John A Keith

List of Publications by Year in descending order

80 papers	5,109 citations	87843 38 h-index	88593 70 g-index
99 all docs	99 docs citations	99 times ranked	6419 citing authors

#	Article	IF	Citations
1	Water Oxidation on Pure and Doped Hematite (0001) Surfaces: Prediction of Co and Ni as Effective Dopants for Electrocatalysis. Journal of the American Chemical Society, 2012, 134, 13296-13309.	6.6	492
2	Using natureâ€™s blueprint to expand catalysis with Earth-abundant metals. Science, 2020, 369, .	6.0	306
3	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. Chemical Reviews, 2021, 121, 9816-9872.	23.0	287
4	The Mechanism of the Wacker Reaction: A Tale of Two Hydroxypalladations. Angewandte Chemie - International Edition, 2009, 48, 9038-9049.	7.2	261
5	Elucidation of the Selectivity of Proton-Dependent Electrocatalytic CO₂ Reduction by fac-Re(bpy)(CO)₃Cl. Journal of the American Chemical Society, 2013, 135, 15823-15829.	6.6	238
6	Theoretical Studies of Potentialâ€Dependent and Competing Mechanisms of the Electrocatalytic Oxygen Reduction Reaction on Pt(111). Angewandte Chemie - International Edition, 2010, 49, 9521-9525.	7.2	214
7	Theoretical Investigations of the Oxygen Reduction Reaction on Pt(111). ChemPhysChem, 2010, 11, 2779-2794.	1.0	200
8	Theoretical Elucidation of the Competitive Electro-oxidation Mechanisms of Formic Acid on Pt(111). Journal of the American Chemical Society, 2010, 132, 18377-18385.	6.6	189
9	Theoretical Insights into Pyridinium-Based Photoelectrocatalytic Reduction of CO₂. Journal of the American Chemical Society, 2012, 134, 7580-7583.	6.6	161
10	Ab Initio DFT+U Analysis of Oxygen Vacancy Formation and Migration in La_{1-x}Sr_xFeO_{3-Î´}(x= 0, 0.25, 0.50). Chemistry of Materials, 2013, 25, 3011-3019.	3.2	153
11	The Inner-Sphere Process in the Enantioselective Tsuji Allylation Reaction with (S)-t-Bu-phosphinooxazoline Ligands. Journal of the American Chemical Society, 2007, 129, 11876-11877.	6.6	129
12	Oxygen Transport in Perovskite-Type Solid Oxide Fuel Cell Materials: Insights from Quantum Mechanics. Accounts of Chemical Research, 2014, 47, 3340-3348.	7.6	121
13	The Electronic States of Rhenium Bipyridyl Electrocatalysts for CO₂ Reduction as Revealed by Xâ€ray Absorption Spectroscopy and Computational Quantum Chemistry. Angewandte Chemie - International Edition, 2013, 52, 4841-4844.	7.2	119
14	Unraveling the Wacker Oxidation Mechanisms. Journal of the American Chemical Society, 2007, 129, 12342-12343.	6.6	110
15	Electrochemical reactivities of pyridinium in solution: consequences for CO2 reduction mechanisms. Chemical Science, 2013, 4, 1490.	3.7	110
16	The Reaction Mechanism of the Enantioselective Tsuji Allylation: Inner-Sphere and Outer-Sphere Pathways, Internal Rearrangements, and Asymmetric Câ€“C Bond Formation. Journal of the American Chemical Society, 2012, 134, 19050-19060.	6.6	103
17	Size-extensivity-corrected multireference configuration interaction schemes to accurately predict bond dissociation energies of oxygenated hydrocarbons. Journal of Chemical Physics, 2014, 140, 044317.	1.2	85
18	Quantum Chemical Benchmarking, Validation, and Prediction of Acidity Constants for Substituted Pyridinium Ions and Pyridinyl Radicals. Journal of Chemical Theory and Computation, 2012, 8, 3187-3206.	2.3	81

