Xun-Lei Ding

List of Publications by Year in Descending Order

139 papers	4,151 citations	37 h-index	58 g-index
147 ext. papers	4,695 ext. citations	4.9 avg, IF	5.58 L-index

#	Paper	IF	Citations
139	Mechanochemical bromination of unburned carbon in fly ash and its mercury removal mechanism: DFT study. *Journal of Hazardous Materials*, **2022**, 423, 127198	12.8	3
138	Exploring the Effects of Ionic Defects on the Stability of CsPbI with a Deep Learning Potential.. *ChemPhysChem*, **2022**, e202100841	3.2	0
137	A descriptor for the structural stability of organic-inorganic hybrid perovskites based on binding mechanism in electronic structure.. *Journal of Molecular Modeling*, **2022**, 28, 80	2	1
136	Single-atom iron on penta-graphene assisted with non-bonding interaction as superior demercurizer: A DFT exploration. *Applied Surface Science*, **2022**, 590, 153060	6.7	0
135	Comparison of Nitrogen Activation on Trinuclear Niobium and Tungsten Sulfide Clusters Nb S and W S (n=0-3): A DFT Study.. *ChemPhysChem*, **2022**, e202200124	3.2	0
134	Facile N?N Bond Cleavage by Anionic Trimetallic Clusters V Ta C (x=0-3): A DFT Study. *ChemPhysChem*, **2021**,	3.2	5
133	Non-Dissociative Activation of Chemisorbed Dinitrogen on One or Two Vanadium Atoms Supported by a Mo S Cluster. *ChemPhysChem*, **2021**, 22, 1645-1654	3.2	7
132	Non-stoichiometric molybdenum sulfide clusters and their reactions with the hydrogen molecule. *Physical Chemistry Chemical Physics*, **2021**, 23, 347-355	3.6	4
131	A new perspective for evaluating the photoelectric performance of organic-inorganic hybrid perovskites based on the DFT calculations of excited states. *Physical Chemistry Chemical Physics*, **2021**, 23, 11548-11556	3.6	8
130	Infrared photodissociation spectroscopic and theoretical study of HnC4O+ (n = 1, 2) cation clusters in the gas phase. *Molecular Physics*, **2021**, 119, e1879301	1.7	
129	Design of (C3N2H5)(1-x)CsxPbI3 as a novel hybrid perovskite with strong stability and excellent photoelectric performance: A theoretical prediction. *Solar Energy Materials and Solar Cells*, **2021**, 233, 111401	6.4	3
128	Screening for lead-free inorganic double perovskites with suitable band gaps and high stability using combined machine learning and DFT calculation. *Applied Surface Science*, **2021**, 568, 150916	6.7	8
127	Oxygen Molecule Activation on Single-Atom Catalysts with Cu, Ag, and Au: A Cluster Model Study. *Journal of Materials Science and Chemical Engineering*, **2021**, 09, 46-59	0.3	
126	Identifying the active sites of carbonaceous surface for the adsorption of gaseous arsenic trioxide: A theoretical study. *Chemical Engineering Journal*, **2020**, 402, 125800	14.7	9
125	Cooperativity effects between regium-bonding and pnicogen-bonding interactions in ternary MF□□PH3O□□MF (M = Cu, Ag, Au): an ab initio study. *Molecular Physics*, **2020**, 118, e1784478	1.7	6
124	Methane activation by heteronuclear diatomic AuRh cation: comparison with homonuclear Au and Rh. *Physical Chemistry Chemical Physics*, **2020**, 22, 6231-6238	3.6	4
123	The effect of coordination environment on the kinetic and thermodynamic stability of single-atom iron catalysts. *Physical Chemistry Chemical Physics*, **2020**, 22, 3983-3989	3.6	23

