Djamaladdin G Musaev

List of Publications by Year in Descending Order

259 papers	14,323 citations	66 h-index	109 g-index
264 ext. papers	15,482 ext. citations	9.2 avg, IF	6.51 L-index

#	Paper	IF	Citations
259	Unconventional mechanism and selectivity of the Pd-catalyzed C-H bond lactonization in aromatic carboxylic acid.. *Nature Communications*, **2022**, 13, 315	17.4	3
258	Light-Promoted Dearomative Cross-Coupling of Heteroarenium Salts and Aryl Iodides via Nickel Catalysis. *ACS Catalysis*, **2022**, 12, 1818-1829	13.1	2
257	Computational Study of Key Mechanistic Details for a Proposed Copper (I)-Mediated Deconstructive Fluorination of -Protected Cyclic Amines.. *Topics in Catalysis*, **2022**, 65, 418-432	2.3	1
256	Hydrogen-Bonding as a Factor to Determine the Regioselectivity for Pd-mediated C–H Activation of Pyridine. *ChemCatChem*, **2021**, 13, 1201-1206	5.2	0
255	Key Mechanistic Features of the Silver(I)-Mediated Deconstructive Fluorination of Cyclic Amines: Multistate Reactivity versus Single-Electron Transfer. *Journal of the American Chemical Society*, **2021**, 143, 3889-3900	16.4	8
254	An All-Atom Theory of Electron Transfer at Nanocrystal/Molecule Interfaces: A Hybrid LCAO/DFT Approach. *Journal of Physical Chemistry C*, **2021**, 125, 5116-5126	3.8	1
253	A solvent-free solid catalyst for the selective and color-indicating ambient-air removal of sulfur mustard. *Communications Chemistry*, **2021**, 4,	6.3	6
252	C–H activation. *Nature Reviews Methods Primers*, **2021**, 1,		52
251	Polyniobate Nanothreads for Decomposition of the Nerve Agent Simulant Dimethyl Chlorophosphate. *ACS Applied Nano Materials*, **2021**, 4, 5649-5654	5.6	0
250	An Active-Site Sulfonate Group Creates a Fast Water Oxidation Electrocatalyst That Exhibits High Activity in Acid. *Angewandte Chemie - International Edition*, **2021**, 60, 1540-1545	16.4	6
249	Influence of Aryl Substituents on the Alignment of Ligands in the Dirhodium Tetrakis(1,2,2-Triarylcyclopropane- carboxylate) Catalysts. *ChemCatChem*, **2021**, 13, 174-179	5.2	4
248	Pyochelin Biosynthetic Metabolites Bind Iron and Promote Growth in Demonstrating Siderophore-like Activity. *ACS Infectious Diseases*, **2021**, 7, 544-551	5.5	3
247	Sequential Norrish-Yang Cyclization and C-C Cleavage/Cross-Coupling of a [4.1.0] Fused Saturated Azacycle. *Journal of Organic Chemistry*, **2021**, 86, 12436-12442	4.2	1
246	Nanoscale TiO Protection Layer Enhances the Built-In Field and Charge Separation Performance of GaP Photoelectrodes. *Nano Letters*, **2021**, 21, 8017-8024	11.5	2
245	Tafel Slope Analyses for Homogeneous Catalytic Reactions. *Catalysts*, **2021**, 11, 87	4	1
244	Reactivity and Selectivity Controlling Factors in the Pd/Dialkylbiarylphosphine-Catalyzed C-C Cleavage/Cross-Coupling of an N-Fused Bicyclo-Hydroxy-Lactam. *Journal of the American Chemical Society*, **2020**, 142, 21140-21152	16.4	11
243	Mechanistic details of the cobalt-mediated dehydrogenative dimerization of aminoquinoline-directed benzamides. *Chemical Science*, **2020**, 11, 6085-6096	9.4	7

242	C-C Cleavage Approach to C-H Functionalization of Saturated Aza-Cycles. *ACS Catalysis*, **2020**, 10, 2929-2941	13.1	26
241	Metal-Organic Framework- and Polyoxometalate-Based Sorbents for the Uptake and Destruction of Chemical Warfare Agents. *ACS Applied Materials & Interfaces*, **2020**, 12, 14641-14661	9.5	23
240	Roles of Base in the Pd-Catalyzed Annulative Chlorophenylene Dimerization. *ACS Catalysis*, **2020**, 10, 3059-3073	13.1	7
239	Rhodium-Stabilized Diarylcarbenes Behaving as Donor/Acceptor Carbenes. *ACS Catalysis*, **2020**, 10, 6240-6247	13.1	27
