Zongtang Fang

List of Publications by Year
in descending order

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45 papers	835 citations	516710 16 h-index	526287 27 g-index
47 all docs	47 docs citations	47 times ranked	986 citing authors

#	Article	IF	Citations
1	Prediction of Bond Dissociation Energies/Heats of Formation for Diatomic Transition Metal Compounds: CCSD(T) Works. Journal of Chemical Theory and Computation, 2017, 13, 1057-1066.	5.3	92
2	Ethanol Conversion on Cyclic (MO3)3 (M = Mo, W) Clusters. Journal of Physical Chemistry C, 2014, 118, 4869-4877.	3.1	62
3	Computational Study of the Hydrolysis Reactions of the Ground and First Excited Triplet States of Small TiO₂ Nanoclusters. Journal of Physical Chemistry C, 2011, 115, 9344-9360.	3.1	61
4	Structural and Electronic Property Study of (ZnO)_n, n â‰ 168: Transition from Zinc Oxide Molecular Clusters to Ultrasmall Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 20400-20418.	3.1	53
5	Computational Study of H2 and O2 Production from Water Splitting by Small (MO2)n Clusters (M = Ti,) Tj ETQq1 1 0.784314 rgBT /Ove	2.5	45
6	Use of Improved Orbitals for CCSD(T) Calculations for Predicting Heats of Formation of Group IV and Group VI Metal Oxide Monomers and Dimers and UCl₆. Journal of Chemical Theory and Computation, 2016, 12, 3583-3592.	5.3	43
7	Oxidation, Reduction, and Condensation of Alcohols over (MO3)3 (M = Mo, W) Nanoclusters. Journal of Physical Chemistry C, 2014, 118, 22620-22634.	3.1	37
8	Computational Study of the Hydrolysis Reactions of Small MO₂ (M = Zr and Hf) Nanoclusters with Water. Journal of Physical Chemistry C, 2012, 116, 8475-8492.	3.1	35
9	Computational Study of Ethanol Conversion on Al₈O₁₂ as a Model for Î³-Al₂O₃. Journal of Physical Chemistry C, 2015, 119, 23413-23421.	3.1	33
10	Benchmark Calculations of Energetic Properties of Groups 4 and 6 Transition Metal Oxide Nanoclusters Including Comparison to Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 3689-3710.	5.3	32
11	Reactions of laser-ablated U atoms with (CN)2: infrared spectra and electronic structure calculations of UNC, U(NC)2, and U(NC)4 in solid argon. Chemical Communications, 2015, 51, 3899-3902.	4.1	26
12	Hydrolysis of ZrCl₄ and HfCl₄: The Initial Steps in the High-Temperature Oxidation of Metal Chlorides to Produce ZrO₂ and HfO₂. Journal of Physical Chemistry C, 2013, 117, 7459-7474.	3.1	25
13	Properties of Cerium Hydroxides from Matrix Infrared Spectra and Electronic Structure Calculations. Inorganic Chemistry, 2016, 55, 1702-1714.	4.0	24
14	Formation of Surface Impurities on Lithiumâ€“Nickelâ€“Manganeseâ€“Cobalt Oxides in the Presence of CO₂ and H₂O. Journal of the American Chemical Society, 2021, 143, 10261-10274.	13.7	21
15	Formation and Characterization of Homoleptic Thorium Isocyanide Complexes. Inorganic Chemistry, 2017, 56, 5060-5068.	4.0	20
16	A Comparison of Solid Electrolyte Interphase Formation and Evolution on Highly Oriented Pyrolytic and Disordered Graphite Negative Electrodes in Lithiumâ€ion Batteries. Small, 2021, 17, e2105292.	10.0	18
17	The surprising oxidation state of fumed silica and the nature of water binding to silicon oxides and hydroxides. Chemical Physics Letters, 2011, 501, 159-165.	2.6	15
18	Structures and Properties of the Products of the Reaction of Lanthanide Atoms with H₂O: Dominance of the +II Oxidation State. Journal of Physical Chemistry A, 2016, 120, 793-804.	2.5	15