122	Theoretical study on the stability of the complexes A□BX [A = CHNH, NHCHNH, NHCHOH; B = Sn, Pb; X = F, Cl, Br, I]. *Journal of Molecular Modeling*, **2020**, 26, 46	2	4
121	CO2 hydrogenation to formic acid over platinum cluster doped defective graphene: A DFT study. *Applied Surface Science*, **2020**, 517, 146200	6.7	11
120	Geometric structures, electronic characteristics, stabilities, catalytic activities, and descriptors of graphene-based single-atom catalysts. *Nano Materials Science*, **2020**, 2, 120-131	10.2	24
119	Theoretical prediction of graphene-based single-atom iron as a novel catalyst for catalytic oxidation of Hg0 by O2. *Applied Surface Science*, **2020**, 508, 145035	6.7	11
118	Theoretical study on double-atom catalysts supported with graphene for electroreduction of nitrogen into ammonia. *Electrochimica Acta*, **2020**, 335, 135667	6.7	35
117	Mechanism study on CO2 reforming of methane over platinum cluster doped graphene: A DFT calculation. *Molecular Catalysis*, **2020**, 497, 111205	3.3	5
116	Synthesis of 2D MoSSe semiconductor alloy by chemical vapor deposition.. *RSC Advances*, **2020**, 10, 42173-42177	3.7	4
115	A comprehensive exploration of mercury adsorption sites on the carbonaceous surface: A DFT study. *Fuel*, **2020**, 282, 118781	7.1	11
114	C/C Exchange in Activation/Coupling Reaction of Acetylene and Methane Mediated by Os: A Comparison with Ir, Pt, and Au. *Journal of Physical Chemistry Letters*, **2020**, 11, 8346-8351	6.4	3
113	Screening the activity of single-atom catalysts for the catalytic oxidation of sulfur dioxide with a kinetic activity model. *Chemical Communications*, **2020**, 56, 11657-11660	5.8	5
112	Simultaneous catalytic oxidation of nitric oxide and elemental mercury by single-atom Pd/g-C3N4 catalyst: A DFT study. *Molecular Catalysis*, **2020**, 488, 110901	3.3	11
111	Hg0 oxidation and SO3, Pb0, PbO, PbCl2 and As2O3 adsorption by graphene-based bimetallic catalyst ((Fe,Co)@N-GN): A DFT study. *Applied Surface Science*, **2019**, 496, 143686	6.7	20
110	Theoretical insights into the stability of perovskite clusters by studying water adsorption on (CH3NH3)4SnI6. *Solar Energy Materials and Solar Cells*, **2019**, 202, 110126	6.4	3
109	Directly catalytic reduction of NO without NH3 by single atom iron catalyst: A DFT calculation. *Fuel*, **2019**, 243, 262-270	7.1	54
108	Regium bonds formed by MX (M?Cu, Ag, Au; X?F, Cl, Br) with phosphine-oxide/phosphinous acid: comparisons between oxygen-shared and phosphine-shared complexes. *Molecular Physics*, **2019**, 117, 2443-2455	1.7	18
107	Adsorption behavior of mercuric oxide clusters on activated carbon and the effect of SO on this adsorption: a theoretical investigation. *Journal of Molecular Modeling*, **2019**, 25, 142	2	15
106	Activity of Atomically Precise Titania Nanoparticles in CO Oxidation. *Angewandte Chemie - International Edition*, **2019**, 58, 8002-8006	16.4	14
105	Density functional study of the adsorption of NO on Nin (n = 1, 2, 3 and 4) clusters doped functionalized graphene support. *Applied Surface Science*, **2019**, 481, 940-950	6.7	18

104	Adsorption characteristics of Co-anchored different graphene substrates toward O2 and NO molecules. *Applied Surface Science*, **2019**, 480, 779-791	6.7	18
103	Bimetallic sites supported on N-doped graphene ((Fe,Co)/N-GN) as a new catalyst for NO oxidation: A theoretical investigation. *Molecular Catalysis*, **2019**, 470, 56-66	3.3	23
