

# Xun-Lei Ding

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	C-H bond activation by oxygen-centered radicals over atomic clusters. <i>Accounts of Chemical Research</i> , <b>2012</b> , 45, 382-90	24.3	229
138	Characterization and reactivity of oxygen-centred radicals over transition metal oxide clusters. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 1925-38	3.6	149
137	Adsorption energies of molecular oxygen on Au clusters. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 9594-6009	3.9	149
136	Carbon dioxide hydrogenation on Ni(110). <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 11417-22	16.4	132
135	Active sites of stoichiometric cerium oxide cations (Ce <sub>m</sub> O <sub>2m+</sub> ) probed by reactions with carbon monoxide and small hydrocarbon molecules. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 3984-97	3.6	123
134	Ratiometric fluorescent sensor based on inhibition of resonance for detection of cadmium in aqueous solution and living cells. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 3680-90	5.1	114
133	Transition metal oxide clusters with character of oxygen-centered radical: a DFT study. <i>Theoretical Chemistry Accounts</i> , <b>2010</b> , 127, 449-465	1.9	113
132	Hydrogen-Assisted Transformation of CO <sub>2</sub> on Nickel: The Role of Formate and Carbon Monoxide. <i>Journal of Physical Chemistry Letters</i> , <b>2010</b> , 1, 402-406	6.4	99
131	Hydrogen-atom abstraction from methane by stoichiometric early transition metal oxide cluster cations. <i>Chemical Communications</i> , <b>2010</b> , 46, 1736-8	5.8	93
130	Room-temperature methane activation by a bimetallic oxide cluster. <i>Chemical Physics Letters</i> , <b>2010</b> , 489, 25-29	2.5	91
129	Methane activation by V <sub>3</sub> PO <sub>10</sub> (H <sup>+</sup> ) and V <sub>4</sub> O <sub>10</sub> (H <sup>+</sup> ) clusters: a comparative study. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 12223-8	3.6	82
128	Hydrogen-atom abstraction from methane by stoichiometric vanadium-silicon heteronuclear oxide cluster cations. <i>Chemistry - A European Journal</i> , <b>2010</b> , 16, 11463-70	4.8	82
127	Theoretical study of nitric oxide adsorption on Au clusters. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 2558-62	6.2	74
126	Experimental and Theoretical Study of the Reactions between Cerium Oxide Cluster Anions and Carbon Monoxide: Size-Dependent Reactivity of Ce <sub>n</sub> O <sub>2n+1</sub> <sup>-</sup> (n = 1-11). <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 13329-13337	3.8	71
125	Experimental and Theoretical Study of the Reactions between Vanadium-Silicon Heteronuclear Oxide Cluster Anions with n-Butane. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 12271-12279	3.8	71
124	Reactivity of atomic oxygen radical anions bound to titania and zirconia nanoparticles in the gas phase: low-temperature oxidation of carbon monoxide. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 2991-8	16.4	68
123	C=C bond cleavage on neutral VO <sub>3</sub> (V <sub>2</sub> O <sub>5</sub> ) <sub>n</sub> clusters. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 1057-66	16.4	68

122	Benzodithiophene bridged dimeric perylene diimide amphiphiles as efficient solution-processed non-fullerene small molecules. <i>Polymer Chemistry</i> , <b>2013</b> , 4, 4631	4.9	64
121	Methane activation by yttrium-doped vanadium oxide cluster cations: local charge effects. <i>Chemistry - A European Journal</i> , <b>2011</b> , 17, 11728-33	4.8	64
120	Formation, distribution, and structures of oxygen-rich iron and cobalt oxide clusters. <i>International Journal of Mass Spectrometry</i> , <b>2009</b> , 281, 72-78	1.9	63
119	Self-assembled hollow nanospheres strongly enhance photoluminescence. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 11022-5	16.4	59
