Ke R Yang

List of Publications by Year
in descending order

44 papers	4,101 citations	147801 31 h-index	243625 44 g-index
45 all docs	45 docs citations	45 times ranked	6473 citing authors

#	Article	IF	Citations
1	Nitrogen-doped tungsten carbide nanoarray as an efficient bifunctional electrocatalyst for water splitting in acid. Nature Communications, 2018, 9, 924.	12.8	571
2	Active sites of copper-complex catalytic materials for electrochemical carbon dioxide reduction. Nature Communications, 2018, 9, 415.	12.8	527
3	Facet-Dependent Photoelectrochemical Performance of TiO₂ Nanostructures: An Experimental and Computational Study. Journal of the American Chemical Society, 2015, 137, 1520-1529.	13.7	242
4	Stable iridium dinuclear heterogeneous catalysts supported on metal-oxide substrate for solar water oxidation. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2902-2907.	7.1	229
5	Investigating the Role of Copper Oxide in Electrochemical CO₂ Reduction in Real Time. ACS Applied Materials & Interfaces, 2018, 10, 8574-8584.	8.0	207
6	Tests of the RPBE, revPBE, Ï„-HCTHhyb, Ï‰B97X-D, and MOHLYP density functional approximations and 29 others against representative databases for diverse bond energies and barrier heights in catalysis. Journal of Chemical Physics, 2010, 132, 164117.	3.0	206
7	Multihole water oxidation catalysis on haematite photoanodes revealed by operando spectroelectrochemistry and DFT. Nature Chemistry, 2020, 12, 82-89.	13.6	189
8	Global ab initio ground-state potential energy surface of N4. Journal of Chemical Physics, 2013, 139, 044309.	3.0	175
9	New Pathways for Formation of Acids and Carbonyl Products in Low-Temperature Oxidation: The Korcek Decomposition of Î³-Ketohydroperoxides. Journal of the American Chemical Society, 2013, 135, 11100-11114.	13.7	153
10	Enantioselective Propargylation of Polyols and Desymmetrization of meso 1,2â€Diols by Copper/Borinic Acid Dual Catalysis. Angewandte Chemie - International Edition, 2017, 56, 7213-7217.	13.8	114
11	Photodissociation Dynamics of Phenol: Multistate Trajectory Simulations including Tunneling. Journal of the American Chemical Society, 2014, 136, 16378-16386.	13.7	102
12	Full-dimensional potentials and state couplings and multidimensional tunneling calculations for the photodissociation of phenol. Chemical Science, 2014, 5, 4661-4680.	7.4	90
13	Ultrathin dendrimerâ€“graphene oxide composite film for stable cycling lithiumâ€“sulfur batteries. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3578-3583.	7.1	90
14	Mechanistic Insights into Surface Chemical Interactions between Lithium Polysulfides and Transition Metal Oxides. Journal of Physical Chemistry C, 2017, 121, 14222-14227.	3.1	86
15	End-On Bound Iridium Dinuclear Heterogeneous Catalysts on WO₃ for Solar Water Oxidation. ACS Central Science, 2018, 4, 1166-1172.	11.3	69
16	Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. Journal of Chemical Theory and Computation, 2014, 10, 102-121.	5.3	65
17	Potential energy surfaces of quintet and singlet O₄. Journal of Chemical Physics, 2017, 147, 034301.	3.0	65
18	Solution Structures of Highly Active Molecular Ir Water-Oxidation Catalysts from Density Functional Theory Combined with High-Energy X-ray Scattering and EXAFS Spectroscopy. Journal of the American Chemical Society, 2016, 138, 5511-5514.	13.7	63