238	Multimodal Characterization of Materials and Decontamination Processes for Chemical Warfare Protection. *ACS Applied Materials & Interfaces*, **2020**, 12, 14721-14738	9.5	12
237	Tailored quinones support high-turnover Pd catalysts for oxidative C-H arylation with O. *Science*, **2020**, 370, 1454-1460	33.3	16
236	Can Donor Ligands Make Pd(OAc) a Stronger Oxidant? Access to Elusive Palladium(II) Reduction Potentials and Effects of Ancillary Ligands via Palladium(II)/Hydroquinone Redox Equilibria. *Journal of the American Chemical Society*, **2020**, 142, 19678-19688	16.4	13
235	Ion-pairing in polyoxometalate chemistry: impact of fully hydrated alkali metal cations on properties of the keggin [PWO] anion. *Dalton Transactions*, **2020**, 49, 11170-11178	4.3	0
234	Enhanced intersystem crossing of boron dipyrromethene by TEMPO radical. *Journal of Chemical Physics*, **2020**, 153, 154201	3.9	3
233	Comparison of 1,2-Diarylcyclopropanecarboxylates with 1,2,2-Triarylcyclopropanecarboxylates as Chiral Ligands for Dirhodium-Catalyzed Cyclopropanation and C-H Functionalization. *Journal of Organic Chemistry*, **2020**, 85, 12199-12211	4.2	5
232	Correlated Multimodal Approach Reveals Key Details of Nerve-Agent Decomposition by Single-Site Zr-Based Polyoxometalates. *Journal of Physical Chemistry Letters*, **2019**, 10, 2295-2299	6.4	17
231	Modulating electronic coupling at the quantum dot/molecule interface by wavefunction engineering. *Journal of Chemical Physics*, **2019**, 150, 124704	3.9	2
230	Predictive Model for the [Rh2(esp)2]-Catalyzed Intermolecular C(sp3)H Bond Insertion of Carbonyl Ester Carbenes: Interplay between Theory and Experiment. *ACS Catalysis*, **2019**, 9, 4526-4538	13.1	14
229	Effect of Carbon Dioxide on the Degradation of Chemical Warfare Agent Simulant in the Presence of Zr Metal Organic Framework MOF-808. *Chemistry of Materials*, **2019**, 31, 9904-9914	9.6	17
228	Di-Palladium Complexes are Active Catalysts for Mono-N-Protected Amino Acid-Accelerated Enantioselective CH Functionalization. *ACS Catalysis*, **2019**, 9, 11386-11397	13.1	15
227	Key mechanistic details of paraoxon decomposition by polyoxometalates: Critical role of para-nitro substitution. *Chemical Physics*, **2019**, 518, 30-37	2.3	7
226	A bulk adjusted linear combination of atomic orbitals (BA-LCAO) approach for nanoparticles. *Journal of Computational Chemistry*, **2019**, 40, 212-221	3.5	2
225	Understanding Regiodivergence in a Pd(II)-Mediated Site-Selective CH Alkynylation. *ACS Catalysis*, **2018**, 8, 4516-4527	13.1	27

224	Keiji Morokuma. *Journal of Physical Chemistry A*, **2018**, 122, 880-881	2.8	
223	Key mechanistic insights into the intramolecular C-H bond amination and double bond aziridination in sulfamate esters catalyzed by dirhodium tetracarboxylate complexes. *Journal of Organometallic Chemistry*, **2018**, 867, 183-192	2.3	11
222	Site-Selective Carbene-Induced C–H Functionalization Catalyzed by Dirhodium Tetrakis(triarylcyclopropanecarboxylate) Complexes. *ACS Catalysis*, **2018**, 8, 678-682	13.1	40
221	Impact of ambient gases on the mechanism of [CsNbO]-promoted nerve-agent decomposition. *Chemical Science*, **2018**, 9, 2147-2158	9.4	16
220	Unveiling the Role of Base and Additive in the Ullmann-Type of Arene-Aryl C–C Coupling Reaction. *ACS Catalysis*, **2018**, 8, 4829-4837	13.1	18
219	Design of catalysts for site-selective and enantioselective functionalization of non-activated primary C-H bonds. *Nature Chemistry*, **2018**, 10, 1048-1055	17.6	86
218	Generality and Strength of Transition Metal–Effects. *Journal of the American Chemical Society*, **2018**, 140, 10612-10618	16.4	10