118	Single-atom iron catalyst with single-vacancy graphene-based substrate as a novel catalyst for NO oxidation: a theoretical study. <i>Catalysis Science and Technology</i> , <b>2018</b> , 8, 4159-4168	5.5	55
117	Support effects in single atom iron catalysts on adsorption characteristics of toxic gases (NO <sub>2</sub> , NH <sub>3</sub> , SO <sub>3</sub> and H <sub>2</sub> S). <i>Applied Surface Science</i> , <b>2018</b> , 436, 585-595	6.7	55
116	Directly catalytic reduction of NO without NH <sub>3</sub> by single atom iron catalyst: A DFT calculation. <i>Fuel</i> , <b>2019</b> , 243, 262-270	7.1	54
115	C <sub>6</sub> H <sub>6</sub> activation on aluminum-vanadium bimetallic oxide cluster anions. <i>Chemistry - A European Journal</i> , <b>2011</b> , 17, 3449-57	4.8	52
114	Collision-induced dissociation and density functional theory studies of CO adsorption over zirconium oxide cluster ions: oxidative and nonoxidative adsorption. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 5238-46	2.8	49
113	Activation of multiple C-H bonds promoted by gold in AuNbO(3)(+) clusters. <i>Angewandte Chemie - International Edition</i> , <b>2013</b> , 52, 2444-8	16.4	48
112	Density-functional global optimization of (La <sub>2</sub> O <sub>3</sub> ) <sub>n</sub> clusters. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 21433-4	3.4	46
111	Ground state structures of Fe(2)O(4-6)(+) clusters probed by reactions with N(2). <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 5302-9	2.8	44
110	Partial oxidation of propylene catalyzed by VO <sub>3</sub> clusters: a density functional theory study. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 5984-93	2.8	44
109	The adsorption characteristics of As <sub>2</sub> O <sub>3</sub> , PbO, PbO and PbCl <sub>2</sub> on single atom iron adsorbent with graphene-based substrates. <i>Chemical Engineering Journal</i> , <b>2019</b> , 361, 304-313	14.7	44
108	Facile synthesis of 1-bromo-7-alkoxyl perylene diimide dyes: toward unsymmetrical functionalizations at the 1,7-positions. <i>Tetrahedron Letters</i> , <b>2012</b> , 53, 1094-1097	2	42
107	Density functional study on cage and noncage (Fe <sub>2</sub> O <sub>3</sub> ) <sub>n</sub> clusters. <i>Journal of Chemical Physics</i> , <b>2009</b> , 130, 014303	3.9	42
106	Adsorption sensitivity of Fe decorated different graphene supports toward toxic gas molecules (CO and NO). <i>Applied Surface Science</i> , <b>2018</b> , 456, 351-359	6.7	39
105	Support effects on adsorption and catalytic activation of O in single atom iron catalysts with graphene-based substrates. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 7333-7341	3.6	38

104	N-(1-naphthyl) ethylenediamine dinitrate: a new matrix for negative ion MALDI-TOF MS analysis of small molecules. <i>Journal of the American Society for Mass Spectrometry</i> , <b>2012</b> , 23, 1454-60	3.5	38
103	The adsorption characteristics of mercury species on single atom iron catalysts with different graphene-based substrates. <i>Applied Surface Science</i> , <b>2018</b> , 455, 940-951	6.7	37
102	Experimental and theoretical study of the reactions between vanadium oxide cluster cations and water. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 2049-54	2.8	36
101	Theoretical study on double-atom catalysts supported with graphene for electroreduction of nitrogen into ammonia. <i>Electrochimica Acta</i> , <b>2020</b> , 335, 135667	6.7	35
100	Electronic structure and reactivity of a biradical cluster: Sc <sub>3</sub> O <sub>6</sub> (-). <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 10084-90	3.6	32
99	Characterization of mononuclear oxygen-centered radical (O(-*)) in Zr(2)O(8)(-) cluster. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 10024-7	2.8	32
98	Theoretical research on heterogeneous reduction of N <sub>2</sub> O by char. <i>Applied Thermal Engineering</i> , <b>2017</b> , 126, 28-36	5.8	30