102	Side-on-End-on Coordination of Dinitrogen on a Polynuclear Vanadium Nitride Cluster Anion [V N]. *Chemistry - A European Journal*, **2019**, 25, 16523	4.8	15
101	Methane Activation on (Au/Ag)1-Doped Vanadium Oxide Clusters. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2019**, 35, 1005-1013	3.8	6
100	Boron nitride supported NiCoP nanoparticles as noble metal-free catalyst for highly efficient hydrogen generation from ammonia borane. *International Journal of Hydrogen Energy*, **2019**, 44, 4764-4770	4.7	27
99	Highly efficient adsorption of benzothiophene from model fuel on a metal-organic framework modified with dodeca-tungstophosphoric acid. *Chemical Engineering Journal*, **2019**, 362, 30-40	14.7	21
98	The adsorption characteristics of As2O3, Pb0, PbO and PbCl2 on single atom iron adsorbent with graphene-based substrates. *Chemical Engineering Journal*, **2019**, 361, 304-313	14.7	44
97	Halogen bonds and metal bonds involving superalkalies M2OCN/M2NCO (M = Li, Na) complexes. *Structural Chemistry*, **2019**, 30, 965-977	1.8	11
96	Support effects on adsorption and catalytic activation of O in single atom iron catalysts with graphene-based substrates. *Physical Chemistry Chemical Physics*, **2018**, 20, 7333-7341	3.6	38
95	Small stoichiometric (MoS) clusters with the 1T phase. *Physical Chemistry Chemical Physics*, **2018**, 20, 6365-6373	3.6	22
94	Single-atom iron catalyst with single-vacancy graphene-based substrate as a novel catalyst for NO oxidation: a theoretical study. *Catalysis Science and Technology*, **2018**, 8, 4159-4168	5.5	55
93	Adsorption sensitivity of Fe decorated different graphene supports toward toxic gas molecules (CO and NO). *Applied Surface Science*, **2018**, 456, 351-359	6.7	39
92	The adsorption characteristics of mercury species on single atom iron catalysts with different graphene-based substrates. *Applied Surface Science*, **2018**, 455, 940-951	6.7	37
91	Support effects in single atom iron catalysts on adsorption characteristics of toxic gases (NO2, NH3, SO3 and H2S). *Applied Surface Science*, **2018**, 436, 585-595	6.7	55
90	Comparison of halide donators based on pi⋯M (M = Cu, Ag, Au), pi⋯H and pi⋯halogen bonds. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	6
89	14.1% efficiency hybrid planar-Si/organic heterojunction solar cells with SnO2 insertion layer. *Solar Energy*, **2018**, 174, 549-555	6.8	20
88	Mechanistic Variants in Methane Activation Mediated by Gold(I) Supported on Silicon Oxide Clusters. *Chemistry - A European Journal*, **2018**, 24, 17506-17512	4.8	6
87	A theoretical investigation on Cu/Ag/Au bonding in XHP?MY(X = H, CH, F, CN, NO; M = Cu, Ag, Au; Y = F, Cl, Br, I) complexes. *Journal of Chemical Physics*, **2018**, 148, 194106	3.9	16

86	First-Principles Study of Molecular Clusters Formed by Nitric Acid and Ammonia. *Journal of Physical Chemistry A*, **2017**, 121, 661-668	2.8	9
85	H Oxidation Mediated by Au-Doped Vanadium Oxide Cluster Cation AuVO: A Comparative Study with AuCeO. *Journal of Physical Chemistry A*, **2017**, 121, 4069-4075	2.8	4
84	A theoretical investigation on doping superalkali for triggering considerable nonlinear optical properties of Si C nanostructure. *Journal of Computational Chemistry*, **2017**, 38, 1574-1582	3.5	28