217	Quantum Confinement Theory of Auger-Assisted Biexciton Recombination Dynamics in Type-I and Quasi Type-II Quantum Dots. *Journal of Physical Chemistry C*, **2018**, 122, 18742-18750	3.8	9
216	Multi-Tasking POM Systems. *Frontiers in Chemistry*, **2018**, 6, 365	5	16
215	Synthesis of [3a,7a]-Dihydroindoles by a Tandem Arene Cyclopropanation/3,5-Sigmatropic Rearrangement Reaction. *Journal of Organic Chemistry*, **2018**, 83, 7939-7949	4.2	7
214	Buffer-Induced Acceleration and Inhibition in Polyoxometalate-Catalyzed Organophosphorus Ester Hydrolysis. *ACS Catalysis*, **2018**, 8, 7068-7076	13.1	22
213	The mechanism of directed Ni(ii)-catalyzed C-H iodination with molecular iodine. *Chemical Science*, **2018**, 9, 1144-1154	9.4	31
212	Desymmetrization of cyclohexanes by site- and stereoselective C-H functionalization. *Nature*, **2018**, 564, 395-399	50.4	61
211	Mechanism of Permanganate-Promoted Dihydroxylation of Complex Diketopiperazines: Critical Roles of Counter-cation and Ion-Pairing. *Journal of the American Chemical Society*, **2018**, 140, 13375-13386	16.4	10
210	Catalyst-Controlled Selective Functionalization of Unactivated C-H Bonds in the Presence of Electronically Activated C-H Bonds. *Journal of the American Chemical Society*, **2018**, 140, 12247-12255	16.4	43
209	Comparison of Reactivity and Enantioselectivity between Chiral Bimetallic Catalysts: Bismuth–Rhodium- and Dirhodium-Catalyzed Carbene Chemistry. *ACS Catalysis*, **2018**, 8, 10676-10682	13.1	24
208	Biologically Inspired Total Synthesis of Ulbactin F, an Iron-Binding Natural Product. *Organic Letters*, **2018**, 20, 5922-5926	6.2	12
207	Tetracobalt-polyoxometalate catalysts for water oxidation: Key mechanistic details. *Journal of Catalysis*, **2017**, 350, 56-63	7.3	47

206	Mono--protected amino acid ligands stabilize dimeric palladium(ii) complexes of importance to C-H functionalization. *Chemical Science*, **2017**, 8, 5746-5756	9.4	30
205	Enantioselectivity Model for Pd-Catalyzed C□H Functionalization Mediated by the Mono-N-protected Amino Acid (MPAA) Family of Ligands. *ACS Catalysis*, **2017**, 7, 4344-4354	13.1	24
204	A Role for Pd(IV) in Catalytic Enantioselective C-H Functionalization with Monoprotected Amino Acid Ligands under Mild Conditions. *Journal of the American Chemical Society*, **2017**, 139, 9238-9245	16.4	38
203	Effects of Competitive Active-Site Ligand Binding on Proton- and Electron-Transfer Properties of the [Co4(H2O)2(PW9O34)2]10□Polyoxometalate Water Oxidation Catalyst. *Journal of Cluster Science*, **2017**, 28, 839-852	3	4
202	Site-selective and stereoselective functionalization of non-activated tertiary C-H bonds. *Nature*, **2017**, 551, 609-613	50.4	173
201	Cu-Catalyzed aromatic C-H imidation with -fluorobenzenesulfonimide: mechanistic details and predictive models. *Chemical Science*, **2017**, 8, 988-1001	9.4	44
200	Rh -Catalyzed □C(sp)-H Alkylation of Enol Ethers, Enamides and Enecarbamates with □Diazo Dicarbonyl Compounds. *Chemistry - A European Journal*, **2017**, 23, 1129-1135	4.8	6
199	Reaction Mechanism of Nerve-Agent Hydrolysis with the Cs8Nb6O19 Lindqvist Hexaniobate Catalyst. *Journal of Physical Chemistry C*, **2016**, 120, 16822-16830	3.8	17
198	Broad-Spectrum Liquid- and Gas-Phase Decontamination of Chemical Warfare Agents by One-Dimensional Heteropolyniobates. *Angewandte Chemie - International Edition*, **2016**, 55, 7403-7	16.4	82
197	Cu-based Polyoxometalate Catalyst for Efficient Catalytic Hydrogen Evolution. *Inorganic Chemistry*, **2016**, 55, 6750-8	5.1	34
196	Rh2(II,III) Catalysts with Chelating Carboxylate and Carboxamidate Supports: Electronic Structure and Nitrene Transfer Reactivity. *Journal of the American Chemical Society*, **2016**, 138, 2327-41	16.4	82