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19	Data driven reaction mechanism estimation via transient kinetics and machine learning. Chemical Engineering Journal, 2021, 420, 129610.	12.7	14
20	The Molybdenum(V) and Tungsten(VI) Oxoazides [MoO(N₃)₃], [MoO(N₃)₃â‹…2â€‰CH₃CN], [(bipy)MoO(N₃)₃], [MoO(N₃)₅]^{2â^’}, [WO(N₃)₄], and [WO(N₃)₄â‹…CH₃CN]. Angewandte Chemie - International Edition, 2015, 54, 15550-15555.	13.8	12
21	Extending the Row of Lanthanide Tetrafluorides: A Combined Matrixâ€Isolation and Quantumâ€Chemical Study. Chemistry - A European Journal, 2016, 22, 2406-2416.	3.3	12
22	Laser-Ablated U Atom Reactions with (CN)₂ to Form UNC, U(NC)₂, and U(NC)₄: Matrix Infrared Spectra and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2018, 122, 516-528.	2.5	12
23	Properties of Lanthanide Hydroxide Molecules Produced in Reactions of Lanthanide Atoms with H₂O₂ and H₂ + O₂ Mixtures: Roles of the +I, +II, +III, and +IV Oxidation States. Journal of Physical Chemistry A, 2017, 121, 1779-1796.	2.5	11
24	Nature of Oxygen Adsorption on Defective Carbonaceous Materials. Journal of Physical Chemistry C, 2021, 125, 20686-20696.	3.1	11
25	The presence of Ti(II) centers in doped nanoscale TiO2 and TiO2â^’xNx. Chemical Physics Letters, 2012, 539-540, 58-63.	2.6	10
26	The First Molybdenum(VI) and Tungsten(VI) Oxoazides MO₂(N₃)₂, MO₂(N₃)₂â‹…2â€‰CH₃CN, (bipy)MO₂(N₃)₂, and [MO₂(N₃)₄]^{2â^’} (M=Mo, W). Angewandte Chemie - International Edition, 2015, 54, 9581-9585.	13.8	9
27	TAPsolver: A Python package for the simulation and analysis of TAP reactor experiments. Chemical Engineering Journal, 2021, 420, 129377.	12.7	9
28	1,2-Ethanediol and 1,3-Propanediol Conversions over (MO₃)₃ (M = Mo, W) Nanoclusters: A Computational Study. Journal of Physical Chemistry A, 2016, 120, 1897-1907.	2.5	8
29	Infrared Spectroscopic and Theoretical Studies on the OMF₂ and OMF (M = Cr, Mo, W) Molecules in Solid Argon. Journal of Physical Chemistry A, 2017, 121, 7603-7612.	2.5	8
30	Electronic Structures of Small (RuO₂)_n (n = 1â€“4) Nanoclusters and Their Anions and the Hydrolysis Reactions with Water. Journal of Physical Chemistry A, 2017, 121, 7726-7744.	2.5	6
31	Infrared Spectroscopic and Theoretical Studies of the 3d Transition Metal Oxyfluoride Molecules. Inorganic Chemistry, 2019, 58, 9796-9810.	4.0	6
32	Understanding Reaction Networks through Controlled Approach to Equilibrium Experiments Using Transient Methods. Journal of the American Chemical Society, 2021, 143, 10998-11006.	13.7	6
33	Die MolybdÃn(V)â€•und Wolfram(VI)â€oxoazide [MoO(N 3) 3], [MoO(N 3) 3 â‹…2â€‰CH 3 CN], [(bipy)MoO(N 3) 3], [MoO(N 3) 5] 2â^’ , [WO(N 3) 4] und [WO(N 3) 4 â‹…CH 3. Angewandte Chemie, 2015, 127, 15771-15776.	2.0	5
34	Synthesis of nanoscale silicon oxide oxidation state distributions: The transformation from hydrophilicity to hydrophobicity. Chemical Physics Letters, 2016, 653, 137-143.	2.6	5
35	Computational Study of Molecular Hydrogen Adsorption over Small (MO₂)_n Nanoclusters (M = Ti, Zr, Hf; n = 1 to 4). Journal of Physical Chemistry A, 2018, 122, 4338-4349.	2.5	5
36	Pt-Assisted Carbon Remediation of Mo₂C Materials for CO Disproportionation. ACS Catalysis, 2020, 10, 1894-1911.	11.2	5

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37	The First Molybdenum(VI) and Tungsten(VI) Oxoazides MO 2 (N 3) 2 , MO 2 (N 3) 2 â‹…2â€‰CH 3 CN, (bipy)MO 2 (N 3) 2 , and [MO 2 (N 3) 4] 2â¯ (M=Mo, W). Angewandte Chemie, 2015, 127, 9717-9721.	2.0	4
38	Energetic Properties and Electronic Structure of [Si,N,S] and [Si,P,S] Isomers. Journal of Physical Chemistry A, 2016, 120, 1691-1697.	2.5	4
39	Methods for determining the intrinsic kinetic characteristics of irreversible adsorption processes. Chemical Engineering Science, 2019, 207, 344-351.	3.8	4
40	Computational Study of Triphosphine-Ligated Cu(I) Catalysts for Hydrogenation of CO₂ to Formate. Journal of Physical Chemistry A, 2021, 125, 6600-6610.	2.5	4
41	Formation of Cerium and Neodymium Isocyanides in the Reactions of Cyanogen with Ce and Nd Atoms in Argon Matrices. Journal of Physical Chemistry A, 2019, 123, 8208-8219.	2.5	3
42	Mechanistic pathways and role of oxygen in oxidative coupling of methane derived from transient kinetic studies. Catalysis Today, 2022, , .	4.4	3
43	Quantifying the impact of temporal analysis of products reactor initial state uncertainties on kinetic parameters. AICHE Journal, 2022, 68, .	3.6	2
44	Tungsten Hydride Phosphorus- and Arsenic-Bearing Molecules with Double and Triple Wâ€“P and Wâ€“As Bonds. Inorganic Chemistry, 2018, 57, 5320-5332.	4.0	0
45	Internal Calibration of Transient Kinetic Data via Machine Learning. Catalysis Today, 2022, , .	4.4	0