Xin Xu

List of Publications by Year in Descending Order

196 papers	9,522 citations	42 h-index	94 g-index
217 ext. papers	10,824 ext. citations	5.6 avg, IF	6.37 L-index

#	Paper	IF	Citations
196	A general principle enabling the design of ultrastable metal nanocatalysts. *Science China Chemistry*, **2022**, 65, 641-642	7.9	
195	Structure-Reactivity Relationship for Nano-Catalysts in the Hydrogenation/Dehydrogenation Controlled Reaction Systems. *Angewandte Chemie*, **2021**, 133, 26546	3.6	0
194	Structure-Reactivity Relationship for Nano-Catalysts in the Hydrogenation/Dehydrogenation Controlled Reaction Systems. *Angewandte Chemie - International Edition*, **2021**, 60, 26342-26345	16.4	1
193	Exploring the Limits of the XYG3-Type Doubly Hybrid Approximations for the Main-Group Chemistry: The xDH@B3LYP Model. *Journal of Physical Chemistry Letters*, **2021**, 12, 2638-2644	6.4	6
192	Dynamic and Intermediate-Specific Local Coverage Controls the Syngas Conversion on Rh(111) Surfaces: An Operando Theoretical Analysis. *ACS Catalysis*, **2021**, 11, 3830-3841	13.1	3
191	Comprehensive Analysis of the Prognosis and Correlations With Immune Infiltration of S100 Protein Family Members in Hepatocellular Carcinoma. *Frontiers in Genetics*, **2021**, 12, 648156	4.5	6
190	Doubly Hybrid Functionals Close to Chemical Accuracy for Both Finite and Extended Systems: Implementation and Test of XYG3 and XYGJ-OS. *Jacs Au*, **2021**, 1, 543-549		4
189	A Good Prediction of the Overall Reaction Rate May Not Mean a Correct Description of the Reaction Kinetics: A Case Study for CO Oxidation on RuO2(110) Surfaces. *Journal of Physical Chemistry C*, **2021**, 125, 9169-9177	3.8	2
188	Perturbation theory made efficient and effective for predictions of ionization potential and electron affinity. *Journal of Chemical Physics*, **2021**, 154, 174101	3.9	0
187	Conformational Features of Ras: Key Hydrogen-Bonding Interactions of Gln61 in the Intermediate State during GTP Hydrolysis. *Journal of Physical Chemistry B*, **2021**, 125, 8805-8813	3.4	6
186	Second-Order Analytic Derivatives for XYG3 Type of Doubly Hybrid Density Functionals: Theory, Implementation, and Application to Harmonic and Anharmonic Vibrational Frequency Calculations. *Journal of Chemical Theory and Computation*, **2021**, 17, 4860-4871	6.4	0
185	Coverage-Dependent Microkinetics in Heterogeneous Catalysis Powered by the Maximum Rate Analysis. *ACS Catalysis*, **2021**, 11, 9333-9344	13.1	3
184	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of SIE and NCE. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11,	7.9	12
183	Highly Efficient and Selective N-Formylation of Amines with CO2 and H2 Catalyzed by Porous Organometallic Polymers. *Angewandte Chemie*, **2021**, 133, 4171-4178	3.6	1
182	Highly Efficient and Selective N-Formylation of Amines with CO and H Catalyzed by Porous Organometallic Polymers. *Angewandte Chemie - International Edition*, **2021**, 60, 4125-4132	16.4	14
181	2,2-difluorovinyl benzoates for diverse synthesis of gem-difluoroenol ethers by Ni-catalyzed cross-coupling reactions. *Nature Communications*, **2021**, 12, 412	17.4	6
180	Prediction of Heats of Formation of Polycyclic Saturated Hydrocarbons Using the XYG3 Double Hybrid Functionals. *Springer Series in Materials Science*, **2021**, 245-255	0.9	

179	New Insights into the Ion-Specific Behaviors and Design Strategies for Ion□Interactions. *CCS Chemistry*, **2021**, 3, 904-915	7.2	6
178	Rhodium-Catalyzed Regiodivergent Synthesis of Alkylboronates via Deoxygenative Hydroboration of Aryl Ketones: Mechanism and Origin of Selectivities. *ACS Catalysis*, **2021**, 11, 9495-9505	13.1	5
177	Enantioselective Rh-Catalyzed Hydroboration of Silyl Enol Ethers. *Journal of the American Chemical Society*, **2021**, 143, 10902-10909	16.4	5
176	Revealing Thermodynamics and Kinetics of Lipid Self-Assembly by Markov State Model Analysis. *Journal of the American Chemical Society*, **2020**, 142, 21344-21352	16.4	3
