# Ke R Yang

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | 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 |
| 2 | 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 |
| 3 | Is Deprotonation of the Oxygen-Evolving Complex of Photosystem II during the S<sub>1</sub> â†' S<sub>2</sub> Transition Suppressed by Proton Quantum Delocalization?. Journal of the American Chemical Society, 2021, 143, 8324-8332. | 13.7 | 21 |
| 4 | Development of an Enantioselective Synthesis of (â^')-Euonyminol. Journal of Organic Chemistry, 2021, 86, 17011-17035. | 3.2 | 6 |
| 5 | 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 |
| 6 | Multihole water oxidation catalysis on haematite photoanodes revealed by operando spectroelectrochemistry and DFT. Nature Chemistry, 2020, 12, 82-89. | 13.6 | 189 |
| 7 | 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 |
| 8 | Facet-Dependent Kinetics and Energetics of Hematite for Solar Water Oxidation Reactions. ACS Applied Materials & Interfaces, 2019, 11, 5616-5622. | 8.0 | 46 |
| 9 | Catalytic manganese oxide nanostructures for the reverse water gas shift reaction. Nanoscale, 2019, 11, 16677-16688. | 5.6 | 31 |
| 10 | Thermodynamics of the S<sub>2</sub>-to-S<sub>3</sub> state transition of the oxygen-evolving complex of photosystem II. Physical Chemistry Chemical Physics, 2019, 21, 20840-20848. | 2.8 | 21 |
| 11 | Nitrogen-doped tungsten carbide nanoarray as an efficient bifunctional electrocatalyst for water splitting in acid. Nature Communications, 2018, 9, 924. | 12.8 | 571 |
| 12 | 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 |
| 13 | Investigating the Role of Copper Oxide in Electrochemical CO<sub>2</sub> Reduction in Real Time. ACS Applied Materials & Interfaces, 2018, 10, 8574-8584. | 8.0 | 207 |
| 14 | Active sites of copper-complex catalytic materials for electrochemical carbon dioxide reduction. Nature Communications, 2018, 9, 415. | 12.8 | 527 |
| 15 | Hydrophobic CuO Nanosheets Functionalized with Organic Adsorbates. Journal of the American Chemical Society, 2018, 140, 1824-1833. | 13.7 | 59 |
| 16 | End-On Bound Iridium Dinuclear Heterogeneous Catalysts on WO<sub>3</sub> for Solar Water Oxidation. ACS Central Science, 2018, 4, 1166-1172. | 11.3 | 69 |
| 17 | Water-Nucleophilic Attack Mechanism for the Cu<sup>II</sup>(pyalk)<sub>2</sub> Water-Oxidation Catalyst. ACS Catalysis, 2018, 8, 7952-7960. | 11.2 | 37 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Antimony Complexes for Electrocatalysis: Activity of a Mainâ€Group Element in Proton Reduction. Angewandte Chemie - International Edition, 2017, 56, 9111-9115. | 13.8 | 51 |
| 20 | 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 |
| 21 | 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 |
| 22 | Potential energy surfaces of quintet and singlet O<sub>4</sub>. Journal of Chemical Physics, 2017, 147, 034301. | 3.0 | 65 |
| 23 | Antimony Complexes for Electrocatalysis: Activity of a Mainâ€Group Element in Proton Reduction. Angewandte Chemie, 2017, 129, 9239-9243. | 2.0 | 12 |
| 24 | 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 |
| 25 | 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 |
| 26 | Ferroceneâ€Promoted Longâ€Cycle Lithiumâ€“Sulfur Batteries. Angewandte Chemie, 2016, 128, 15038-15042. | 2.0 | 11 |
| 27 | Ferroceneâ€Promoted Longâ€Cycle Lithiumâ€“Sulfur Batteries. Angewandte Chemie - International Edition, 2016, 55, 14818-14822. | 13.8 | 46 |
| 28 | Facet-Dependent Photoelectrochemical Performance of TiO<sub>2</sub> Nanostructures: An Experimental and Computational Study. Journal of the American Chemical Society, 2015, 137, 1520-1529. | 13.7 | 242 |
| 29 | Triplet Oxygen Evolution Catalyzed by a Biomimetic Oxomanganese Complex: Functional Role of the Carboxylate Buffer. ACS Catalysis, 2015, 5, 2384-2390. | 11.2 | 15 |
| 30 | Mechanism of Manganese-Catalyzed Oxygen Evolution from Experimental and Theoretical Analyses of <sup>18</sup>O Kinetic Isotope Effects. ACS Catalysis, 2015, 5, 7104-7113. | 11.2 | 41 |
| 31 | Anchor Points Reactive Potential for Bond-Breaking Reactions. Journal of Chemical Theory and Computation, 2014, 10, 924-933. | 5.3 | 16 |
| 32 | 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 |
| 33 | Photodissociation Dynamics of Phenol: Multistate Trajectory Simulations including Tunneling. Journal of the American Chemical Society, 2014, 136, 16378-16386. | 13.7 | 102 |
| 34 | Full-dimensional potentials and state couplings and multidimensional tunneling calculations for the photodissociation of phenol. Chemical Science, 2014, 5, 4661-4680. | 7.4 | 90 |
| 35 | 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 |
| 36 | Quantum Mechanical Fragment Methods Based on Partitioning Atoms or Partitioning Coordinates. Accounts of Chemical Research, 2014, 47, 2731-2738. | 15.6 | 27 |

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|---|---|---|---|
| 37 | Quasiclassical Trajectory Analysis of the N2 + N2 Reaction Using a New Ab Initio Potential Energy Surface. , 2014, , . | | 10 |
| 38 | 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 |
| 39 | Global ab initio ground-state potential energy surface of N4. Journal of Chemical Physics, 2013, 139, 044309. | 3.0 | 175 |
| 40 | 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 |
| 41 | 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 |
| 42 | 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 |
| 43 | 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 |
| 44 | 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 |