Michael B Hall

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348 papers	13,334 citations	59 h-index	97 g-index
367 ext. papers	14,058 ext. citations	8.2 avg, IF	6.64 L-index

#	Paper	IF	Citations
348	Theoretical studies on reactions of transition-metal complexes. *Chemical Reviews*, **2000**, 100, 353-406	68.1	744
347	Electronic structure and bonding in methyl- and perfluoromethyl(pentacarbonyl)manganese. *Inorganic Chemistry*, **1972**, 11, 768-775	5.1	477
346	Basis sets for transition metals: Optimized outer p functions. *Journal of Computational Chemistry*, **1996**, 17, 1359-70	3.5	384
345	Computational studies of [NiFe] and [FeFe] hydrogenases. *Chemical Reviews*, **2007**, 107, 4414-35	68.1	364
344	A capable bridging ligand for Fe-only hydrogenase: density functional calculations of a low-energy route for heterolytic cleavage and formation of dihydrogen. *Journal of the American Chemical Society*, **2001**, 123, 3828-9	16.4	315
343	Rhodium boryl complexes in the catalytic, terminal functionalization of alkanes. *Journal of the American Chemical Society*, **2005**, 127, 2538-52	16.4	288
342	Monomeric and oligomeric amine-borane sigma-complexes of rhodium. intermediates in the catalytic dehydrogenation of amine-boranes. *Journal of the American Chemical Society*, **2009**, 131, 15440-56	16.4	175
341	Fundamental properties of small molecule models of Fe-only hydrogenase: computations relative to the definition of an entatic state in the active site. *Coordination Chemistry Reviews*, **2003**, 238-239, 255-266	23.2	175
340	Thermally Stable Homogeneous Catalysts for Alkane Dehydrogenation S.O. thanks the German Academic Exchange Service (DAAD) for financing a research stay with W.C.K. in the USA. This work was supported by the National Science Foundation (CHE 9800184 to M.B.H.), by the University of California Energy Institute and University of California Santa Barbara (to W.C.K.), and by the	16.4	167
339	Theoretical Characterization of the Reaction Intermediates in a Model of the Nickel–Iron Hydrogenase of Desulfovibrio gigas. *Journal of the American Chemical Society*, **1999**, 121, 4000-4007	16.4	164
338	Experimental and computational evidence for a boron-assisted, sigma-bond metathesis pathway for alkane borylation. *Journal of the American Chemical Society*, **2003**, 125, 858-9	16.4	156
337	Modeling the active sites in metalloenzymes. 3. Density functional calculations on models for [Fe]-hydrogenase: structures and vibrational frequencies of the observed redox forms and the reaction mechanism at the Diiron Active Center. *Journal of the American Chemical Society*, **2001**, 123, 3734-42	16.4	156
336	Monoiron hydrogenase catalysis: hydrogen activation with the formation of a dihydrogen, Fe-H(delta-)...H(delta+)-O, bond and methenyl-H4MPT+ triggered hydride transfer. *Journal of the American Chemical Society*, **2009**, 131, 10901-8	16.4	143
335	Flexible Zirconium Metal-Organic Frameworks as Bioinspired Switchable Catalysts. *Angewandte Chemie - International Edition*, **2016**, 55, 10776-80	16.4	143
334	Tetrarhena-heterocycle from the palladium-catalyzed dimerization of Re2(CO)8(μ-SbPh2)(μ-H) exhibits an unusual host-guest behavior. *Journal of the American Chemical Society*, **2011**, 133, 12994-7	16.4	138
333	Electronic effects steer the mechanism of asymmetric hydrogenations of unfunctionalized aryl-substituted alkenes. *Journal of the American Chemical Society*, **2004**, 126, 16688-9	16.4	135
332	De novo design of synthetic di-iron(I) complexes as structural models of the reduced form of iron-iron hydrogenase. *Inorganic Chemistry*, **2006**, 45, 1552-9	5.1	133