175	Selective Catalytic Dehydrogenative Oxidation of Bio-Polyols to Lactic Acid. *Angewandte Chemie - International Edition*, **2020**, 59, 13871-13878	16.4	18
174	Selective Catalytic Dehydrogenative Oxidation of Bio-Polyols to Lactic Acid. *Angewandte Chemie*, **2020**, 132, 13975-13982	3.6	3
173	Structural Phase Transitions of Molecular Self-Assembly Driven by Nonbonded Metal Adatoms. *ACS Nano*, **2020**, 14, 6331-6338	16.7	3
172	XO-PBC: An Accurate and Efficient Method for Molecular Crystals. *Journal of Chemical Theory and Computation*, **2020**, 16, 4271-4285	6.4	2
171	Selective mono-N-methylation of nitroarenes with methanol catalyzed by atomically dispersed NHC-Ir solid assemblies. *Journal of Catalysis*, **2020**, 389, 337-344	7.3	18
170	Iridium-Catalyzed Selective Cross-Coupling of Ethylene Glycol and Methanol to Lactic Acid. *Angewandte Chemie - International Edition*, **2020**, 59, 10421-10425	16.4	15
169	Iridium-Catalyzed Selective Cross-Coupling of Ethylene Glycol and Methanol to Lactic Acid. *Angewandte Chemie*, **2020**, 132, 10507-10511	3.6	3
168	Identification of Water Hexamer on Cu(111) Surfaces. *Journal of the American Chemical Society*, **2020**, 142, 6902-6906	16.4	5
167	xOPBE: A Specialized Functional for Accurate Prediction of C Chemical Shifts. *Journal of Physical Chemistry A*, **2020**, 124, 5824-5831	2.8	3
166	The enhanced extended phenomenological kinetics method to deal with timescale disparity problem among different reaction pathways. *Journal of Computational Chemistry*, **2020**, 41, 2115-2123	3.5	4
165	An accurate single descriptor for ion-□nteractions. *National Science Review*, **2020**, 7, 1036-1045	10.8	6
164	Extended Koopmans' theorem at the second-order perturbation theory. *Journal of Computational Chemistry*, **2020**, 41, 1165-1174	3.5	11
163	Boosting CO2 Electroreduction to CH4 via Tuning Neighboring Single-Copper Sites. *ACS Energy Letters*, **2020**, 5, 1044-1053	20.1	154
162	Extending nudged elastic band method to reaction pathways involving multiple spin states. *Journal of Chemical Physics*, **2020**, 153, 134114	3.9	1

161	Theoretical analysis of an anion-π complex: IF···C6F6. *Chinese Journal of Chemical Physics*, **2020**, 33, 285-290	0.9	1
160	Theory-Guided Design of Anode Catalysts for Hydrogenous Liquid Fuels. *Journal of Physical Chemistry C*, **2020**, 124, 17494-17502	3.8	1
159	Extended Koopmans' theorem in the adiabatic connection formalism: Applied to doubly hybrid density functionals. *Journal of Chemical Physics*, **2020**, 153, 044109	3.9	3
158	A correlation-relaxation-balanced direct method at the second order perturbation theory for accurate ionization potential predictions. *Physical Chemistry Chemical Physics*, **2020**, 22, 22342-22348	3.6	1
157	Involvement of the Unoccupied Site Changes the Kinetic Trend Significantly: A Case Study on Formic Acid Decomposition. *ACS Catalysis*, **2020**, 10, 5153-5162	13.1	10
156	The XPK package: A comparison between the extended phenomenological kinetic (XPK) method and the conventional kinetic Monte Carlo (KMC) method. *Chinese Journal of Chemical Physics*, **2019**, 32, 143-150	0.9	11
155	Janus Mesoporous Sensor Devices for Simultaneous Multivariable Gases Detection. *Matter*, **2019**, 1, 1274-1284	21	23
154	Conformation Search Across Multiple-Level Potential-Energy Surfaces (CSAMP): A Strategy for Accurate Prediction of Protein-Ligand Binding Structures. *Journal of Chemical Theory and Computation*, **2019**, 15, 4264-4279	6.4	8
153	Simultaneous Attenuation of Both Self-Interaction Error and Nondynamic Correlation Error in Density Functional Theory: A Spin-Pair Distinctive Adiabatic-Connection Approximation. *Journal of Physical Chemistry Letters*, **2019**, 10, 2617-2623	6.4	12