83	Theoretical study on the interactions of halogen-bonds and pnicogen-bonds in phosphine derivatives with Br2, BrCl, and BrF. *International Journal of Quantum Chemistry*, **2017**, 117, e25443	2.1	21
82	Theoretical research on heterogeneous reduction of N2O by char. *Applied Thermal Engineering*, **2017**, 126, 28-36	5.8	30
81	DFT investigations on AuVO3+, a barrier-free catalyst for oxidation of CO with O2. *Chemical Physics*, **2016**, 475, 69-76	2.3	5
80	Adsorption of a single gold or silver atom on vanadium oxide clusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 9497-503	3.6	10
79	Ligand-free nano-grain Cu2SnS3 as a potential cathode alternative for both cobalt and iodine redox electrolyte dye-sensitized solar cells. *Journal of Materials Chemistry A*, **2016**, 4, 14865-14876	13	17
78	Geometric and electronic properties of gold clusters doped with a single oxygen atom. *Physical Chemistry Chemical Physics*, **2016**, 18, 28960-28972	3.6	5
77	Investigation of protonated and sodiated leucine-enkephalin by hydrogen–deuterium exchange and theoretical calculations. *Analytical Methods*, **2015**, 7, 5551-5556	3.2	8
76	High reactivity of nanosized niobium oxide cluster cations in methane activation: A comparison with vanadium oxides. *Journal of Chemical Physics*, **2015**, 143, 124312	3.9	15
75	Hydrogen Atom Abstraction from CH4 by Nanosized Vanadium Oxide Cluster Cations. *Journal of Physical Chemistry C*, **2014**, 118, 24062-24071	3.8	19
74	Reactivity of oxygen radical anions bound to scandia nanoparticles in the gas phase: C-H bond activation. *Chemistry - A European Journal*, **2014**, 20, 1167-75	4.8	18
73	Benzodithiophene bridged dimeric perylene diimide amphiphiles as efficient solution-processed non-fullerene small molecules. *Polymer Chemistry*, **2013**, 4, 4631	4.9	64
72	Experimental and theoretical study of the reactions between MO2- (M = Fe, Co, Ni, Cu, and Zn) cluster anions and hydrogen sulfide. *Journal of Physical Chemistry A*, **2013**, 117, 8377-87	2.8	14
71	Reactions of $Sc_2O_4^-$ and $La_2O_4^-$ clusters with CO: A comparative study. *International Journal of Mass Spectrometry*, **2013**, 334, 1-7	1.9	12
70	The leverage effect of the relative strength of molecular solvophobicity vs. solvophilicity on fine-tuning nanomorphologies of perylene diimide bolaamphiphiles. *Soft Matter*, **2013**, 9, 3089	3.6	12
69	Theoretical characters and nature of the intermolecular lithium bonded interactions B?LiCN/LiNC (B=pyridine, furan and thiophene). *Computational and Theoretical Chemistry*, **2013**, 1017, 153-158	2	6

68	Reactivity of atomic oxygen radical anions bound to titania and zirconia nanoparticles in the gas phase: low-temperature oxidation of carbon monoxide. *Journal of the American Chemical Society*, **2013**, 135, 2991-8	16.4	68
67	Chromism based on supramolecular H-bonds. *Physical Chemistry Chemical Physics*, **2013**, 15, 11960-5	3.6	3
66	Collision-induced dissociation and infrared photodissociation studies of methane adsorption on V5O12(+) and V5O13(+) clusters. *Journal of Physical Chemistry A*, **2013**, 117, 2961-70	2.8	15
65	Activation of Multiple C?H Bonds Promoted by Gold in AuNbO3+ Clusters. *Angewandte Chemie*, **2013**, 125, 2504-2508	3.6	22
64	Fabrication and optical properties of pyrene-Eu hybrid materials. *Journal of Nanoscience and Nanotechnology*, **2013**, 13, 819-23	1.3	1