#	Article	IF	Citations
19	Diabatic Molecular Orbitals, Potential Energies, and Potential Energy Surface Couplings by the 4-fold Way for Photodissociation of Phenol. Journal of Chemical Theory and Computation, 2013, 9, 3612-3625.	5.3	61
20	Hydrophobic CuO Nanosheets Functionalized with Organic Adsorbates. Journal of the American Chemical Society, 2018, 140, 1824-1833.	13.7	59
21	In Situ Identification of Reaction Intermediates and Mechanistic Understandings of Methane Oxidation over Hematite: A Combined Experimental and Theoretical Study. Journal of the American Chemical Society, 2020, 142, 17119-17130.	13.7	59
22	High-resolution cryo-electron microscopy structure of photosystem II from the mesophilic cyanobacterium, Synechocystis sp. PCC 6803. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	58
23	Density functional study of multiplicity-changing valence and Rydberg excitations of p-block elements: Delta self-consistent field, collinear spin-flip time-dependent density functional theory (DFT), and conventional time-dependent DFT. Journal of Chemical Physics, 2011, 135, 044118.	3.0	57
24	Antimony Complexes for Electrocatalysis: Activity of a Mainâ€Group Element in Proton Reduction. Angewandte Chemie - International Edition, 2017, 56, 9111-9115.	13.8	51
25	Ferroceneâ€Promoted Longâ€Cycle Lithiumâ€“Sulfur Batteries. Angewandte Chemie - International Edition, 2016, 55, 14818-14822.	13.8	46
26	Facet-Dependent Kinetics and Energetics of Hematite for Solar Water Oxidation Reactions. ACS Applied Materials & Interfaces, 2019, 11, 5616-5622.	8.0	46
27	Direct diabatization of electronic states by the fourfold-way: Including dynamical correlation by multi-configuration quasidegenerate perturbation theory with complete active space self-consistent-field diabatic molecular orbitals. Chemical Physics Letters, 2013, 573, 84-89.	2.6	42
28	Mechanism of Manganese-Catalyzed Oxygen Evolution from Experimental and Theoretical Analyses of ¹⁸O Kinetic Isotope Effects. ACS Catalysis, 2015, 5, 7104-7113.	11.2	41
29	Water-Nucleophilic Attack Mechanism for the Cu^{II}(pyalk)₂ Water-Oxidation Catalyst. ACS Catalysis, 2018, 8, 7952-7960.	11.2	37
30	Which Ab Initio Wave Function Methods Are Adequate for Quantitative Calculations of the Energies of Biradicals? The Performance of Coupled-Cluster and Multi-Reference Methods Along a Single-Bond Dissociation Coordinate. Journal of Chemical Theory and Computation, 2013, 9, 418-431.	5.3	35
31	Testing Noncollinear Spin-Flip, Collinear Spin-Flip, and Conventional Time-Dependent Density Functional Theory for Predicting Electronic Excitation Energies of Closed-Shell Atoms. Journal of Chemical Theory and Computation, 2014, 10, 2070-2084.	5.3	33
32	Catalytic manganese oxide nanostructures for the reverse water gas shift reaction. Nanoscale, 2019, 11, 16677-16688.	5.6	31
33	Quantum Mechanical Fragment Methods Based on Partitioning Atoms or Partitioning Coordinates. Accounts of Chemical Research, 2014, 47, 2731-2738.	15.6	27
34	Enantioselective Propargylation of Polyols and Desymmetrization of meso 1,2â€Diols by Copper/Borinic Acid Dual Catalysis. Angewandte Chemie, 2017, 129, 7319-7323.	2.0	23
35	Thermodynamics of the S₂-to-S₃ state transition of the oxygen-evolving complex of photosystem II. Physical Chemistry Chemical Physics, 2019, 21, 20840-20848.	2.8	21
36	Is Deprotonation of the Oxygen-Evolving Complex of Photosystem II during the S₁ â†' S₂ Transition Suppressed by Proton Quantum Delocalization?. Journal of the American Chemical Society, 2021, 143, 8324-8332.	13.7	21

#	Article	IF	Citations
37	Anchor Points Reactive Potential for Bond-Breaking Reactions. Journal of Chemical Theory and Computation, 2014, 10, 924-933.	5.3	16
38	Triplet Oxygen Evolution Catalyzed by a Biomimetic Oxomanganese Complex: Functional Role of the Carboxylate Buffer. ACS Catalysis, 2015, 5, 2384-2390.	11.2	15
39	Antimony Complexes for Electrocatalysis: Activity of a Mainâ€Group Element in Proton Reduction. Angewandte Chemie, 2017, 129, 9239-9243.	2.0	12
40	Ferroceneâ€Promoted Longâ€Cycle Lithiumâ€“Sulfur Batteries. Angewandte Chemie, 2016, 128, 15038-15042.	2.0	11
41	Quasiclassical Trajectory Analysis of the N2 + N2 Reaction Using a New Ab Initio Potential Energy Surface. , 2014, , .		10
42	Understanding the Separation Mechanism of C2H6/C2H4 on Zeolitic Imidazolate Framework ZIF-7 by Periodic DFT Investigations. Journal of Physical Chemistry C, 2020, 124, 256-266.	3.1	9
43	Development of an Enantioselective Synthesis of (â^')-Euonyminol. Journal of Organic Chemistry, 2021, 86, 17011-17035.	3.2	6
44	Glycerol binding at the narrow channel of photosystem II stabilizes the low-spin S2 state of the oxygen-evolving complex. Photosynthesis Research, 2022, , 1.	2.9	1