152	Insights into Direct Methods for Predictions of Ionization Potential and Electron Affinity in Density Functional Theory. *Journal of Physical Chemistry Letters*, **2019**, 10, 2692-2699	6.4	11
151	HHLA2 in intrahepatic cholangiocarcinoma: an immune checkpoint with prognostic significance and wider expression compared with PD-L1 **2019**, 7, 77		49
150	High expression of Oct4 and Nanog predict poor prognosis in intrahepatic cholangiocarcinoma patients after curative resection. *Journal of Cancer*, **2019**, 10, 1313-1324	4.5	5
149	Doping strain induced bi-Ti pairs for efficient N activation and electrocatalytic fixation. *Nature Communications*, **2019**, 10, 2877	17.4	173
148	Bistability for CO Oxidation: An Understanding from Extended Phenomenological Kinetics Simulations. *ACS Catalysis*, **2019**, 9, 11116-11124	13.1	12
147	Accurate heats of formation of polycyclic saturated hydrocarbons predicted by using the XYG3 type of doubly hybrid functionals. *Journal of Computational Chemistry*, **2019**, 40, 1113-1122	3.5	3
146	Beyond Mean-Field Microkinetics: Toward Accurate and Efficient Theoretical Modeling in Heterogeneous Catalysis. *ACS Catalysis*, **2018**, 8, 5816-5826	13.1	29
145	Doubly hybrid density functionals that correctly describe both density and energy for atoms. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 2287-2292	11.5	20
144	The harpooning mechanism as evidenced in the oxidation reaction of the Al atom. *Chemical Science*, **2018**, 9, 488-494	9.4	9

143	Single-Atomic Cu with Multiple Oxygen Vacancies on Ceria for Electrocatalytic CO2 Reduction to CH4. *ACS Catalysis*, **2018**, 8, 7113-7119	13.1	323
142	Understanding the Nonplanarity in Aromatic Metallabenzenes: A Control Mechanism. *Inorganic Chemistry*, **2018**, 57, 9205-9214	5.1	12
141	Accurate prediction of nuclear magnetic resonance shielding constants: An extension of the focal-point analysis method for magnetic parameter calculations (FPA-M) with improved efficiency. *Journal of Chemical Physics*, **2018**, 149, 184101	3.9	1
140	Prognostic Nomogram Based on Histological Characteristics of Fibrotic Tumor Stroma in Patients Who Underwent Curative Resection for Intrahepatic Cholangiocarcinoma. *Oncologist*, **2018**, 23, 1482-1493	5.7	18
139	Development of New Density Functional Approximations. *Annual Review of Physical Chemistry*, **2017**, 68, 155-182	15.7	32
138	When does a functional correctly describe both the structure and the energy of the transition state?. *Journal of Molecular Modeling*, **2017**, 23, 65	2	5
137	Rational design of model Pd(ii)-catalysts for C-H activation involving ligands with charge-shift bonding characteristics. *Physical Chemistry Chemical Physics*, **2017**, 19, 2417-2424	3.6	8
136	Albumin to gamma-glutamyltransferase ratio as a prognostic indicator in intrahepatic cholangiocarcinoma after curative resection. *Oncotarget*, **2017**, 8, 13293-13303	3.3	30
135	Accurate potential energy surfaces for hydrogen abstraction reactions: A benchmark study on the XYG3 doubly hybrid density functional. *Journal of Computational Chemistry*, **2017**, 38, 2326-2334	3.5	3
134	The XYG3 type of doubly hybrid density functionals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 721-747	7.9	40
133	Improving B3LYP heats of formation with three-dimensional molecular descriptors. *Journal of Computational Chemistry*, **2016**, 37, 1175-90	3.5	8
132	Second-Order Perturbation Theory for Fractional Occupation Systems: Applications to Ionization Potential and Electron Affinity Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 2285-97	6.4	11
131	Understanding the anion- interactions with tetraoxacalix[2]arene[2]triazine. *Physical Chemistry Chemical Physics*, **2016**, 18, 6913-24	3.6	32
130	How well can B3LYP heats of formation be improved by dispersion correction models?. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	7
