetics. *Journal of Chemical Physics*, **1999**, 110, 12082-12088	3.9	23
20	Lateral potential energy surfaces for molecular chemisorption on metals from experiment and theory: NO on Pt{110}-(1×2). *Chemical Physics Letters*, **1999**, 299, 253-259	2.5	23
19	The chemisorption and dissociation of ethylene on Pt{111} from first principles. *Journal of Chemical Physics*, **1999**, 110, 4699-4702	3.9	66
18	Multilayer influences on the monolayer structure for NO on Pt{110}-(1×2). *Physical Chemistry Chemical Physics*, **1999**, 1, 1995-2000	3.6	14
17	Energetics, geometry and spin density of NO chemisorbed on Pt{111}. *Chemical Physics Letters*, **1998**, 285, 15-20	2.5	94
16	Kinetics of ethylene conversion to ethylidyne on Rh{111} from laser-induced thermal desorption. *Surface Science*, **1998**, 397, 13-22	1.8	4
15	First principles calculation of the energy and structure of two solid surface phases on Ir{100}. *Surface Science*, **1998**, 418, 529-535	1.8	34

14	Imaging the Pore Structure and Polytypic Intergrowths in Mesoporous Silica. *Journal of Physical Chemistry B*, **1998**, 102, 6933-6936	3.4	65
13	Ordering of ruthenium cluster carbonyls in mesoporous silica. *Science*, **1998**, 280, 705-8	33.3	215
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11	Dynamics of hydrogen dissociation on Pt{100}: Steering, screening and thermal roughening effects. *Journal of Chemical Physics*, **1997**, 106, 8896-8904	3.9	38
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