James T Muckerman

List of Publications by Year
in descending order

70 papers	6,827 citations	66343 42 h-index	82547 72 g-index
75 all docs	75 docs citations	75 times ranked	7487 citing authors

#	Article	IF	Citations
1	The Trans Effect in Electrocatalytic CO₂ Reduction: Mechanistic Studies of Asymmetric Ruthenium Pyridyl-Carbene Catalysts. Journal of the American Chemical Society, 2019, 141, 6658-6671.	13.7	51
2	Picolinamideâ€Based Iridium Catalysts for Dehydrogenation of Formic Acid in Water: Effect of Amide N Substituent on Activity and Stability. Chemistry - A European Journal, 2018, 24, 18389-18392.	3.3	35
3	Photocatalytic CO₂ Reduction by Trigonal-Bipyramidal Cobalt(II) Polypyridyl Complexes: The Nature of Cobalt(I) and Cobalt(0) Complexes upon Their Reactions with CO₂, CO, or Proton. Inorganic Chemistry, 2018, 57, 5486-5498.	4.0	53
4	Highly Efficient and Selective Methanol Production from Paraformaldehyde and Water at Room Temperature. ACS Catalysis, 2018, 8, 5233-5239.	11.2	20
5	Additive-Free Ruthenium-Catalyzed Hydrogen Production from Aqueous Formaldehyde with High Efficiency and Selectivity. ACS Catalysis, 2018, 8, 8600-8605.	11.2	36
6	CO₂ Hydrogenation Catalysts with Deprotonated Picolinamide Ligands. ACS Catalysis, 2017, 7, 6426-6429.	11.2	70
7	Efficient Hydrogen Storage and Production Using a Catalyst with an Imidazolineâ€Based, Protonâ€Responsive Ligand. ChemSusChem, 2017, 10, 1071-1075.	6.8	57
8	Iridium Complexes with Protonâ€Responsive Azoleâ€Type Ligands as Effective Catalysts for CO₂ Hydrogenation. ChemSusChem, 2017, 10, 4535-4543.	6.8	41
9	Noninnocent Proton-Responsive Ligand Facilitates Reductive Deprotonation and Hinders CO₂ Reduction Catalysis in [Ru(tpy)(6DHBP)(NCCH₃)]²⁺ (6DHBP =) Tj ETQq1 1 0.784314 rgBT	4.0	43
10	Mechanism of Photocatalytic Reduction of CO₂ by Re(bpy)(CO)₃Cl from Differences in Carbon Isotope Discrimination. ACS Catalysis, 2016, 6, 5473-5481.	11.2	58
11	Direction to practical production of hydrogen by formic acid dehydrogenation with Cp*Ir complexes bearing imidazoline ligands. Catalysis Science and Technology, 2016, 6, 988-992.	4.1	69
12	Efficient Cp*Ir Catalysts with Imidazoline Ligands for CO2Hydrogenation. European Journal of Inorganic Chemistry, 2015, 2015, 5591-5594.	2.0	39
13	Striking Differences in Properties of Geometric Isomers of [Ir(tpy)(ppy)H]⁺: Experimental and Computational Studies of their Hydricities, Interaction with CO₂, and Photochemistry. Angewandte Chemie - International Edition, 2015, 54, 14128-14132.	13.8	51
14	Push or Pull? Proton Responsive Ligand Effects in Rhenium Tricarbonyl CO₂ Reduction Catalysts. Journal of Physical Chemistry B, 2015, 119, 7457-7466.	2.6	88
15	CO₂ Hydrogenation Catalyzed by Iridium Complexes with a Proton-Responsive Ligand. Inorganic Chemistry, 2015, 54, 5114-5123.	4.0	106
16	Biomass-derived high-performance tungsten-based electrocatalysts on graphene for hydrogen evolution. Journal of Materials Chemistry A, 2015, 3, 18572-18577.	10.3	43
17	Mechanistic Studies of Hydrogen Evolution in Aqueous Solution Catalyzed by a Tertpyridineâ€“Amine Cobalt Complex. Inorganic Chemistry, 2015, 54, 4310-4321.	4.0	64
18	Highly Robust Hydrogen Generation by Bioinspired Ir Complexes for Dehydrogenation of Formic Acid in Water: Experimental and Theoretical Mechanistic Investigations at Different pH. ACS Catalysis, 2015, 5, 5496-5504.	11.2	134