129	Theoretical Investigation on the Role of the Central Carbon Atom and Close Protein Environment on the Nitrogen Reduction in Mo Nitrogenase. *ACS Catalysis*, **2016**, 6, 1567-1577	13.1	49
128	A comparative study of the xDH-PBE0 and DSD-PBEPBE-D3BJ doubly hybrid density functionals. *Molecular Physics*, **2016**, 114, 1207-1217	1.7	10
127	Benchmarking Density Functionals on Structural Parameters of Small-/Medium-Sized Organic Molecules. *Journal of Chemical Theory and Computation*, **2016**, 12, 459-65	6.4	110
126	Quantum Reaction Dynamics Based on a New Generation Density Functional and Neural Network Potential Energy Surfaces. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2016**, 32, 119-130	3.8	5

125	DOX: A new computational protocol for accurate prediction of the protein-ligand binding structures. *Journal of Computational Chemistry*, **2016**, 37, 336-44	3.5	19
124	Self-consistent field for fragmented quantum mechanical model of large molecular systems. *Journal of Computational Chemistry*, **2016**, 37, 321-6	3.5	2
123	The mechanism of hydrogen abstraction by high valence transition metal oxo compounds. *Journal of Energy Chemistry*, **2016**, 25, 1045-1050	12	
122	Beyond energies: geometry predictions with the XYG3 type of doubly hybrid density functionals. *Chemical Communications*, **2016**, 52, 13840-13860	5.8	15
121	H + H2 quantum dynamics using potential energy surfaces based on the XYG3 type of doubly hybrid density functionals: validation of the density functionals. *Journal of Chemical Physics*, **2015**, 142, 084107	3.9	10
120	Integration approach at the second-order perturbation theory: applications to ionization potential and electron affinity calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 4677-88	6.4	13
119	Toward the construction of parameter-free doubly hybrid density functionals. *International Journal of Quantum Chemistry*, **2015**, 115, 589-595	2.1	18
118	Double hybrid functionals and the □system bond length alternation challenge: rivaling accuracy of post-HF methods. *Journal of Chemical Theory and Computation*, **2015**, 11, 832-8	6.4	19
117	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
116	The X1 family of methods that combines B3LYP with neural network corrections for an accurate yet efficient prediction of thermochemistry. *International Journal of Quantum Chemistry*, **2015**, 115, 1021-1031	2.1	16
115	Response to □Comment on □Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0□[J. Chem. Phys. 143, 187101 (2015)]. *Journal of Chemical Physics*, **2015**, 143, 187102	3.9	7
114	Error accumulations in adhesive energies of dihydrogen molecular chains: performances of the XYG3 type of doubly hybrid density functionals. *Journal of Physical Chemistry A*, **2015**, 119, 1590-9	2.8	13
113	Construction of a parameter-free doubly hybrid density functional from adiabatic connection. *Journal of Chemical Physics*, **2014**, 140, 18A512	3.9	48
112	A New-Generation Density Functional. *Springer Briefs in Molecular Science*, **2014**,	0.6	18
111	Formation of Acrylates from Ethylene and CO2on Ni Complexes: A Mechanistic Viewpoint from a Hybrid DFT Approach. *Organometallics*, **2014**, 33, 6369-6380	3.8	33
110	NO adsorption and transformation on the BaO surfaces from density functional theory calculations. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	3
109	Fractional charge behavior and band gap predictions with the XYG3 type of doubly hybrid density functionals. *Journal of Physical Chemistry A*, **2014**, 118, 9201-11	2.8	43
108	RRS-PBC: a molecular approach for periodic systems. *Science China Chemistry*, **2014**, 57, 1399-1404	7.9	7

107	Perturbative treatment of anharmonic vibrational effects on bond distances: an extended Langevin dynamics method. *Journal of Computational Chemistry*, **2014**, 35, 467-78	3.5	1
106	Global Potential Energy Surface for the H+CH4<-H2+CH3 Reaction using Neural Networks. *Chinese Journal of Chemical Physics*, **2014**, 27, 373-379	0.9	43