63	Activation of multiple C-H bonds promoted by gold in AuNbO(3)(+) clusters. *Angewandte Chemie - International Edition*, **2013**, 52, 2444-8	16.4	48
62	Facile synthesis of 1-bromo-7-alkoxyl perylene diimide dyes: toward unsymmetrical functionalizations at the 1,7-positions. *Tetrahedron Letters*, **2012**, 53, 1094-1097	2	42
61	C-H bond activation by oxygen-centered radicals over atomic clusters. *Accounts of Chemical Research*, **2012**, 45, 382-90	24.3	229
60	Density-functional global optimization of (La2O3)n clusters. *Journal of Chemical Physics*, **2012**, 137, 214311	3.9	46
59	Alkali metal cations control over nucleophilic substitutions on aromatic fused pyrimidine-2,4-[1H,3H]-diones: towards new PNA monomers. *Tetrahedron*, **2012**, 68, 8908-8915	2.4	12
58	Interaction of vanadium oxide cluster anions with water: an experimental and theoretical study on reactivity and mechanism. *Dalton Transactions*, **2012**, 41, 5562-70	4.3	22
57	Experimental and theoretical study of the reactions between vanadium oxide cluster cations and water. *Journal of Physical Chemistry A*, **2012**, 116, 2049-54	2.8	36
56	Synthesis and charge-transporting properties of electron-deficient CN2Fluorene based DA copolymers. *Polymer Chemistry*, **2012**, 3, 2170	4.9	24
55	Comparisons of the halogen-bonded and hydrogen-bonded complexes of furan, thiophene and pyridine with Lewis acids (ClF, HCl). *Computational and Theoretical Chemistry*, **2012**, 981, 1-6	2	19
54	Chiral structures and tunable magnetic moments in 3d transition metal doped Pt 6 clusters. *Chinese Physics B*, **2012**, 21, 093601	1.2	2
53	Experimental and Theoretical Study of the Reactions between Vanadium Oxide Cluster Cations and Hydrogen Sulfide. *Journal of Physical Chemistry C*, **2012**, 116, 9043-9048	3.8	17
52	Experimental and Theoretical Study of the Reactions between Manganese Oxide Cluster Anions and Hydrogen Sulfide. *Journal of Physical Chemistry C*, **2012**, 116, 24184-24192	3.8	23
51	Reactivity control of C-H bond activation over vanadium-silver bimetallic oxide cluster cations. *Chemistry - A European Journal*, **2012**, 18, 10998-1006	4.8	22

50	Structures and reactivity of oxygen-rich scandium cluster anions ScO(3-5)-. *ChemPhysChem*, **2012**, 13, 1282-8	3.2	29
49	N-(1-naphthyl) ethylenediamine dinitrate: a new matrix for negative ion MALDI-TOF MS analysis of small molecules. *Journal of the American Society for Mass Spectrometry*, **2012**, 23, 1454-60	3.5	38
48	Electronic structure and reactivity of a biradical cluster: Sc3O6(-). *Physical Chemistry Chemical Physics*, **2011**, 13, 10084-90	3.6	32
47	Experimental and theoretical study of hydrogen atom abstraction from n-butane by lanthanum oxide cluster anions. *Journal of Physical Chemistry A*, **2011**, 115, 10245-50	2.8	30
46	Experimental and Theoretical Study of the Reactions between Cerium Oxide Cluster Anions and Carbon Monoxide: Size-Dependent Reactivity of CenO2n+1□(n = 1□1). *Journal of Physical Chemistry C*, **2011**, 115, 13329-13337	3.8	71
45	Nearly monodispersed perylene nanotablets: easy fabrication and unique optical properties. *Journal of Nanoscience and Nanotechnology*, **2011**, 11, 10696-700	1.3	
44	Double-oxygen-atom transfer in reactions of Ce(m)O(2m)(+) (m=2-6) with C2H2. *ChemPhysChem*, **2011**, 12, 2110-7	3.2	25