195	Enhancing photo-reduction quantum efficiency using quasi-type II core/shell quantum dots. *Chemical Science*, **2016**, 7, 4125-4133	9.4	29
194	Factors Controlling Stability and Reactivity of Dimeric Pd(II) Complexes in C□H Functionalization Catalysis. *ACS Catalysis*, **2016**, 6, 829-839	13.1	47
193	Broad-Spectrum Liquid- and Gas-Phase Decontamination of Chemical Warfare Agents by One-Dimensional Heteropolyniobates. *Angewandte Chemie*, **2016**, 128, 7529-7533	3.6	13
192	Transition Metal Substitution Effects on Metal-to-Polyoxometalate Charge Transfer. *Inorganic Chemistry*, **2016**, 55, 4308-19	5.1	19
191	Site-selective and stereoselective functionalization of unactivated C-H bonds. *Nature*, **2016**, 533, 230-4	50.4	220
190	Flexible Reaction Pocket on Bulky Diphosphine□Ir Complex Controls Regioselectivity in para-Selective C□H Borylation of Arenes. *ACS Catalysis*, **2016**, 6, 7536-7546	13.1	52
189	Water splitting with polyoxometalate-treated photoanodes: enhancing performance through sensitizer design. *Chemical Science*, **2015**, 6, 5531-5543	9.4	58

188	Mechanistic Details of Pd(II)-Catalyzed C-H Iodination with Molecular I2: Oxidative Addition vs Electrophilic Cleavage. *Journal of the American Chemical Society*, **2015**, 137, 9022-31	16.4	49
187	Decarbonylative organoboron cross-coupling of esters by nickel catalysis. *Nature Communications*, **2015**, 6, 7508	17.4	199
186	A Hybrid Quantum Mechanical Approach: Intimate Details of Electron Transfer between Type-I CdSe/ZnS Quantum Dots and an Anthraquinone Molecule. *Journal of Physical Chemistry B*, **2015**, 119, 7651-8	3.4	23
185	Factors Impacting the Mechanism of the Mono-N-Protected Amino Acid Ligand-Assisted and Directing-Group-Mediated C□H Activation Catalyzed by Pd(II) Complex. *ACS Catalysis*, **2015**, 5, 830-840	13.1	61
184	All-inorganic networks and tetramer based on tin(II)-containing polyoxometalates: tuning structural and spectral properties with lone-pairs. *Journal of the American Chemical Society*, **2014**, 136, 12085-91	16.4	39
183	Comparative Investigations of Cp*-Based Group 9 Metal-Catalyzed Direct C□H Amination of Benzamides. *Organometallics*, **2014**, 33, 4076-4085	3.8	105
182	An Infinite Order Discrete Variable Representation of an Effective Mass Hamiltonian: Application to Exciton Wave Functions in Quantum Confined Nanostructures. *Journal of Chemical Theory and Computation*, **2014**, 10, 3409-16	6.4	3
181	Key mechanistic features of Ni-catalyzed C-H/C-O biaryl coupling of azoles and naphthalen-2-yl pivalates. *Journal of the American Chemical Society*, **2014**, 136, 14834-44	16.4	147
180	Versatile reactivity of Pd-catalysts: mechanistic features of the mono-N-protected amino acid ligand and cesium-halide base in Pd-catalyzed C-H bond functionalization. *Chemical Society Reviews*, **2014**, 43, 5009-31	58.5	129
179	Extending metal-to-polyoxometalate charge transfer lifetimes: the effect of heterometal location. *Chemistry - A European Journal*, **2014**, 20, 4297-307	4.8	29
178	A noble-metal-free, tetra-nickel polyoxotungstate catalyst for efficient photocatalytic hydrogen evolution. *Journal of the American Chemical Society*, **2014**, 136, 14015-8	16.4	165
177	An exceptionally fast homogeneous carbon-free cobalt-based water oxidation catalyst. *Journal of the American Chemical Society*, **2014**, 136, 9268-71	16.4	225
176	Can bis(imino)pyridine iron, (PDI)FeL1L2, complexes catalyze C□H bond functionalization?. *Chemical Science*, **2013**, 4, 3758	9.4	22