#	Article	IF	Citations
19	Free Standing Nanoporous Palladium Alloys as CO Poisoning Tolerant Electrocatalysts for the Electrochemical Reduction of CO₂ to Formate. ACS Catalysis, 2019, 9, 5290-5301.	5.5	78
20	Ab initio DFT+U analysis of oxygen transport in LaCoO₃: the effect of Co³⁺ magnetic states. Journal of Materials Chemistry A, 2014, 2, 8060-8074.	5.2	76
21	Neural network and ReaxFF comparison for Au properties. International Journal of Quantum Chemistry, 2016, 116, 979-987.	1.0	66
22	Thermodynamic Hydricities of Biomimetic Organic Hydride Donors. Journal of the American Chemical Society, 2018, 140, 4569-4579.	6.6	65
23	Reactive forcefield for simulating gold surfaces and nanoparticles. Physical Review B, 2010, 81, .	1.1	64
24	Quantifying solvation energies at solid/liquid interfaces using continuum solvation methods. Molecular Simulation, 2017, 43, 420-427.	0.9	64
25	Inaccessibility of Î²-Hydride Elimination from â^'OH Functional Groups in Wacker-Type Oxidation. Journal of the American Chemical Society, 2006, 128, 3132-3133.	6.6	62
26	A Heterobimetallic Mechanism for Câ€“H Borylation Elucidated from Experimental and Computational Data. ACS Catalysis, 2015, 5, 3689-3699.	5.5	61
27	Oxidation of formic acid on the Pt(111) surface in the gas phase. Dalton Transactions, 2010, 39, 8450.	1.6	59
28	Experimental and Computational Study of a Direct O₂-Coupled Wacker Oxidation: Water Dependence in the Absence of Cu Salts. Journal of the American Chemical Society, 2010, 132, 11872-11874.	6.6	58
29	Theoretical Insights into Electrochemical CO₂ Reduction Mechanisms Catalyzed by Surface-Bound Nitrogen Heterocycles. Journal of Physical Chemistry Letters, 2013, 4, 4058-4063.	2.1	57
30	Significant Reduction in NiO Band Gap Upon Formation of Li_xNi_{1â^'x}O alloys: Applications To Solar Energy Conversion. ChemSusChem, 2014, 7, 195-201.	3.6	56
31	Machine Learning-Guided Approach for Studying Solvation Environments. Journal of Chemical Theory and Computation, 2020, 16, 633-642.	2.3	52
32	Alchemical Predictions for Computational Catalysis: Potential and Limitations. Journal of Physical Chemistry Letters, 2017, 8, 5002-5007.	2.1	48
33	Thermodynamic Descriptors for Molecules That Catalyze Efficient CO₂ Electroreductions. ACS Catalysis, 2015, 5, 1123-1130.	5.5	46
34	Accurate Bond Energies of Biodiesel Methyl Esters from Multireference Averaged Coupled-Pair Functional Calculations. Journal of Physical Chemistry A, 2014, 118, 7392-7403.	1.1	44
35	Computational investigation of CO₂ electroreduction on tin oxide and predictions of Ti, V, Nb and Zr dopants for improved catalysis. Journal of Materials Chemistry A, 2017, 5, 11756-11763.	5.2	44
36	A sobering assessment of smallâ€molecule force field methods for low energy conformer predictions. International Journal of Quantum Chemistry, 2018, 118, e25512.	1.0	43