105	A New Generation of Doubly Hybrid Density Functionals (DHDFs). *Springer Briefs in Molecular Science*, **2014**, 25-45	0.6	2
104	Benchmarking the Performance of DHDFs for the Main Group Chemistry. *Springer Briefs in Molecular Science*, **2014**, 47-77	0.6	
103	An Overview of Modern Density Functional Theory. *Springer Briefs in Molecular Science*, **2014**, 1-24	0.6	
102	XYG3 Results for Some Selected Applications. *Springer Briefs in Molecular Science*, **2014**, 79-101	0.6	
101	Nonfitting protein-ligand interaction scoring function based on first-principles theoretical chemistry methods: development and application on kinase inhibitors. *Journal of Computational Chemistry*, **2013**, 34, 1636-46	3.5	32
100	Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. *Journal of Computational Chemistry*, **2013**, 34, 1759-74	3.5	20
99	Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. *Journal of Physical Chemistry Letters*, **2013**, 4, 1669-75	6.4	57
98	Performance enhancement of dye-sensitized solar cells using an ester-functionalized imidazolium iodide as the solid state electrolyte. *ACS Applied Materials & Interfaces*, **2013**, 5, 3219-23	9.5	15
97	Oxidation Mechanism of Si(111)-7 × 7 by Water: A Theoretical Study. *Journal of Physical Chemistry C*, **2013**, 117, 15763-15772	3.8	3
96	A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0. *Journal of Chemical Physics*, **2013**, 139, 174106	3.9	30
95	Accurate prediction of nuclear magnetic resonance shielding constants: towards the accuracy of CCSD(T) complete basis set limit. *Journal of Chemical Physics*, **2013**, 138, 124113	3.9	16
94	A new insight into the initial step in the Fischer-Tropsch synthesis: CO dissociation on Ru surfaces. *Physical Chemistry Chemical Physics*, **2012**, 14, 16686-94	3.6	23
93	Vanadium Distribution in Four-Component Mo-V-Te-Nb Mixed-Oxide Catalysts from First Principles: How to Explore the Numerous Configurations?. *Angewandte Chemie*, **2012**, 124, 13026-13030	3.6	7
92	Innentitelbild: Vanadium Distribution in Four-Component Mo-V-Te-Nb Mixed-Oxide Catalysts from First Principles: How to Explore the Numerous Configurations? (Angew. Chem. 51/2012). *Angewandte Chemie*, **2012**, 124, 12800-12800	3.6	
91	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. *Journal of Chemical Physics*, **2012**, 136, 174103	3.9	86
90	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. *Physical Chemistry Chemical Physics*, **2012**, 14, 12554-70	3.6	29

89	Mechanistic Insights into Selective Oxidation of Light Alkanes by Transition Metal Compounds/Complexes **2012**, 113-141		
88	Theoretical Studies on Dehydrogenation Reactions in Mg2(BH4)2(NH2)2 Compounds. *Chinese Journal of Chemical Physics*, **2012**, 25, 676-680	0.9	7
87	DCMB that combines divide-and-conquer and mixed-basis set methods for accurate geometry optimizations, total energies, and vibrational frequencies of large molecules. *Journal of Computational Chemistry*, **2012**, 33, 1421-32	3.5	4
86	XO: an extended ONIOM method for accurate and efficient modeling of large systems. *Journal of Computational Chemistry*, **2012**, 33, 2142-60	3.5	30
85	Gas-phase thermodynamics as a validation of computational catalysis on surfaces: a case study of Fischer-Tropsch synthesis. *ChemPhysChem*, **2012**, 13, 1486-94	3.2	19
84	Hybrid molecular dynamics and first-principles study on the work function of a Pt(111) electrode immersed in aqueous solution at room temperature. *Physical Review B*, **2012**, 86,	3.3	16
83	Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. *Frontiers of Chemistry in China: Selected Publications From Chinese Universities*, **2011**, 6, 269-279		17
82	Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. *Journal of Computational Chemistry*, **2011**, 32, 1824-38	3.5	25
