# 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 | Evaluating quantum alchemy of atoms with thermodynamic cycles: Beyond ground electronic states. Journal of Chemical Physics, 2022, 156, 064106. | 1.2 | 5 |
| 2 | Quantum alchemy beyond singlets: Bonding in diatomic molecules with hydrogen. Journal of Chemical Physics, 2022, 156, . | 1.2 | 2 |
| 3 | Deeper learning in electrocatalysis: realizing opportunities and addressing challenges. Current Opinion in Chemical Engineering, 2022, 36, 100824. | 3.8 | 6 |
| 4 | A Bond-Energy/Bond-Order and Populations Relationship. Journal of Chemical Theory and Computation, 2022, 18, 4774-4794. | 2.3 | 5 |
| 5 | Acceleration of catalyst discovery with easy, fast, and reproducible computational alchemy. International Journal of Quantum Chemistry, 2021, 121, e26380. | 1.0 | 15 |
| 6 | 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 |
| 7 | A Tribute to Emily A. Carter. Journal of Physical Chemistry A, 2021, 125, 1669-1670. | 1.1 | 0 |
| 8 | A Tribute to Emily A. Carter. Journal of Physical Chemistry C, 2021, 125, 4331-4332. | 1.5 | 0 |
| 9 | Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. Chemical Reviews, 2021, 121, 9816-9872. | 23.0 | 287 |
| 10 | 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 |
| 11 | Quantifying Uncertainties in Solvation Procedures for Modeling Aqueous Phase Reaction Mechanisms. Journal of Physical Chemistry A, 2021, 125, 154-164. | 1.1 | 24 |
| 12 | <scp>Gdâ€Niâ€Sbâ€SnO<sub>2</sub></scp> electrocatalysts for active and selective ozone production. AIChE Journal, 2021, 67, e17486. | 1.8 | 8 |
| 13 | 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 |
| 14 | Machine Learning-Guided Approach for Studying Solvation Environments. Journal of Chemical Theory and Computation, 2020, 16, 633-642. | 2.3 | 52 |
| 15 | Using natureâ€™s blueprint to expand catalysis with Earth-abundant metals. Science, 2020, 369, . | 6.0 | 306 |
| 16 | Machine learning corrected alchemical perturbation density functional theory for catalysis applications. AIChE Journal, 2020, 66, e17041. | 1.8 | 10 |
| 17 | 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 |
| 18 | Sugar Acetate-based Low Molecular Weight Organogelators. Chemistry Letters, 2020, 49, 1026-1029. | 0.7 | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Combined Neural Network Potential and Density Functional Theory Study of TiAl<sub>2</sub>O<sub>5</sub> Surface Morphology and Oxygen Reduction Reaction Overpotentials. Journal of Physical Chemistry C, 2020, 124, 15171-15179. | 1.5 | 9 |
| 20 | Computational Quantum Chemical Explorations of Chemical/Material Space for Efficient Electrocatalysts. Electrochemical Society Interface, 2020, 29, 63-66. | 0.3 | 0 |
| 21 | First-principles modeling of chemistry in mixed solvents: Where to go from here?. Journal of Chemical Physics, 2020, 152, 130902. | 1.2 | 15 |
| 22 | Free Standing Nanoporous Palladium Alloys as CO Poisoning Tolerant Electrocatalysts for the Electrochemical Reduction of CO<sub>2</sub> to Formate. ACS Catalysis, 2019, 9, 5290-5301. | 5.5 | 78 |
| 23 | Benchmarking Computational Alchemy for Carbide, Nitride, and Oxide Catalysts. Advanced Theory and Simulations, 2019, 2, 1800142. | 1.3 | 16 |
| 24 | Liquids That Freeze When Mixed: Cocrystallization and Liquidâ€“Liquid Equilibrium in Polyoxacyclobutaneâ€“Water Mixtures. Macromolecules, 2018, 51, 3176-3183. | 2.2 | 7 |
| 25 | Thermodynamic Hydricities of Biomimetic Organic Hydride Donors. Journal of the American Chemical Society, 2018, 140, 4569-4579. | 6.6 | 65 |
| 26 | 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 |