#	Article	IF	Citations
37	Advances and challenges in modeling solvated reaction mechanisms for renewable fuels and chemicals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1446.	6.2	42
38	Regioselective De Novo Synthesis of Cyanohydroxypyridines with a Concerted Cycloaddition Mechanism. Journal of the American Chemical Society, 2008, 130, 13219-13221.	6.6	40
39	Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by ab Initio Molecular Dynamics and Nudged Elastic-Band Studies of NaBH₄ Hydrolysis. Journal of Physical Chemistry C, 2014, 118, 21385-21399.	1.5	37
40	Trends in Bond Dissociation Energies of Alcohols and Aldehydes Computed with Multireference Averaged Coupled-Pair Functional Theory. Journal of Physical Chemistry A, 2014, 118, 3039-3050.	1.1	36
41	Examining the selectivity of borohydride for carbon dioxide and bicarbonate reduction in protic conditions. Fuel, 2015, 150, 139-145.	3.4	34
42	A paramedic treatment for modeling explicitly solvated chemical reaction mechanisms. Chemical Science, 2018, 9, 5341-5346.	3.7	34
43	Cluster Models for Studying CO2 Reduction on Semiconductor Photoelectrodes. Topics in Catalysis, 2015, 58, 46-56.	1.3	30
44	Ab initio evaluation of oxygen diffusivity in LaFeO3: the role of lanthanum vacancies. MRS Communications, 2013, 3, 161-166.	0.8	26
45	Quantifying Uncertainties in Solvation Procedures for Modeling Aqueous Phase Reaction Mechanisms. Journal of Physical Chemistry A, 2021, 125, 154-164.	1.1	24
46	Nitrogen-doped nanocarbon materials under electroreduction operating conditions and implications for electrocatalysis of CO2. Carbon, 2017, 111, 859-866.	5.4	22
47	Comment on â€œMechanism and Kinetics of the Wacker Process: A Quantum Mechanical Approachâ€. Organometallics, 2009, 28, 1618-1619.	1.1	20
48	Insufficient Hartreeâ€“Fock Exchange in Hybrid DFT Functionals Produces Bent Alkynyl Radical Structures. Journal of Physical Chemistry Letters, 2012, 3, 289-293.	2.1	19
49	Firstâ€Principles Modeling of Electrochemical Water Oxidation on MnO:ZnO(001). ChemElectroChem, 2014, 1, 407-415.	1.7	19
50	Doped Amorphous Ti Oxides To Deoptimize Oxygen Reduction Reaction Catalysis. Journal of Physical Chemistry C, 2017, 121, 16825-16830.	1.5	19
51	Mechanism of Isobutylene Polymerization: Quantum Chemical Insight into AlCl₃/H₂O-Catalyzed Reactions. ACS Catalysis, 2018, 8, 8006-8013.	5.5	19
52	Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. International Journal of Quantum Chemistry, 2018, 118, e25516.	1.0	17
53	Benchmarking Computational Alchemy for Carbide, Nitride, and Oxide Catalysts. Advanced Theory and Simulations, 2019, 2, 1800142.	1.3	16
54	First-principles modeling of chemistry in mixed solvents: Where to go from here?. Journal of Chemical Physics, 2020, 152, 130902.	1.2	15