97	Experimental and theoretical study of hydrogen atom abstraction from n-butane by lanthanum oxide cluster anions. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 10245-50	2.8	30
96	Structures and reactivity of oxygen-rich scandium cluster anions ScO(3-5)-. <i>ChemPhysChem</i> , <b>2012</b> , 13, 1282-8	3.2	29
95	A theoretical investigation on doping superalkali for triggering considerable nonlinear optical properties of Si C nanostructure. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 1574-1582	3.5	28
94	Theoretical study of molecular nitrogen adsorption on Au clusters. <i>Computational and Theoretical Chemistry</i> , <b>2005</b> , 755, 9-17		27
93	Density functional theory study of W <sub>n</sub> (n=2-4) clusters. <i>Computational and Theoretical Chemistry</i> , <b>2005</b> , 757, 113-118		27
92	Boron nitride supported NiCoP nanoparticles as noble metal-free catalyst for highly efficient hydrogen generation from ammonia borane. <i>International Journal of Hydrogen Energy</i> , <b>2019</b> , 44, 4764-4770	6.7	27
91	Theoretical Investigation of the Selective Oxidation of Methanol to Formaldehyde on Vanadium Oxide Species Supported on Silica: Umbrella Model. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 3161-3169	3.8	26
90	Modeling adsorption of CO <sub>2</sub> on Ni(110) surface. <i>Materials Science and Engineering C</i> , <b>2007</b> , 27, 1355-1358	3.3	26
89	Double-oxygen-atom transfer in reactions of Ce(m)O(2m)(+) (m=2-6) with C <sub>2</sub> H <sub>2</sub> . <i>ChemPhysChem</i> , <b>2011</b> , 12, 2110-7	3.2	25
88	Synthesis and charge-transporting properties of electron-deficient CN <sub>2</sub> fluorene based D-A copolymers. <i>Polymer Chemistry</i> , <b>2012</b> , 3, 2170	4.9	24
87	Geometric structures, electronic characteristics, stabilities, catalytic activities, and descriptors of graphene-based single-atom catalysts. <i>Nano Materials Science</i> , <b>2020</b> , 2, 120-131	10.2	24

86	Bimetallic sites supported on N-doped graphene ((Fe,Co)/N-GN) as a new catalyst for NO oxidation: A theoretical investigation. <i>Molecular Catalysis</i> , <b>2019</b> , 470, 56-66	3.3	23
85	The effect of coordination environment on the kinetic and thermodynamic stability of single-atom iron catalysts. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 3983-3989	3.6	23
84	Experimental and Theoretical Study of the Reactions between Manganese Oxide Cluster Anions and Hydrogen Sulfide. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 24184-24192	3.8	23
83	A theoretical study on the mechanism of C(2)H(4) oxidation over a neutral V(3)O(8) cluster. <i>ChemPhysChem</i> , <b>2010</b> , 11, 1718-25	3.2	23
82	Small stoichiometric (MoS) clusters with the 1T phase. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 6365-6373	3.6	22
81	Interaction of vanadium oxide cluster anions with water: an experimental and theoretical study on reactivity and mechanism. <i>Dalton Transactions</i> , <b>2012</b> , 41, 5562-70	4.3	22
80	Reactivity control of C-H bond activation over vanadium-silver bimetallic oxide cluster cations. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 10998-1006	4.8	22
79	Activation of Multiple C-H Bonds Promoted by Gold in AuNbO <sub>3</sub> <sup>+</sup> Clusters. <i>Angewandte Chemie</i> , <b>2013</b> , 125, 2504-2508	3.6	22
78	Theoretical study on the interactions of halogen-bonds and pnictogen-bonds in phosphine derivatives with Br <sub>2</sub> , BrCl, and BrF. <i>International Journal of Quantum Chemistry</i> , <b>2017</b> , 117, e25443	2.1	21
77	Highly efficient adsorption of benzothiophene from model fuel on a metal-organic framework modified with dodeca-tungstophosphoric acid. <i>Chemical Engineering Journal</i> , <b>2019</b> , 362, 30-40	14.7	21
76	Hg <sup>0</sup> oxidation and SO <sub>3</sub> , Pb <sup>0</sup> , PbO, PbCl <sub>2</sub> and As <sub>2</sub> O <sub>3</sub> adsorption by graphene-based bimetallic catalyst ((Fe,Co)@N-GN): A DFT study. <i>Applied Surface Science</i> , <b>2019</b> , 496, 143686	6.7	20