43	Inside Cover: Double-Oxygen-Atom Transfer in Reactions of CemO2m+ (m=2□) with C2H2 (ChemPhysChem 11/2011). *ChemPhysChem*, **2011**, 12, 2046-2046	3.2	1
42	C□H activation on aluminum-vanadium bimetallic oxide cluster anions. *Chemistry - A European Journal*, **2011**, 17, 3449-57	4.8	52
41	Methane activation by yttrium-doped vanadium oxide cluster cations: local charge effects. *Chemistry - A European Journal*, **2011**, 17, 11728-33	4.8	64
40	Characterization and reactivity of oxygen-centred radicals over transition metal oxide clusters. *Physical Chemistry Chemical Physics*, **2011**, 13, 1925-38	3.6	149
39	Collision-induced dissociation and density functional theory studies of CO adsorption over zirconium oxide cluster ions: oxidative and nonoxidative adsorption. *Journal of Physical Chemistry A*, **2011**, 115, 5238-46	2.8	49
38	Self-assembled hollow nanospheres strongly enhance photoluminescence. *Journal of the American Chemical Society*, **2011**, 133, 11022-5	16.4	59
37	Ratiometric fluorescent sensor based on inhibition of resonance for detection of cadmium in aqueous solution and living cells. *Inorganic Chemistry*, **2011**, 50, 3680-90	5.1	114
36	Classification of VxOyq Clusters by □= 2y+q□x. *Chinese Journal of Chemical Physics*, **2011**, 24, 586-596	0.9	19
35	Experimental and Theoretical Study of Hydrogen Atom Abstraction from C2H6 and C4H10 by Zirconium Oxide Clusters Anions. *Chinese Journal of Chemical Physics*, **2010**, 23, 133-137	0.9	20
34	Hydrogen-atom abstraction from methane by stoichiometric early transition metal oxide cluster cations. *Chemical Communications*, **2010**, 46, 1736-8	5.8	93
33	Characterization of mononuclear oxygen-centered radical (O(-*)) in Zr(2)O(8)(-) cluster. *Journal of Physical Chemistry A*, **2010**, 114, 10024-7	2.8	32

32	Experimental and Theoretical Study of the Reactions between Vanadium□Silicon Heteronuclear Oxide Cluster Anions with n-Butane. *Journal of Physical Chemistry C*, **2010**, 114, 12271-12279	3.8	71
31	Hydrogen-Assisted Transformation of CO2 on Nickel: The Role of Formate and Carbon Monoxide. *Journal of Physical Chemistry Letters*, **2010**, 1, 402-406	6.4	99
30	Active sites of stoichiometric cerium oxide cations (CemO2m+) probed by reactions with carbon monoxide and small hydrocarbon molecules. *Physical Chemistry Chemical Physics*, **2010**, 12, 3984-97	3.6	123
29	Methane activation by V3PO10(□) and V4O10(□) clusters: a comparative study. *Physical Chemistry Chemical Physics*, **2010**, 12, 12223-8	3.6	82
28	Theoretical Investigation of the Selective Oxidation of Methanol to Formaldehyde on Vanadium Oxide Species Supported on Silica: Umbrella Model. *Journal of Physical Chemistry C*, **2010**, 114, 3161-3169	3.8	26
27	Transition metal oxide clusters with character of oxygen-centered radical: a DFT study. *Theoretical Chemistry Accounts*, **2010**, 127, 449-465	1.9	113
26	Room-temperature methane activation by a bimetallic oxide cluster . *Chemical Physics Letters*, **2010** , 489, 25-29	2.5	91
25	A theoretical study on the mechanism of C(2)H(4) oxidation over a neutral V(3)O(8) cluster. *ChemPhysChem*, **2010**, 11, 1718-25	3.2	23
24	Hydrogen-atom abstraction from methane by stoichiometric vanadium-silicon heteronuclear oxide cluster cations. *Chemistry - A European Journal*, **2010**, 16, 11463-70	4.8	82