331	Dual electron uptake by simultaneous iron and ligand reduction in an N-heterocyclic carbene substituted [FeFe] hydrogenase model compound. *Inorganic Chemistry*, **2005**, 44, 5550-2	5.1	132
330	The catalytic dehydrogenation of ammonia-borane involving an unexpected hydrogen transfer to ligated carbene and subsequent carbon-hydrogen activation. *Journal of the American Chemical Society*, **2008**, 130, 1798-9	16.4	128
329	Mechanism of water splitting and oxygen-oxygen bond formation by a mononuclear ruthenium complex. *Journal of the American Chemical Society*, **2010**, 132, 120-30	16.4	125
328	Hydrogen-substituted osmium silylene complexes: effect of charge localization on catalytic hydrosilation. *Journal of the American Chemical Society*, **2006**, 128, 428-9	16.4	122
327	Two-State Reactivity in Low-Valent Iron-Mediated C-H Activation and the Implications for Other First-Row Transition Metals. *Journal of the American Chemical Society*, **2016**, 138, 3715-30	16.4	108
326	Series of mixed valent Fe(II)Fe(I) complexes that model the Hox state of [FeFe]hydrogenase: redox properties, density-functional theory investigation, and reactivities with extrinsic CO. *Inorganic Chemistry*, **2008**, 47, 7009-24	5.1	106
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324	Synthesis of Carboxylic Acid-Modified [FeFe]-Hydrogenase Model Complexes Amenable to Surface Immobilization. *Organometallics*, **2007**, 26, 3976-3984	3.8	102
323	Theoretical Calculations of Metal-Dioxygen Complexes. *Chemical Reviews*, **1994**, 94, 639-658	68.1	101
322	Origins of the selectivity for borylation of primary over secondary C-H bonds catalyzed by Cp*-rhodium complexes. *Journal of the American Chemical Society*, **2010**, 132, 3078-91	16.4	97
321	Theoretical studies of inorganic and organometallic reaction mechanisms. 2. The trans effect in square-planar platinum(II) and rhodium(I) substitution reactions. *Inorganic Chemistry*, **1991**, 30, 646-651	5.1	94
320	Carbon-hydrogen bond activation: two, three, or more mechanisms?. *Journal of the American Chemical Society*, **2007**, 129, 12068-9	16.4	92
319	Theoretical Studies on Models for the Oxo-Transfer Reaction of Dioxomolybdenum Enzymes. *Inorganic Chemistry*, **1996**, 35, 1273-1278	5.1	92
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317	Mechanistic insights into iridium-catalyzed asymmetric hydrogenation of dienes. *Chemistry - A European Journal*, **2005**, 11, 6859-68	4.8	84
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315	Synthesis, reactivity, and DFT studies of tantalum complexes incorporating diamido-N-heterocyclic carbene ligands. Facile endocyclic C-H bond activation. *Journal of the American Chemical Society*, **2006**, 128, 12531-43	16.4	81
314	Density functional study of the catalytic cycle of nickel-iron [NiFe] hydrogenases and the involvement of high-spin nickel(II). *Journal of Biological Inorganic Chemistry*, **2006**, 11, 286-306	3.7	81

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312	A theoretical investigation of ruthenium-catalyzed alkene hydrosilation: evidence to support an exciting new mechanistic proposal. *Journal of the American Chemical Society*, **2004**, 126, 13564-5	16.4	75
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310	Prediction of the Geometries of Simple Transition Metal Polyhydride Complexes by Symmetry Analysis. *Journal of the American Chemical Society*, **1999**, 121, 1348-1358	16.4	74
309	Structural and spectroscopic features of mixed valent Fe(II)Fe(I) complexes and factors related to the rotated configuration of diiron hydrogenase. *Journal of the American Chemical Society*, **2012**, 134, 13089-102	16.4	73
308	The molecular and electronic structure of carbon–hydrogen bond activation and transition metal assisted hydrogen transfer. *Coordination Chemistry Reviews*, **2009**, 253, 1202-1218	23.2	72
307	Noncovalent bonding: Stacking interactions of chelate rings of transition metal complexes. *Coordination Chemistry Reviews*, **2017**, 345, 318-341	23.2	71
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