81	Theoretical studies of Na+ location in ZSM-5: Model selection for accurate coordination structure and energetics. *Catalysis Today*, **2011**, 165, 112-119	5.3	7
80	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. *International Reviews in Physical Chemistry*, **2011**, 30, 115-160	7	106
79	Br□sted-NH(4)(+) mechanism versus nitrite mechanism: new insight into the selective catalytic reduction of NO by NH(3). *Physical Chemistry Chemical Physics*, **2011**, 13, 453-60	3.6	41
78	Mechanisms for Selective Catalytic Oxidation of Ammonia over Vanadium Oxides. *Journal of Physical Chemistry C*, **2011**, 115, 21218-21229	3.8	33
77	How to prepare a chiral Grignard reagent: a theoretical proposal. *Organic Letters*, **2011**, 13, 2046-9	6.2	4
76	Exploring the Sodium Cation Location and Aluminum Distribution in ZSM-5: A Systematic Study by the Extended ONIOM (XO) Method. *Journal of Physical Chemistry C*, **2011**, 115, 14754-14761	3.8	14
75	Theoretical studies on thermochemistry for conversion of 5-chloromethylfurfural into valuable chemicals. *Journal of Physical Chemistry A*, **2011**, 115, 13628-41	2.8	24
74	Assessment of Some Density Functional Theory Methods and Force Field Models in Describing Various Interaction Modes of Benzene Dimer. *Chinese Journal of Chemical Physics*, **2011**, 24, 635-639	0.9	7
73	Pyrolysis of D-Glucose to Acrolein. *Chinese Journal of Chemical Physics*, **2011**, 24, 249-252	0.9	18
72	A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 19896-900	11.5	124

71	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. *Journal of Chemical Physics*, **2010**, 132, 194105	3.9	37
70	Basis set dependence of the doubly hybrid XYG3 functional. *Journal of Chemical Physics*, **2010**, 133, 104105	3.9	39
69	Fishing-Mode Tip-enhanced Raman Spectroscopy (FM-TERS) for Studying Single-Molecule Junctions **2010**,		1
68	Spectroscopic and DFT study on the interaction system of vanadium with L-proline in aqueous solution. *Journal of Physical Chemistry A*, **2010**, 114, 5211-6	2.8	5
67	Extending the reliability and applicability of B3LYP. *Chemical Communications*, **2010**, 46, 3057-70	5.8	145
66	Trends in R-X Bond Dissociation Energies (R = Me, Et, i-Pr, t-Bu, X = H, Me, Cl, OH). *Journal of Chemical Theory and Computation*, **2010**, 6, 1462-9	6.4	37
65	Ion strength and pH sensitive phase transition of N-isobutyryl-L-(D)-cysteine monolayers on Au(111) surfaces. *Langmuir*, **2010**, 26, 7343-8	4	9
64	Density functional theory study of 1:1 glycine-water complexes in the gas phase and in solution. *Science China Chemistry*, **2010**, 53, 383-395	7.9	18
63	The X1s method for accurate bond dissociation energies. *ChemPhysChem*, **2010**, 11, 2561-7	3.2	23
62	XO: An extended ONIOM method for accurate and efficient geometry optimization of large molecules. *Chemical Physics Letters*, **2010**, 498, 203-208	2.5	46
61	Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 4963-8	11.5	280
60	Accurate prediction of heats of formation by a combined method of B3LYP and neural network correction. *Journal of Computational Chemistry*, **2009**, 30, 1424-44	3.5	25
59	O-atom transfer reaction from N2O to CO: A theoretical investigation. *Chemical Physics Letters*, **2009**, 475, 202-207	2.5	8
58	Dissociative Adsorption of PH3 on the Si(111)-7 7 Surface: A Theoretical Investigation. *Journal of Physical Chemistry C*, **2009**, 113, 7843-7850	3.8	4
57	Performance of Several Density Functional Theory Methods on Describing Hydrogen-Bond Interactions. *Journal of Chemical Theory and Computation*, **2009**, 5, 86-96	6.4	117
56	Binding interaction analysis of the active site and its inhibitors for neuraminidase (N1 subtype) of human influenza virus by the integration of molecular docking, FMO calculation and 3D-QSAR CoMFA modeling. *Journal of Chemical Information and Modeling*, **2008**, 48, 1802-12	6.1	27