#	Article	IF	Citations
55	Acceleration of catalyst discovery with easy, fast, and reproducible computational alchemy. International Journal of Quantum Chemistry, 2021, 121, e26380.	1.0	15
56	Explicitly Unraveling the Roles of Counterions, Solvent Molecules, and Electron Correlation in Solution Phase Reaction Pathways. Journal of Physical Chemistry B, 2016, 120, 10797-10807.	1.2	13
57	Structural and Substituent Group Effects on Multielectron Standard Reduction Potentials of Aromatic N-Heterocycles. Journal of Physical Chemistry A, 2016, 120, 6888-6894.	1.1	13
58	Unveiling the Synergistic Role of Oxygen Functional Groups in the Graphene-Mediated Oxidation of Glutathione. ACS Applied Materials & Interfaces, 2020, 12, 45753-45762.	4.0	12
59	Atomicâ€Level Elucidation of the Initial Stages of Selfâ€Assembled Monolayer Metallization and Nanoparticle Formation. Chemistry - A European Journal, 2010, 16, 12381-12386.	1.7	10
60	Machine learning corrected alchemical perturbation density functional theory for catalysis applications. AICHE Journal, 2020, 66, e17041.	1.8	10
61	Multiscale Modeling of Au-Island Ripening on Au(100). Advances in Physical Chemistry, 2011, 2011, 1-11.	2.0	9
62	Water adsorption on MnO:ZnO(001) â€" From single molecules to bilayer coverage. Surface Science, 2013, 617, 218-224.	0.8	9
63	Combined Neural Network Potential and Density Functional Theory Study of TiAl₂O₅ Surface Morphology and Oxygen Reduction Reaction Overpotentials. Journal of Physical Chemistry C, 2020, 124, 15171-15179.	1.5	9
64	Theoretical studies of Pd metal deposition on the âˆš3Ã—âˆš3 4-mercaptopyridine self-assembled monolayer. Electrochimica Acta, 2010, 55, 8258-8262.	2.6	8
65	<scp>Gdâ€Niâ€Sbâ€SnO₂</scp> electrocatalysts for active and selective ozone production. AICHE Journal, 2021, 67, e17486.	1.8	8
66	Quantum Chemical Analyses of BH 4 â^' and BH 3 OH â^' Hydride Transfers to CO 2 in Aqueous Solution with Potentials of Mean Force. ChemPhysChem, 2017, 18, 3148-3152.	1.0	7
67	Liquids That Freeze When Mixed: Cocrystallization and Liquidâ€"Liquid Equilibrium in Polyoxacyclobutaneâ€"Water Mixtures. Macromolecules, 2018, 51, 3176-3183.	2.2	7
68	Oligomer Hydrate Crystallization Improves Carbon Nanotube Memory. Chemistry of Materials, 2018, 30, 3813-3818.	3.2	6
69	Deeper learning in electrocatalysis: realizing opportunities and addressing challenges. Current Opinion in Chemical Engineering, 2022, 36, 100824.	3.8	6
70	Standard redox potentials, pK_as, and hydricities of inorganic complexes under electrochemical conditions and implications for CO₂ reduction. Dalton Transactions, 2016, 45, 15336-15341.	1.6	5
71	Evaluating quantum alchemy of atoms with thermodynamic cycles: Beyond ground electronic states. Journal of Chemical Physics, 2022, 156, 064106.	1.2	5
72	A Bond-Energy/Bond-Order and Populations Relationship. Journal of Chemical Theory and Computation, 2022, 18, 4774-4794.	2.3	5

#	Article	IF	Citations
73	Computationally Guided Searches for Efficient Catalysts through Chemical/Materials Space: Progress and Outlook. Journal of Physical Chemistry C, 2021, 125, 6495-6507.	1.5	4
74	Computational predictions of metalâ€“macrocycle stability constants require accurate treatments of local solvent and pH effects. Physical Chemistry Chemical Physics, 2021, 23, 9189-9197.	1.3	4
75	Quantum Chemical Analyses of BH4 â^' and BH3 OHâ^' Hydride Transfers to CO2 in Aqueous Solution with Potentials of Mean Force. ChemPhysChem, 2017, 18, 3090-3090.	1.0	2
76	Quantum alchemy beyond singlets: Bonding in diatomic molecules with hydrogen. Journal of Chemical Physics, 2022, 156, .	1.2	2
77	Sugar Acetate-based Low Molecular Weight Organogelators. Chemistry Letters, 2020, 49, 1026-1029.	0.7	0
78	Computational Quantum Chemical Explorations of Chemical/Material Space for Efficient Electrocatalysts. Electrochemical Society Interface, 2020, 29, 63-66.	0.3	0
79	A Tribute to Emily A. Carter. Journal of Physical Chemistry A, 2021, 125, 1669-1670.	1.1	0
80	A Tribute to Emily A. Carter. Journal of Physical Chemistry C, 2021, 125, 4331-4332.	1.5	0