75	Experimental and Theoretical Study of Hydrogen Atom Abstraction from C <sub>2</sub> H <sub>6</sub> and C <sub>4</sub> H <sub>10</sub> by Zirconium Oxide Clusters Anions. <i>Chinese Journal of Chemical Physics</i> , <b>2010</b> , 23, 133-137	0.9	20
74	Conduction mechanism of Aviram-Ratner rectifiers with single pyridine-sigma-C(60) oligomers. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 24505-12	3.4	20
73	14.1% efficiency hybrid planar-Si/organic heterojunction solar cells with SnO <sub>2</sub> insertion layer. <i>Solar Energy</i> , <b>2018</b> , 174, 549-555	6.8	20
72	Hydrogen Atom Abstraction from CH <sub>4</sub> by Nanosized Vanadium Oxide Cluster Cations. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 24062-24071	3.8	19
71	Comparisons of the halogen-bonded and hydrogen-bonded complexes of furan, thiophene and pyridine with Lewis acids (ClF, HCl). <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 981, 1-6	2	19
70	Classification of V <sub>x</sub> O <sub>y</sub> Clusters by $\frac{1}{2}2y+q\frac{1}{2}x$ . <i>Chinese Journal of Chemical Physics</i> , <b>2011</b> , 24, 586-596	0.9	19
69	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. <i>Molecular Physics</i> , <b>2019</b> , 117, 2443-2455	1.7	18

68	Density functional study of the adsorption of NO on Nin (n = 1, 2, 3 and 4) clusters doped functionalized graphene support. <i>Applied Surface Science</i> , <b>2019</b> , 481, 940-950	6.7	18
67	Adsorption characteristics of Co-anchored different graphene substrates toward O2 and NO molecules. <i>Applied Surface Science</i> , <b>2019</b> , 480, 779-791	6.7	18
66	Reactivity of oxygen radical anions bound to scandia nanoparticles in the gas phase: C-H bond activation. <i>Chemistry - A European Journal</i> , <b>2014</b> , 20, 1167-75	4.8	18
65	Theoretical study of molecular nitrogen adsorption on Wn clusters. <i>Computational and Theoretical Chemistry</i> , <b>2008</b> , 867, 17-21		18
64	Experimental and Theoretical Study of the Reactions between Vanadium Oxide Cluster Cations and Hydrogen Sulfide. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 9043-9048	3.8	17
63	Assignment of photoelectron spectra of AunO2 <sup>-</sup> (n=2,4,6) clusters. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 621-3	3.9	17
62	Ligand-free nano-grain Cu2SnS3 as a potential cathode alternative for both cobalt and iodine redox electrolyte dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 14865-14876	13	17
61	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. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 194106	3.9	16
60	Adsorption behavior of mercuric oxide clusters on activated carbon and the effect of SO on this adsorption: a theoretical investigation. <i>Journal of Molecular Modeling</i> , <b>2019</b> , 25, 142	2	15
59	Side-on-End-on Coordination of Dinitrogen on a Polynuclear Vanadium Nitride Cluster Anion [V <sub>n</sub> N <sub>n</sub> ]. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 16523	4.8	15
58	High reactivity of nanosized niobium oxide cluster cations in methane activation: A comparison with vanadium oxides. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 124312	3.9	15
57	Collision-induced dissociation and infrared photodissociation studies of methane adsorption on V5O12(+) and V5O13(+) clusters. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 2961-70	2.8	15
56	Activity of Atomically Precise Titania Nanoparticles in CO Oxidation. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 8002-8006	16.4	14
55	Experimental and theoretical study of the reactions between MO2 <sup>-</sup> (M = Fe, Co, Ni, Cu, and Zn) cluster anions and hydrogen sulfide. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 8377-87	2.8	14