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19	CO₂ Hydrogenation to Formate and Methanol as an Alternative to Photo- and Electrochemical CO₂ Reduction. Chemical Reviews, 2015, 115, 12936-12973.	47.7	1,244
20	Positional Effects of Hydroxy Groups on Catalytic Activity of Proton-Responsive Half-Sandwich Cp*Iridium(III) Complexes. Organometallics, 2014, 33, 6519-6530.	2.3	104
21	First-Principles Approach to Calculating Energy Level Alignment at Aqueous Semiconductor Interfaces. Physical Review Letters, 2014, 113, 176802.	7.8	72
22	Formic Acid Dehydrogenation with Bioinspired Iridium Complexes: A Kinetic Isotope Effect Study and Mechanistic Insight. ChemSusChem, 2014, 7, 1976-1983.	6.8	123
23	Efficient H₂generation from formic acid using azole complexes in water. Catalysis Science and Technology, 2014, 4, 34-37.	4.1	118
24	New Water Oxidation Chemistry of a Seven-Coordinate Ruthenium Complex with a Tetradentate Polypyridyl Ligand. Inorganic Chemistry, 2014, 53, 6904-6913.	4.0	48
25	Cp*Co(III) Catalysts with Proton-Responsive Ligands for Carbon Dioxide Hydrogenation in Aqueous Media. Inorganic Chemistry, 2013, 52, 12576-12586.	4.0	142
26	Density Functional Kinetic Monte Carlo Simulation of Waterâ€“Gas Shift Reaction on Cu/ZnO. Journal of Physical Chemistry C, 2013, 117, 3414-3425.	3.1	48
27	Mechanistic Insight through Factors Controlling Effective Hydrogenation of CO₂ Catalyzed by Bioinspired Proton-Responsive Iridium(III) Complexes. ACS Catalysis, 2013, 3, 856-860.	11.2	169
28	Biomass-derived electrocatalytic composites for hydrogen evolution. Energy and Environmental Science, 2013, 6, 1818.	30.8	343
29	Hydroxy-substituted pyridine-like N-heterocycles: versatile ligands in organometallic catalysis. New Journal of Chemistry, 2013, 37, 1860.	2.8	36
30	Toward the accurate calculation of pKa values in water and acetonitrile. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 882-891.	1.0	112
31	Aluminum Hydride Separation Using N-Alkylmorpholine. Journal of Physical Chemistry C, 2013, 117, 14983-14991.	3.1	5
32	Calculation of thermodynamic hydricities and the design of hydride donors for CO ₂ reduction. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15657-15662.	7.1	71
33	Nickel(ii) macrocycles: highly efficient electrocatalysts for the selective reduction of CO2 to CO. Energy and Environmental Science, 2012, 5, 9502.	30.8	180
34	Reversible hydrogen storage using CO2 and a proton-switchable iridium catalyst in aqueous media under mild temperatures and pressures. Nature Chemistry, 2012, 4, 383-388.	13.6	830
35	Second-coordination-sphere and electronic effects enhance iridium(iii)-catalyzed homogeneous hydrogenation of carbon dioxide in water near ambient temperature and pressure. Energy and Environmental Science, 2012, 5, 7923.	30.8	228
36	Theoretical studies of the mechanism of catalytic hydrogen production by a cobaloxime. Chemical Communications, 2011, 47, 12456.	4.1	213

#	Article	IF	Citations
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55	Quantum dynamics of the photoinitiated unimolecular dissociation of HOCO. Journal of Chemical Physics, 2002, 117, 11139-11145.	3.0	24
56	A K-dependent adiabatic approximation to the Rennerâ€“Teller effect for triatomic molecules. Journal of Chemical Physics, 2002, 116, 1435-1442.	3.0	25
57	Experimental and theoretical studies of the near-infrared spectrum of bromomethylene. Journal of Chemical Physics, 2001, 115, 5433-5444.	3.0	39
58	Competition between photochemistry and energy transfer in ultraviolet-excited diazabenzenes. I. Photofragmentation studies of pyrazine at 248 nm and 266 nm. Journal of Chemical Physics, 2000, 112, 5829-5843.	3.0	38
59	Strong-field optical control of vibrational dynamics: Vibrational Stark effect in planar acetylene. Journal of Chemical Physics, 1999, 110, 2446-2451.	3.0	10
60	Repetitively sampled time-of-flight mass spectrometry for gas-phase kinetics studies. Review of Scientific Instruments, 1999, 70, 3259-3264.	1.3	23
61	Symmetry-adapted filter diagonalization: Calculation of the vibrational spectrum of planar acetylene from correlation functions. Journal of Chemical Physics, 1998, 109, 7128-7136.	3.0	21
62	Vibrational eigenvalues and eigenfunctions for planar acetylene by wave-packet propagation, and its mode-selective infrared excitation. Journal of Chemical Physics, 1997, 107, 3402-3416.	3.0	32
63	Bond selective infrared multiphoton excitation and dissociation of linear monodeuterated acetylene. Journal of Chemical Physics, 1996, 105, 535-550.	3.0	10
64	Modeâ€selective infrared excitation of linear acetylene. Journal of Chemical Physics, 1995, 102, 3897-3910.	3.0	17
65	Studies of the 193 nm photolysis of diethyl ketone and acetone using timeâ€resolved Fourier transform emission spectroscopy. Journal of Chemical Physics, 1995, 102, 6660-6668.	3.0	37
66	Sampling of semiclassically quantized polyatomic molecule vibrations by an adiabatic switching method: Application to quasiclassical trajectory calculations. Journal of Chemical Physics, 1995, 102, 5695-5707.	3.0	28
67	On the valence bond diatomicsâ€inâ€molecules method. II. Application to the valence states of FH2. Journal of Chemical Physics, 1979, 71, 233-254.	3.0	52
68	On the valence bond diatomicsâ€inâ€molecules method. I. A projection operator reformulation. Journal of Chemical Physics, 1979, 71, 225-232.	3.0	50
69	Classical Dynamics of the Reaction of Fluorine Atoms with Hydrogen Molecules. III. The Hotâ€Atom Reactions of 18F with HD. Journal of Chemical Physics, 1972, 57, 3388-3396.	3.0	104
70	Classical Dynamics of the Reaction of Fluorine Atoms with Hydrogen Molecules. II. Dependence on the Potential Energy Surface. Journal of Chemical Physics, 1972, 56, 2997-3006.	3.0	219