175	Visible-light-driven hydrogen evolution from water using a noble-metal-free polyoxometalate catalyst. *Journal of Catalysis*, **2013**, 307, 48-54	7.3	83
174	Understanding the reactivity of Pd(0)/PR3-catalyzed intermolecular C(sp(3))-H bond arylation. *Journal of the American Chemical Society*, **2013**, 135, 14206-14	16.4	71
173	An inorganic chromophore based on a molecular oxide supported metal carbonyl cluster: [P2W17O61{Re(CO)3}3{ORb(H2O)}(□-OH)]9-. *Inorganic Chemistry*, **2013**, 52, 13490-5	5.1	23
172	Long lived charge separation in iridium(III)-photosensitized polyoxometalates: synthesis, photophysical and computational studies of organometallic□redox tunable oxide assemblies. *Chemical Science*, **2013**, 4, 1737	9.4	68
171	Differentiating homogeneous and heterogeneous water oxidation catalysis: confirmation that [Co4(H2O)2(□PW9O34)2]10- is a molecular water oxidation catalyst. *Journal of the American Chemical Society*, **2013**, 135, 14110-8	16.4	173

170	Electron Transfer Dynamics in Semiconductor□Chromophore□Polyoxometalate Catalyst Photoanodes. *Journal of Physical Chemistry C*, **2013**, 117, 918-926	3.8	100
169	Synthesis, structures, and photochemistry of tricarbonyl metal polyoxoanion complexes, [X2W20O70{M(CO)3}2]12□(X = Sb, Bi and M = Re, Mn). *Inorganic Chemistry*, **2013**, 52, 671-8	5.1	46
168	Iridium(III)-bis(oxazolinyl)phenyl catalysts for enantioselective C□H functionalization. *Chemical Science*, **2013**, 4, 2590	9.4	43
167	Rhodium-catalyzed enantioselective cyclopropanation of electron deficient alkenes. *Chemical Science*, **2013**, 4, 2844-2850	9.4	98
166	Parameterization of reactive force field: dynamics of the [Nb6O19H(x)]((8-x)-) Lindqvist polyoxoanion in bulk water. *Journal of Physical Chemistry A*, **2013**, 117, 6967-74	2.8	9
165	Bis(4?-(4-pyridyl)-2,2?:6?,2??-terpyridine)ruthenium(II) complexes and their N-alkylated derivatives in catalytic light-driven water oxidation. *RSC Advances*, **2013**, 3, 20647	3.7	18
164	Scope and mechanistic analysis of the enantioselective synthesis of allenes by rhodium-catalyzed tandem ylide formation/[2,3]-sigmatropic rearrangement between donor/acceptor carbenoids and propargylic alcohols. *Journal of the American Chemical Society*, **2012**, 134, 15497-504	16.4	143
163	Insight into Mechanistic Features of Ruthenium(II)□ybox-Catalyzed C□H Amination. *Organometallics*, **2012**, 31, 4950-4961	3.8	23
162	Mechanistic Insights into the Aerobic Cu(I)-Catalyzed Cross-Coupling of -Acyl Thiosalicylamide Thiol Esters and Boronic Acids. *Organometallics*, **2012**, 31, 7958-7968	3.8	12
161	Structural Modification of TiO2 Surfaces in Bulk Water and Binding Motifs of a Functionalized C60 on TiO2 Anatase and Rutile Surfaces in Vacuo and in Water: Molecular Dynamics Studies. *Journal of Physical Chemistry C*, **2012**, 116, 20937-20948	3.8	4
160	Polyoxometalate water oxidation catalysts and the production of green fuel. *Chemical Society Reviews*, **2012**, 41, 7572-89	58.5	593
159	In situ probe of photocarrier dynamics in water-splitting hematite (□Fe2O3) electrodes. *Energy and Environmental Science*, **2012**, 5, 8923	35.4	109
158	Key mechanistic features of enantioselective C-H bond activation reactions catalyzed by [(chiral mono-N-protected amino acid)-Pd(II)] complexes. *Journal of the American Chemical Society*, **2012**, 134, 1690-8	16.4	145
157	Revisiting the polyoxometalate-based late-transition-metal-oxo complexes: the "oxo wall" stands. *Inorganic Chemistry*, **2012**, 51, 7025-31	5.1	77
156	Catalytic adaptive recognition of thiol (SH) and selenol (SeH) groups toward synthesis of functionalized vinyl monomers. *Journal of the American Chemical Society*, **2012**, 134, 6637-49	16.4	84