54	Experimental and Theoretical Study of Hydrogen Atom Abstraction from Ethylene by Stoichiometric Zirconium Oxide Clusters. <i>Chinese Journal of Chemical Physics</i> , <b>2009</b> , 22, 635-641	0.9	13
53	Reactions of Sc2O4 <sup>+</sup> and La2O4 <sup>+</sup> clusters with CO: A comparative study. <i>International Journal of Mass Spectrometry</i> , <b>2013</b> , 334, 1-7	1.9	12
52	The leverage effect of the relative strength of molecular solvophobicity vs. solvophilicity on fine-tuning nanomorphologies of perylene diimide bolaamphiphiles. <i>Soft Matter</i> , <b>2013</b> , 9, 3089	3.6	12
51	Alkali metal cations control over nucleophilic substitutions on aromatic fused pyrimidine-2,4-[1H,3H]-diones: towards new PNA monomers. <i>Tetrahedron</i> , <b>2012</b> , 68, 8908-8915	2.4	12

50	CO <sub>2</sub> hydrogenation to formic acid over platinum cluster doped defective graphene: A DFT study. <i>Applied Surface Science</i> , <b>2020</b> , 517, 146200	6.7	11
49	Theoretical study of intermolecular interactions in meso-tetraphenylporphyrin diacid dimer (H <sub>4</sub> TPPCl <sub>2</sub> ) <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 2543-52	3.6	11
48	Theoretical prediction of graphene-based single-atom iron as a novel catalyst for catalytic oxidation of Hg <sup>0</sup> by O <sub>2</sub> . <i>Applied Surface Science</i> , <b>2020</b> , 508, 145035	6.7	11
47	A comprehensive exploration of mercury adsorption sites on the carbonaceous surface: A DFT study. <i>Fuel</i> , <b>2020</b> , 282, 118781	7.1	11
46	Halogen bonds and metal bonds involving superalkalies M <sub>2</sub> OCN/M <sub>2</sub> NCO (M = Li, Na) complexes. <i>Structural Chemistry</i> , <b>2019</b> , 30, 965-977	1.8	11
45	Simultaneous catalytic oxidation of nitric oxide and elemental mercury by single-atom Pd/g-C <sub>3</sub> N <sub>4</sub> catalyst: A DFT study. <i>Molecular Catalysis</i> , <b>2020</b> , 488, 110901	3.3	11
44	Adsorption of a single gold or silver atom on vanadium oxide clusters. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 9497-503	3.6	10
43	Theoretical study of partial oxidation of ethylene by vanadium trioxide cluster cation. <i>Science Bulletin</i> , <b>2009</b> , 54, 2814-2821	10.6	10
42	A theoretical study of the Y( $\text{O}_3$ ) clusters. <i>European Physical Journal D</i> , <b>2004</b> , 29, 27-31	1.3	10
41	First-Principles Study of Molecular Clusters Formed by Nitric Acid and Ammonia. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 661-668	2.8	9
40	Identifying the active sites of carbonaceous surface for the adsorption of gaseous arsenic trioxide: A theoretical study. <i>Chemical Engineering Journal</i> , <b>2020</b> , 402, 125800	14.7	9
39	Investigation of protonated and sodiated leucine-enkephalin by hydrogen-deuterium exchange and theoretical calculations. <i>Analytical Methods</i> , <b>2015</b> , 7, 5551-5556	3.2	8
38	DENSITY FUNCTIONAL THEORY STUDY OF W <sub>5</sub> CLUSTERS. <i>International Journal of Modern Physics B</i> , <b>2005</b> , 19, 2427-2432	1.1	8
37	A new perspective for evaluating the photoelectric performance of organic-inorganic hybrid perovskites based on the DFT calculations of excited states. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 11548-11556	3.6	8
36	Screening for lead-free inorganic double perovskites with suitable band gaps and high stability using combined machine learning and DFT calculation. <i>Applied Surface Science</i> , <b>2021</b> , 568, 150916	6.7	8
35	Non-Dissociative Activation of Chemisorbed Dinitrogen on One or Two Vanadium Atoms Supported by a Mo S Cluster. <i>ChemPhysChem</i> , <b>2021</b> , 22, 1645-1654	3.2	7
34	Cooperativity effects between regium-bonding and pnictogen-bonding interactions in ternary MF <sub>3</sub> PH <sub>3</sub> O <sub>2</sub> MF (M = Cu, Ag, Au): an ab initio study. <i>Molecular Physics</i> , <b>2020</b> , 118, e1784478	1.7	6