| 27 | Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. International Journal of Quantum Chemistry, 2018, 118, e25516. | 1.0 | 17 |
| 28 | Oligomer Hydrate Crystallization Improves Carbon Nanotube Memory. Chemistry of Materials, 2018, 30, 3813-3818. | 3.2 | 6 |
| 29 | A paramedic treatment for modeling explicitly solvated chemical reaction mechanisms. Chemical Science, 2018, 9, 5341-5346. | 3.7 | 34 |
| 30 | Mechanism of Isobutylene Polymerization: Quantum Chemical Insight into AlCl<sub>3</sub>/H<sub>2</sub>O-Catalyzed Reactions. ACS Catalysis, 2018, 8, 8006-8013. | 5.5 | 19 |
| 31 | Quantifying solvation energies at solid/liquid interfaces using continuum solvation methods. Molecular Simulation, 2017, 43, 420-427. | 0.9 | 64 |
| 32 | Computational investigation of CO<sub>2</sub> 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 |
| 33 | Alchemical Predictions for Computational Catalysis: Potential and Limitations. Journal of Physical Chemistry Letters, 2017, 8, 5002-5007. | 2.1 | 48 |
| 34 | 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 |
| 35 | 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 |
| 36 | Doped Amorphous Ti Oxides To Deoptimize Oxygen Reduction Reaction Catalysis. Journal of Physical Chemistry C, 2017, 121, 16825-16830. | 1.5 | 19 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Nitrogen-doped nanocarbon materials under electroreduction operating conditions and implications for electrocatalysis of CO2. Carbon, 2017, 111, 859-866. | 5.4 | 22 |
| 38 | Neural network and ReaxFF comparison for Au properties. International Journal of Quantum Chemistry, 2016, 116, 979-987. | 1.0 | 66 |
| 39 | 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 |
| 40 | Standard redox potentials, pK<sub>a</sub>s, and hydricities of inorganic complexes under electrochemical conditions and implications for CO<sub>2</sub> reduction. Dalton Transactions, 2016, 45, 15336-15341. | 1.6 | 5 |
| 41 | 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 |
| 42 | A Heterobimetallic Mechanism for Câ€“H Borylation Elucidated from Experimental and Computational Data. ACS Catalysis, 2015, 5, 3689-3699. | 5.5 | 61 |
| 43 | Thermodynamic Descriptors for Molecules That Catalyze Efficient CO<sub>2</sub> Electroreductions. ACS Catalysis, 2015, 5, 1123-1130. | 5.5 | 46 |
| 44 | Cluster Models for Studying CO2 Reduction on Semiconductor Photoelectrodes. Topics in Catalysis, 2015, 58, 46-56. | 1.3 | 30 |
| 45 | Examining the selectivity of borohydride for carbon dioxide and bicarbonate reduction in protic conditions. Fuel, 2015, 150, 139-145. | 3.4 | 34 |
| 46 | Firstâ€Principles Modeling of Electrochemical Water Oxidation on MnO:ZnO(001). ChemElectroChem, 2014, 1, 407-415. | 1.7 | 19 |
| 47 | Significant Reduction in NiO Band Gap Upon Formation of Li<sub>x</sub>Ni<sub>1â^'x</sub>O alloys: Applications To Solar Energy Conversion. ChemSusChem, 2014, 7, 195-201. | 3.6 | 56 |
| 48 | 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 |
| 49 | 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 |
| 50 | Ab initio DFT+U analysis of oxygen transport in LaCoO<sub>3</sub>: the effect of Co<sup>3+</sup> magnetic states. Journal of Materials Chemistry A, 2014, 2, 8060-8074. | 5.2 | 76 |
| 51 | 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 |
| 52 | 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 |
| 53 | Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by ab Initio Molecular Dynamics and Nudged Elastic-Band Studies of NaBH<sub>4</sub> Hydrolysis. Journal of Physical Chemistry C, 2014, 118, 21385-21399. | 1.5 | 37 |