155	Spectroscopic Studies of Light-driven Water Oxidation Catalyzed by Polyoxometalates. *Industrial & Engineering Chemistry Research*, **2012**, 51, 11850-11859	3.9	36
154	D2-symmetric dirhodium catalyst derived from a 1,2,2-triarylcyclopropanecarboxylate ligand: design, synthesis and application. *Journal of the American Chemical Society*, **2011**, 133, 19198-204	16.4	156
153	Synthesis and characterization of a metal-to-polyoxometalate charge transfer molecular chromophore. *Journal of the American Chemical Society*, **2011**, 133, 20134-7	16.4	74

152	Ditantalum dinitrogen complex: reaction of H2 molecule with "end-on-bridged" [Ta(IV)]2(□(1):□(1)-N2) and Bis(□itrido) [Ta(V)]2(□N)2 complexes. *Inorganic Chemistry*, **2011**, 50, 9481-90	5.1	21
151	A diruthenium catalyst for selective, intramolecular allylic C-H amination: reaction development and mechanistic insight gained through experiment and theory. *Journal of the American Chemical Society*, **2011**, 133, 17207-16	16.4	253
150	Polyoxometalates in the Design of Effective and Tunable Water Oxidation Catalysts. *Israel Journal of Chemistry*, **2011**, 51, 238-246	3.4	36
149	Efficient light-driven carbon-free cobalt-based molecular catalyst for water oxidation. *Journal of the American Chemical Society*, **2011**, 133, 2068-71	16.4	309
148	The role of the heteroatom (X = SiIV, PV, and SVI) on the reactivity of {□(H2O)RuIII(□OH)2RuIII(H2O)][X n+W10O36]}(8□)□with the O2 molecule. *Theoretical Chemistry Accounts*, **2011**, 130, 197-207	1.9	9
147	Insights into photoinduced electron transfer between [Ru(mptpy)2]4+ (mptpy = 4'(4-methylpyridinio)-2,2':6',2''-terpyridine) and [S2O8]2-: computational and experimental studies. *Journal of Physical Chemistry A*, **2010**, 114, 6284-97	2.8	27
146	Insights into the mechanism of O□formation and release from the Mn□O□□'cubane" cluster. *Journal of Physical Chemistry A*, **2010**, 114, 11417-24	2.8	27
145	Computational studies of the geometry and electronic structure of an all-inorganic and homogeneous tetra-Ru-polyoxotungstate catalyst for water oxidation and its four subsequent one-electron oxidized forms. *Journal of Physical Chemistry A*, **2010**, 114, 535-42	2.8	39
144	Insights into photoinduced electron transfer between [Ru(bpy)(3)](2+) and [S(2)O(8)](2-) in water: computational and experimental studies. *Journal of Physical Chemistry A*, **2010**, 114, 73-80	2.8	47
143	Structure and Bonding Energy Analysis of Cobalt, Rhodium, and Iridium Borylene Complexes [(□5-C5H5)(CO)M(BNX2] (X = Me, SiH3, SiMe3) and [(□5-C5H5)(PMe3)M{BN(SiH3)2}] (M = Co, Rh, Ir). *Organometallics*, **2010**, 29, 142-148	3.8	28
142	Computational studies of transition metal selectivity of octapeptide repeat region of prion protein (PrP). *Journal of Physical Chemistry B*, **2010**, 114, 1127-35	3.4	16
141	A fast soluble carbon-free molecular water oxidation catalyst based on abundant metals. *Science*, **2010**, 328, 342-5	33.3	1231
140	Real size of ligands, reactants and catalysts: Studies of structure, reactivity and selectivity by ONIOM and other hybrid computational approaches?. *Journal of Molecular Catalysis A*, **2010**, 324, 104-119		41
139	Synthesis, structure, and characterization of two polyoxometalate□photosensitizer hybrid materials. *Inorganica Chimica Acta*, **2010**, 363, 4381-4386	2.7	31
138	Vicinal dinitridoruthenium-substituted polyoxometalates gamma-[XW10O38{RuN}2]6- (X = Si or Ge). *Chemistry - A European Journal*, **2009**, 15, 10233-43	4.8	30
137	Computational insights to the mechanism of alkene epoxidation by manganese-based catalysts in the presence of bicarbonate. *Computational and Theoretical Chemistry*, **2009**, 903, 115-122		13