23	Inside Cover: Hydrogen-Atom Abstraction from Methane by Stoichiometric Vanadium□Silicon Heteronuclear Oxide Cluster Cations (Chem. Eur. J. 37/2010). *Chemistry - A European Journal*, **2010**, 16, 11194-11194	4.8	
22	Density functional study on cage and noncage (Fe2O3)n clusters. *Journal of Chemical Physics*, **2009**, 130, 014303	3.9	42
21	Experimental and Theoretical Study of Hydrogen Atom Abstraction from Ethylene by Stoichiometric Zirconium Oxide Clusters. *Chinese Journal of Chemical Physics*, **2009**, 22, 635-641	0.9	13
20	Theoretical study of partial oxidation of ethylene by vanadium trioxide cluster cation. *Science Bulletin*, **2009**, 54, 2814-2821	10.6	10
19	Formation, distribution, and structures of oxygen-rich iron and cobalt oxide clusters. *International Journal of Mass Spectrometry*, **2009**, 281, 72-78	1.9	63
18	C=C bond cleavage on neutral VO3(V2O5)n clusters. *Journal of the American Chemical Society*, **2009**, 131, 1057-66	16.4	68
17	Ground state structures of Fe(2)O(4-6)(+) clusters probed by reactions with N(2). *Journal of Physical Chemistry A*, **2009**, 113, 5302-9	2.8	44
16	Theoretical study of intermolecular interactions in meso-tetraphenylporphyrin diacid dimer (H4TPPCl2)2. *Physical Chemistry Chemical Physics*, **2009**, 11, 2543-52	3.6	11
15	Partial oxidation of propylene catalyzed by VO3 clusters: a density functional theory study. *Journal of Physical Chemistry A*, **2008**, 112, 5984-93	2.8	44

14	Carbon dioxide hydrogenation on Ni(110). *Journal of the American Chemical Society*, **2008**, 130, 11417-22	16.4	132
13	Multicolor emission from large-area porous thin films constructed of nanowires of small organic molecules. *Nanotechnology*, **2008**, 19, 505703	3.4	2
12	Theoretical study of molecular nitrogen adsorption on Wn clusters. *Computational and Theoretical Chemistry*, **2008**, 867, 17-21		18
11	Modeling adsorption of CO2 on Ni(110) surface. *Materials Science and Engineering C*, **2007**, 27, 1355-1358	8.3	26
10	Conduction mechanism of Aviram-Ratner rectifiers with single pyridine-sigma-C(60) oligomers. *Journal of Physical Chemistry B*, **2006**, 110, 24505-12	3.4	20
9	Theoretical study of molecular nitrogen adsorption on Au clusters. *Computational and Theoretical Chemistry*, **2005**, 755, 9-17		27
8	Density functional theory study of Wn (n=2-4) clusters. *Computational and Theoretical Chemistry*, **2005**, 757, 113-118		27
7	DENSITY FUNCTIONAL THEORY STUDY OF W5 CLUSTERS. *International Journal of Modern Physics B*, **2005**, 19, 2427-2432	1.1	8
6	A theoretical study of the Y(mathsf{_{3}})O clusters. *European Physical Journal D*, **2004**, 29, 27-31	1.3	10
5	Assignment of photoelectron spectra of AunO2- (n=2,4,6) clusters. *Journal of Chemical Physics*, **2004**, 121, 621-3	3.9	17
4	Theoretical study of nitric oxide adsorption on Au clusters. *Journal of Chemical Physics*, **2004**, 121, 2558-62	3.9	74
3	Adsorption energies of molecular oxygen on Au clusters. *Journal of Chemical Physics*, **2004**, 120, 9594-600	3.9	149
2	First-Principles Study on the Stability and Electronic Properties of Dion□Jacobson Halide A?(MA)n□BnX3n+1 Perovskites. *Journal of Physical Chemistry C*,	3.8	3
1	Exploring trimetallic clusters containing alkali and alkaline earth metal atoms with high activity for nitrogen activation. *Structural Chemistry*,1	1.8	0