| 54 | Elucidation of the Selectivity of Proton-Dependent Electrocatalytic CO<sub>2</sub> Reduction by fac-Re(bpy)(CO)<sub>3</sub>Cl. Journal of the American Chemical Society, 2013, 135, 15823-15829. | 6.6 | 238 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Ab Initio DFT+U Analysis of Oxygen Vacancy Formation and Migration in La<sub>1-x</sub>Sr<sub>x</sub>FeO<sub>3-Î´</sub>(x= 0, 0.25, 0.50). Chemistry of Materials, 2013, 25, 3011-3019. | 3.2 | 153 |
| 56 | Electrochemical reactivities of pyridinium in solution: consequences for CO2 reduction mechanisms. Chemical Science, 2013, 4, 1490. | 3.7 | 110 |
| 57 | Water adsorption on MnO:ZnO(001) â€" From single molecules to bilayer coverage. Surface Science, 2013, 617, 218-224. | 0.8 | 9 |
| 58 | The Electronic States of Rhenium Bipyridyl Electrocatalysts for CO<sub>2</sub> Reduction as Revealed by Xâ€ray Absorption Spectroscopy and Computational Quantum Chemistry. Angewandte Chemie - International Edition, 2013, 52, 4841-4844. | 7.2 | 119 |
| 59 | Theoretical Insights into Electrochemical CO<sub>2</sub> Reduction Mechanisms Catalyzed by Surface-Bound Nitrogen Heterocycles. Journal of Physical Chemistry Letters, 2013, 4, 4058-4063. | 2.1 | 57 |
| 60 | Ab initio evaluation of oxygen diffusivity in LaFeO3: the role of lanthanum vacancies. MRS Communications, 2013, 3, 161-166. | 0.8 | 26 |
| 61 | 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 |
| 62 | 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 |
| 63 | 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 |
| 64 | Theoretical Insights into Pyridinium-Based Photoelectrocatalytic Reduction of CO<sub>2</sub>. Journal of the American Chemical Society, 2012, 134, 7580-7583. | 6.6 | 161 |
| 65 | 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 |
| 66 | Multiscale Modeling of Au-Island Ripening on Au(100). Advances in Physical Chemistry, 2011, 2011, 1-11. | 2.0 | 9 |
| 67 | Theoretical studies of Pd metal deposition on the âˆš3Ã—âˆš3 4-mercaptopyridine self-assembled monolayer. Electrochimica Acta, 2010, 55, 8258-8262. | 2.6 | 8 |
| 68 | Theoretical Investigations of the Oxygen Reduction Reaction on Pt(111). ChemPhysChem, 2010, 11, 2779-2794. | 1.0 | 200 |
| 69 | 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 |
| 70 | 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 |
| 71 | 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 |
| 72 | Reactive forcefield for simulating gold surfaces and nanoparticles. Physical Review B, 2010, 81, . | 1.1 | 64 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Experimental and Computational Study of a Direct O<sub>2</sub>-Coupled Wacker Oxidation: Water Dependence in the Absence of Cu Salts. Journal of the American Chemical Society, 2010, 132, 11872-11874. | 6.6 | 58 |
| 74 | Oxidation of formic acid on the Pt(111) surface in the gas phase. Dalton Transactions, 2010, 39, 8450. | 1.6 | 59 |
| 75 | The Mechanism of the Wacker Reaction: A Tale of Two Hydroxypalladations. Angewandte Chemie - International Edition, 2009, 48, 9038-9049. | 7.2 | 261 |
| 76 | Comment on â€œMechanism and Kinetics of the Wacker Process: A Quantum Mechanical Approachâ€. Organometallics, 2009, 28, 1618-1619. | 1.1 | 20 |
| 77 | Regioselective De Novo Synthesis of Cyanohydroxypyridines with a Concerted Cycloaddition Mechanism. Journal of the American Chemical Society, 2008, 130, 13219-13221. | 6.6 | 40 |
| 78 | Unraveling the Wacker Oxidation Mechanisms. Journal of the American Chemical Society, 2007, 129, 12342-12343. | 6.6 | 110 |
| 79 | 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 |
| 80 | 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 |