136	An experimental and density functional study of the Sb□□ bond activation and organo-Rh bond formation from the spontaneous decay of [RhCl3(SbPh3)3]. *Polyhedron*, **2009**, 28, 3675-3684	2.7	4
135	Density Functional Studies of the Adsorption and Dissociation of NOx (x = 1, 2) Molecules on the W(111) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 5300-5307	3.8	9

134	On the Mechanism of Pd(0)-Catalyzed, Cu(I) Carboxylate-Mediated Thioorganic-Boronic Acid Desulfitative Coupling. A Non-innocent Role for Carboxylate Ligand. *Organometallics*, **2009**, 28, 4639-4642	3.8	30
133	Mechanism of the divanadium-substituted polyoxotungstate [gamma-1,2-H2SiV2W10O40]4- catalyzed olefin epoxidation by H2O2: a computational study. *Inorganic Chemistry*, **2009**, 48, 1871-8	5.1	28
132	Structural, physicochemical, and reactivity properties of an all-inorganic, highly active tetraruthenium homogeneous catalyst for water oxidation. *Journal of the American Chemical Society*, **2009**, 131, 17360-70	16.4	156
131	Homogeneous light-driven water oxidation catalyzed by a tetraruthenium complex with all inorganic ligands. *Journal of the American Chemical Society*, **2009**, 131, 7522-3	16.4	320
130	Dioxygen and water activation processes on multi-Ru-substituted polyoxometalates: comparison with the "blue-dimer" water oxidation catalyst. *Journal of the American Chemical Society*, **2009**, 131, 6844-54	16.4	86
129	Zeolite-supported palladium tetramer and its reactivity toward H2 molecules: computational studies. *Journal of Physical Chemistry A*, **2008**, 112, 5973-83	2.8	11
128	Adsorption and Dissociation of the HCl and Cl2 Molecules on W(111) Surface: A Computational Study. *Journal of Physical Chemistry C*, **2008**, 112, 12342-12348	3.8	8
127	Adsorption and Dissociation of COx(x= 1, 2) on W(111) Surface : A Computational Study. *Journal of Physical Chemistry C*, **2008**, 112, 3341-3348	3.8	19
126	Computational study on kinetics and mechanisms of unimolecular decomposition of succinic acid and its anhydride. *Journal of Physical Chemistry A*, **2008**, 112, 6621-9	2.8	7
125	An all-inorganic, stable, and highly active tetraruthenium homogeneous catalyst for water oxidation. *Angewandte Chemie - International Edition*, **2008**, 47, 3896-9	16.4	526
124	Mechanisms of the reactions of W and W+ with NOx (x=1, 2): a computational study. *Journal of Physical Chemistry A*, **2007**, 111, 982-91	2.8	5
123	The mechanisms of the reactions of W and W+ with COx (x=1, 2): a computational study. *Journal of Physical Chemistry A*, **2007**, 111, 6665-73	2.8	13
122	Terminal gold-oxo complexes. *Journal of the American Chemical Society*, **2007**, 129, 11118-33	16.4	66
121	Why [(eta5-C5Me(n)H5-n)2Ti]2(micro2,eta2,eta2-N2) can not add a H2 molecule to the side-on-coordinated N2 while its Zr and Hf analogues can? insights from computational studies. *Inorganic Chemistry*, **2007**, 46, 2709-15	5.1	17
120	Adsorption and Dissociation of H2O on a W(111) Surface: A Computational Study. *Journal of Physical Chemistry C*, **2007**, 111, 17333-17339	3.8	25
119	Density Functional Study of Platinum(II)-Mediated Bicyclization of 1,6-Dienylphenols. *Organometallics*, **2007**, 26, 2540-2549	3.8	10
118	Mechanistic Aspects of Dinitrogen Hydrogenation Catalyzed by the Geometry-Constrained Zirconium and Titanium Complexes: Computational Studies. *Organometallics*, **2007**, 26, 5978-5986	3.8	21
117	Potential Energy Surfaces of Transition-Metal-Catalyzed Chemical Reactions. *Advances in Chemical Physics*, **2007**, 61-128		13

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