55	Understanding the reactivity of the tetrahedrally coordinated high-valence d0 transition metal oxides toward the C-H bond activation of alkanes: a cluster model study. *Journal of Physical Chemistry A*, **2008**, 112, 717-21	2.8	27
54	One-Step Preparation of Large-Scale Self-Assembled Monolayers of Cyanuric Acid and Melamine Supramolecular Species on Au(111) Surfaces. *Journal of Physical Chemistry C*, **2008**, 112, 4209-4218	3.8	78

53	Chemical Enhancement Effects in SERS Spectra: A Quantum Chemical Study of Pyridine Interacting with Copper, Silver, Gold and Platinum Metals. *Journal of Physical Chemistry C*, **2008**, 112, 4195-4204	3.8	185
52	A hierarchical construction scheme for accurate potential energy surface generation: an application to the F+H2 reaction. *Journal of Chemical Physics*, **2008**, 129, 011103	3.9	48
51	Improving the B3LYP bond energies by using the X1 method. *Journal of Chemical Physics*, **2008**, 129, 164103	3.9	45
50	THEORETICAL STUDY OF GLYCINE CONFORMERS. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 889-909	1.8	20
49	Systematic investigation on the geometric dependence of the calculated nuclear magnetic shielding constants. *Journal of Computational Chemistry*, **2008**, 29, 1798-807	3.5	8
48	ESI-MS and theoretical study on the coordination structures and reaction modes of the diperoxovanadate complexes containing histidine-like ligands. *International Journal of Mass Spectrometry*, **2008**, 269, 138-144	1.9	20
47	Mechanisms for NH3 Decomposition on the Si(111)-7 □7 Surface: A DFT Cluster Model Study. *Journal of Physical Chemistry C*, **2007**, 111, 16974-16981	3.8	15
46	One Step Fabrication of Metal□Organic Coordination Monolayers on Au(111) Surfaces. *Journal of Physical Chemistry C*, **2007**, 111, 7570-7573	3.8	21
45	Theoretical study of the vertical excited states of benzene, pyrimidine, and pyrazine by the symmetry adapted cluster--configuration interaction method. *Journal of Computational Chemistry*, **2007**, 28, 1658-67	3.5	38
44	Systematic studies on the computation of nuclear magnetic resonance shielding constants and chemical shifts: the density functional models. *Journal of Computational Chemistry*, **2007**, 28, 2431-42	3.5	63
43	Isotopic Oxygen Exchange and EPR Studies of Superoxide Species on the SrF2/La2O3 Catalyst. *Catalysis Letters*, **2007**, 118, 238-243	2.8	13
42	DEVELOPING SELECTIVE OXIDATION CATALYSTS OF LIGHT ALKANES: FROM FUNDAMENTAL UNDERSTANDING TO RATIONAL DESIGN. *Surface Review and Letters*, **2007**, 14, 645-656	1.1	8
41	The X1 method for accurate and efficient prediction of heats of formation. *Journal of Chemical Physics*, **2007**, 127, 214105	3.9	79
40	Geometric dependence of the B3LYP-predicted magnetic shieldings and chemical shifts. *Journal of Physical Chemistry A*, **2007**, 111, 9431-7	2.8	66
39	Self-assembly of alkanols on Au(111) surfaces. *Chemistry - A European Journal*, **2006**, 12, 4006-13	4.8	23
38	Selective heterogeneous nucleation and growth of size-controlled metal nanoparticles on carbon nanotubes in solution. *Chemistry - A European Journal*, **2006**, 12, 2542-9	4.8	116
37	A time-dependent density functional theory investigation of the spectroscopic properties of the beta-subunit in C-phycocyanin. *Journal of Physical Chemistry B*, **2006**, 110, 18665-9	3.4	18
36	Mechanism of methane oxidation by transition metal oxides: A cluster model study. *Catalysis Today*, **2006**, 117, 133-137	5.3	25

35	OPBE: A promising density functional for the calculation of nuclear shielding constants. *Chemical Physics Letters*, **2006**, 421, 383-388	2.5	107
34	Mechanisms of methane activation and transformation on molybdenum oxide based catalysts. *Journal of the American Chemical Society*, **2005**, 127, 3989-96	16.4	118
33	Mechanisms of initial propane activation on molybdenum oxides: a density functional theory study. *Journal of Physical Chemistry B*, **2005**, 109, 6416-21	3.4	57
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