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	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
2	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
3	Biomass-derived electrocatalytic composites for hydrogen evolution. Energy and Environmental Science, 2013, 6, 1818.	30.8	343
4	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
5	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
6	Theoretical studies of the mechanism of catalytic hydrogen production by a cobaloxime. Chemical Communications, 2011, 47, 12456.	4.1	213
7	Water Oxidation by a Ruthenium Complex with Noninnocent Quinone Ligands: Possible Formation of an Oâ^'O Bond at a Low Oxidation State of the Metal. Inorganic Chemistry, 2008, 47, 1787-1802.	4.0	200
8	Nickel(ii) macrocycles: highly efficient electrocatalysts for the selective reduction of CO2 to CO. Energy and Environmental Science, 2012, 5, 9502.	30.8	180
9	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
10	Cp*Co(III) Catalysts with Proton-Responsive Ligands for Carbon Dioxide Hydrogenation in Aqueous Media. Inorganic Chemistry, 2013, 52, 12576-12586.	4.0	142
11	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
12	Formic Acid Dehydrogenation with Bioinspired Iridium Complexes: A Kinetic Isotope Effect Study and Mechanistic Insight. ChemSusChem, 2014, 7, 1976-1983.	6.8	123
13	Efficient H₂generation from formic acid using azole complexes in water. Catalysis Science and Technology, 2014, 4, 34-37.	4.1	118
14	First-Principles Studies of the Structural and Electronic Properties of the (Ga₁₋_xZn_x)(N₁₋_xO_x) Solid Solution Photocatalyst. Journal of Physical Chemistry C, 2008, 112, 3439-3446.	4.1	115
15	Toward the accurate calculation of pKa values in water and acetonitrile. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 882-891.	1.0	112
16	CO₂ Hydrogenation Catalyzed by Iridium Complexes with a Proton-Responsive Ligand. Inorganic Chemistry, 2015, 54, 5114-5123.	4.0	106
17	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
18	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

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19	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
20	Desulfurization of SO2and Thiophene on Surfaces and Nanoparticles of Molybdenum Carbide:Â Unexpected Ligand and Steric Effects. Journal of Physical Chemistry B, 2004, 108, 15662-15670.	2.6	72
21	First-Principles Approach to Calculating Energy Level Alignment at Aqueous Semiconductor Interfaces. Physical Review Letters, 2014, 113, 176802.	7.8	72
22	In Situ XRD Studies of ZnO/GaN Mixtures at High Pressure and High Temperature: Synthesis of Zn-Rich (Ga_{1â^'x}Zn_x)(N_{1â^'x}O_x) Photocatalysts. Journal of Physical Chemistry C, 2010, 114, 1809-1814.	3.1	71
23	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
24	CO₂ Hydrogenation Catalysts with Deprotonated Picolinamide Ligands. ACS Catalysis, 2017, 7, 6426-6429.	11.2	70
25	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
26	Mechanistic Studies of Hydrogen Evolution in Aqueous Solution Catalyzed by a Tertpyridineâ€“Amine Cobalt Complex. Inorganic Chemistry, 2015, 54, 4310-4321.	4.0	64
27	Preparation of (Ga_{1â^'x}Zn_x)(N_{1â^'x}O_x) Photocatalysts from the Reaction of NH₃ with Ga₂O₃/ZnO and ZnGa₂O₄: In Situ Time-Resolved XRD and XAFS Studies. Journal of Physical Chemistry C, 2009, 113, 3650-3659.	3.1	63
28	MRCI Calculations of the Lowest Potential Energy Surface for CH3OH and Direct ab Initio Dynamics Simulations of the O(1D) + CH4Reactionâ€. Journal of Physical Chemistry A, 2004, 108, 8615-8623.	2.5	58
29	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
30	Efficient Hydrogen Storage and Production Using a Catalyst with an Imidazolineâ€Based, Protonâ€Responsive Ligand. ChemSusChem, 2017, 10, 1071-1075.	6.8	57
31	Chemical reactivity of metcar Ti8C12, nanocrystal Ti14C13 and a bulk TiC(001) surface: A density functional study. Journal of Chemical Physics, 2003, 118, 7737-7740.	3.0	53
32	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
33	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
34	Water Adsorption on the GaN (101Ì…0) Nonpolar Surface. Journal of Physical Chemistry C, 2009, 113, 3365-3368.	3.1	51
35	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
36	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

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37	On the valence bond diatomicsâ€inâ€molecules method. I. A projection operator reformulation. Journal of Chemical Physics, 1979, 71, 225-232.	3.0	50
38			

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55	A K-dependent adiabatic approximation to the Rennerâ€“Teller effect for triatomic molecules. Journal of Chemical Physics, 2002, 116, 1435-1442.	3.0	25
56	Quantum dynamics of the photoinitiated unimolecular dissociation of HOCO. Journal of Chemical Physics, 2002, 117, 11139-11145.	3.0	24
57	Repetitively sampled time-of-flight mass spectrometry for gas-phase kinetics studies. Review of Scientific Instruments, 1999, 70, 3259-3264.	1.3	23
58	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
59	Highly Efficient and Selective Methanol Production from Paraformaldehyde and Water at Room Temperature. ACS Catalysis, 2018, 8, 5233-5239.	11.2	20
60	Modeâ€selective infrared excitation of linear acetylene. Journal of Chemical Physics, 1995, 102, 3897-3910.	3.0	17
61	Electrodeposition of Pt onto RuO₂(110) Single-Crystal Surface. Journal of Physical Chemistry C, 2007, 111, 15306-15311.	3.1	13
62	Exploring the Multiple Reaction Pathways for the H + cyc-C3H6 Reaction. Journal of Physical Chemistry A, 2004, 108, 10844-10849.	2.5	11
63	Theoretical Investigation of the Binding of Small Molecules and the Intramolecular Agostic Interaction at Tungsten Centers with Carbonyl and Phosphine Ligandsâ€. Journal of Physical Chemistry B, 2007, 111, 6815-6821.	2.6	11
64	Bond selective infrared multiphoton excitation and dissociation of linear monodeuterated acetylene. Journal of Chemical Physics, 1996, 105, 535-550.	3.0	10
65	Strong-field optical control of vibrational dynamics: Vibrational Stark effect in planar acetylene. Journal of Chemical Physics, 1999, 110, 2446-2451.	3.0	10
66	THEORETICAL DETERMINATION OF ROVIBRATIONAL ENERGIES AND ANOMALOUS ISOTOPIC EFFECT OF WEAKLY BOUND CLUSTER HXeOH. Journal of Theoretical and Computational Chemistry, 2003, 02, 573-581.	1.8	7
67	Catalytic Reactions Using Transition-Metal-Complexes Toward Solar Fuel Generation. Bulletin of Japan Society of Coordination Chemistry, 2008, 51, 41-54.	0.2	7
68	Aluminum Hydride Separation Using N-Alkylmorpholine. Journal of Physical Chemistry C, 2013, 117, 14983-14991.	3.1	5
69	Artificial Photosynthesis. ACS Symposium Series, 2010, , 283-312.	0.5	2
70	A Density Functional Theory Study of the Catalytic role of Ti atoms in Reversible Hydrogen Storage in the Complex Metal Hydride, NaAlH4. Materials Research Society Symposia Proceedings, 2005, 884, 1.	0.1	0