33	Theoretical characters and nature of the intermolecular lithium bonded interactions B <sub>2</sub> LiCN/LiNC (B=pyridine, furan and thiophene). <i>Computational and Theoretical Chemistry</i> , <b>2013</b> , 1017, 153-158	2	6

- 32 Methane Activation on (Au/Ag)<sub>1</sub>-Doped Vanadium Oxide Clusters. *Wuli Huaxue Xuebao/Acta Physico - Chimica Sinica*, **2019**, 35, 1005-1013 3.8 6
- 31 Comparison of halide donators based on  $\pi$ - $\pi^*$  (M = Cu, Ag, Au),  $\pi$ -H and  $\pi$ -halogen bonds. *Theoretical Chemistry Accounts*, **2018**, 137, 1 1.9 6
- 30 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
- 29 DFT investigations on AuVO<sub>3</sub><sup>+</sup>, a barrier-free catalyst for oxidation of CO with O<sub>2</sub>. *Chemical Physics*, **2016**, 475, 69-76 2.3 5
- 28 Facile N≡N Bond Cleavage by Anionic Trimetallic Clusters V Ta C (x=0-3): A DFT Study. *ChemPhysChem*, **2021**, 3.2 5
- 27 Mechanism study on CO<sub>2</sub> reforming of methane over platinum cluster doped graphene: A DFT calculation. *Molecular Catalysis*, **2020**, 497, 111205 3.3 5
- 26 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
- 25 Geometric and electronic properties of gold clusters doped with a single oxygen atom. *Physical Chemistry Chemical Physics*, **2016**, 18, 28960-28972 3.6 5
- 24 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
- 23 Methane activation by heteronuclear diatomic AuRh cation: comparison with homonuclear Au and Rh. *Physical Chemistry Chemical Physics*, **2020**, 22, 6231-6238 3.6 4
- 22 Theoretical study on the stability of the complexes A<sub>3</sub>BX [A = CHNH, NHCHNH, NHCHOH; B = Sn, Pb; X = F, Cl, Br, I]. *Journal of Molecular Modeling*, **2020**, 26, 46 2 4
- 21 Synthesis of 2D MoSSe semiconductor alloy by chemical vapor deposition.. *RSC Advances*, **2020**, 10, 42173-42177 3.7 4
- 20 Non-stoichiometric molybdenum sulfide clusters and their reactions with the hydrogen molecule. *Physical Chemistry Chemical Physics*, **2021**, 23, 347-355 3.6 4
- 19 Theoretical insights into the stability of perovskite clusters by studying water adsorption on (CH<sub>3</sub>NH<sub>3</sub>)<sub>4</sub>SnI<sub>6</sub>. *Solar Energy Materials and Solar Cells*, **2019**, 202, 110126 6.4 3
- 18 Chromism based on supramolecular H-bonds. *Physical Chemistry Chemical Physics*, **2013**, 15, 11960-5 3.6 3
- 17 First-Principles Study on the Stability and Electronic Properties of Dion-Jacobson Halide A<sub>2</sub>(MA)<sub>n</sub>B<sub>n</sub>X<sub>3n+1</sub> Perovskites. *Journal of Physical Chemistry C*, 3.8 3
- 16 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
- 15 Design of (C<sub>3</sub>N<sub>2</sub>H<sub>5</sub>)(1-x)Cs<sub>x</sub>PbI<sub>3</sub> 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

14	Mechanochemical bromination of unburned carbon in fly ash and its mercury removal mechanism: DFT study. <i>Journal of Hazardous Materials</i> , <b>2022</b> , 423, 127198	12.8	3
13	Chiral structures and tunable magnetic moments in 3d transition metal doped Pt 6 clusters. <i>Chinese Physics B</i> , <b>2012</b> , 21, 093601	1.2	2
12	Multicolor emission from large-area porous thin films constructed of nanowires of small organic molecules. <i>Nanotechnology</i> , <b>2008</b> , 19, 505703	3.4	2
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10	Inside Cover: Double-Oxygen-Atom Transfer in Reactions of $\text{Ce}(\text{OH})_3^m+$ ( $m=2,3$ ) with $\text{C}_2\text{H}_2$ (ChemPhysChem 11/2011). <i>ChemPhysChem</i> , <b>2011</b> , 12, 2046-2046	3.2	1
9	A descriptor for the structural stability of organic-inorganic hybrid perovskites based on binding mechanism in electronic structure.. <i>Journal of Molecular Modeling</i> , <b>2022</b> , 28, 80	2	1
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7	Exploring trimetallic clusters containing alkali and alkaline earth metal atoms with high activity for nitrogen activation. <i>Structural Chemistry</i> , 1	1.8	0
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