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	Internal Calibration of Transient Kinetic Data via Machine Learning. Catalysis Today, 2022, , .	4.4	0
2	Mechanistic pathways and role of oxygen in oxidative coupling of methane derived from transient kinetic studies. Catalysis Today, 2022, , .	4.4	3
3	Quantifying the impact of temporal analysis of products reactor initial state uncertainties on kinetic parameters. AICHE Journal, 2022, 68, .	3.6	2
4	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
5	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
6	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
7	TAPsolver: A Python package for the simulation and analysis of TAP reactor experiments. Chemical Engineering Journal, 2021, 420, 129377.	12.7	9
8	Nature of Oxygen Adsorption on Defective Carbonaceous Materials. Journal of Physical Chemistry C, 2021, 125, 20686-20696.	3.1	11
9	Data driven reaction mechanism estimation via transient kinetics and machine learning. Chemical Engineering Journal, 2021, 420, 129610.	12.7	14
10	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
11	Pt-Assisted Carbon Remediation of Mo₂C Materials for CO Disproportionation. ACS Catalysis, 2020, 10, 1894-1911.	11.2	5
12	Infrared Spectroscopic and Theoretical Studies of the 3d Transition Metal Oxyfluoride Molecules. Inorganic Chemistry, 2019, 58, 9796-9810.	4.0	6
13	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
14	Methods for determining the intrinsic kinetic characteristics of irreversible adsorption processes. Chemical Engineering Science, 2019, 207, 344-351.	3.8	4
15	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
16	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
17	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
18	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

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19	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
20	Formation and Characterization of Homoleptic Thorium Isocyanide Complexes. Inorganic Chemistry, 2017, 56, 5060-5068.	4.0	20
21	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
22	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
23	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
24	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
25	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
26	Synthesis of nanoscale silicon oxide oxidation state distributions: The transformation from hydrophilicity to hydrophobicity. Chemical Physics Letters, 2016, 653, 137-143.	2.6	5
27	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
28	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
29	Properties of Cerium Hydroxides from Matrix Infrared Spectra and Electronic Structure Calculations. Inorganic Chemistry, 2016, 55, 1702-1714.	4.0	24
30	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
31	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
32	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
33	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
34	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
35	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
36	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

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37	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
38	Ethanol Conversion on Cyclic (MO3)3 (M = Mo, W) Clusters. Journal of Physical Chemistry C, 2014, 118, 4869-4877.	3.1	62
39	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
40	Computational Study of H2 and O2 Production from Water Splitting by Small (MO2)n Clusters (M = Ti,) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	45
41	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
42	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
43	The presence of Ti(II) centers in doped nanoscale TiO2 and TiO2âˆ’xNx. Chemical Physics Letters, 2012, 539-540, 58-63.	2.6	10
44	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
45	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