Djamaladdin G Musaev

List of Publications by Citations

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	A fast soluble carbon-free molecular water oxidation catalyst based on abundant metals. *Science*, **2010**, 328, 342-5	33.3	1231
258	Polyoxometalate water oxidation catalysts and the production of green fuel. *Chemical Society Reviews*, **2012**, 41, 7572-89	58.5	593
257	An all-inorganic, stable, and highly active tetraruthenium homogeneous catalyst for water oxidation. *Angewandte Chemie - International Edition*, **2008**, 47, 3896-9	16.4	526
256	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
255	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
254	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
253	An exceptionally fast homogeneous carbon-free cobalt-based water oxidation catalyst. *Journal of the American Chemical Society*, **2014**, 136, 9268-71	16.4	225
252	Site-selective and stereoselective functionalization of unactivated C-H bonds. *Nature*, **2016**, 533, 230-4	50.4	220
251	Decarbonylative organoboron cross-coupling of esters by nickel catalysis. *Nature Communications*, **2015**, 6, 7508	17.4	199
250	Parameter Calibration of Transition-Metal Elements for the Spin-Polarized Self-Consistent-Charge Density-Functional Tight-Binding (DFTB) Method: Sc, Ti, Fe, Co, and Ni. *Journal of Chemical Theory and Computation*, **2007**, 3, 1349-67	6.4	177
249	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
248	Site-selective and stereoselective functionalization of non-activated tertiary C-H bonds. *Nature*, **2017**, 551, 609-613	50.4	173
247	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
246	A Density Functional Study of the Mechanism of the Diimine Nickel-Catalyzed Ethylene Polymerization Reaction. *Journal of the American Chemical Society*, **1997**, 119, 367-374	16.4	162
245	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
244	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
243	A late-transition metal oxo complex: K7Na9[O=PtIV(H2O)L2], L = [PW9O34]9-. *Science*, **2004**, 306, 2074-7	33.3	151

242	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
241	Theoretical Insight into the C□ Coupling Reactions of the Vinyl, Phenyl, Ethynyl, and Methyl Complexes of Palladium and Platinum. *Organometallics*, **2005**, 24, 715-723	3.8	146
240	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
239	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
238	Theoretical Study of Substituent Effects in the Diimine□M(II) Catalyzed Ethylene Polymerization Reaction Using the IMOMM Method. *Journal of the American Chemical Society*, **1998**, 120, 1581-1587	16.4	141
237	Mechanism of the Methane -jMethanol Conversion Reaction Catalyzed by Methane Monooxygenase: A Density Functional Study. *Journal of the American Chemical Society*, **1999**, 121, 7249-7256	16.4	130
236	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
235	Molecular orbital study of H2 and CH4 activation on small metal clusters. I. Pt, Pd, Pt2, and Pd2. *Journal of Chemical Physics*, **1998**, 108, 8418-8428	3.9	129
234	Effects of the protein environment on the structure and energetics of active sites of metalloenzymes. ONIOM study of methane monooxygenase and ribonucleotide reductase. *Journal of the American Chemical Society*, **2002**, 124, 192-3	16.4	115
233	N2 Cleavage by Three-Coordinate Group 6 Complexes. W(III) Complexes Would Be Better Than Mo(III) Complexes. *Journal of the American Chemical Society*, **1995**, 117, 12366-12367	16.4	112
232	In situ probe of photocarrier dynamics in water-splitting hematite (□Fe2O3) electrodes. *Energy and Environmental Science*, **2012**, 5, 8923	35.4	109
231	Theoretical Studies of Ethylene Polymerization Reactions Catalyzed by Zirconium and Titanium Chelating Alkoxide Complexes. *Journal of the American Chemical Society*, **1997**, 119, 7190-7196	16.4	109
230	Comparative Investigations of Cp*-Based Group 9 Metal-Catalyzed Direct C□H Amination of Benzamides. *Organometallics*, **2014**, 33, 4076-4085	3.8	105
229	Theory Does Not Support an Osmaoxetane Intermediate in the Osmium-Catalyzed Dihydroxylation of Olefins. *Journal of the American Chemical Society*, **1996**, 118, 11660-11661	16.4	104
228	Molecular Orbital Study of the Mechanism of Platinum(0)-Catalyzed Alkene and Alkyne Diboration Reactions. *Organometallics*, **1997**, 16, 1355-1364	3.8	103
227	Ab Initio MO Study of the Full Cycle of Olefin Hydroformylation Catalyzed by a Rhodium Complex, RhH(CO)2(PH3)2. *Organometallics*, **1997**, 16, 1065-1078	3.8	101
226	Four-Coordinate Molybdenum Chalcogenide Complexes Relevant to Nitrous Oxide N□N Bond Cleavage by Three-Coordinate Molybdenum(III): Synthesis, Characterization, Reactivity, and Thermochemistry. *Journal of the American Chemical Society*, **1998**, 120, 2071-2085	16.4	101
225	Electron Transfer Dynamics in Semiconductor□Chromophore□Polyoxometalate Catalyst Photoanodes. *Journal of Physical Chemistry C*, **2013**, 117, 918-926	3.8	100

224	The true nature of the Di-iron(III) gamma-Keggin structure in water: catalytic aerobic oxidation and chemistry of an unsymmetrical trimer. *Journal of the American Chemical Society*, **2006**, 128, 11268-77	16.4	100
223	Rhodium-catalyzed enantioselective cyclopropanation of electron deficient alkenes. *Chemical Science*, **2013**, 4, 2844-2850	9.4	98
222	Density Functional Study on Activation of ortho-CH Bond in Aromatic Ketone by Ru Complex. Role of Unusual Five-Coordinated d6 Metallacycle Intermediate with Agostic Interaction. *Journal of the American Chemical Society*, **1998**, 120, 12692-12693	16.4	97
221	Density Functional Study of the Mechanism of the Palladium(II)-Catalyzed Ethylene Polymerization Reaction. *Organometallics*, **1997**, 16, 1933-1945	3.8	96
220	Vinyl-vinyl coupling on late transition metals through C-C reductive elimination mechanism. A computational study. *Journal of the American Chemical Society*, **2002**, 124, 2839-52	16.4	95
219	Ab Initio Molecular Orbital Study of the Mechanism of H-H, C-H, N-H, O-H and Si-H Bond Activation on Transient Cyclopentadienylcarbonylrhodium. *Journal of the American Chemical Society*, **1995**, 117, 799-805	16.4	94
218	An ab initio molecular orbital study of the mechanism of the rhodium(I)-catalyzed olefin hydroboration reaction. *Journal of the American Chemical Society*, **1994**, 116, 10693-10702	16.4	93
217	Theoretical Study on Bis(imino)pyridylFe(II) Olefin Poly- and Oligomerization Catalysts. Dominance of Different Spin States in Propagation and Hydride Transfer Pathways. *Organometallics*, **2001**, 20, 2007-2026	3.8	92
216	Theoretical Predictions and Single-Crystal Neutron Diffraction and Inelastic Neutron Scattering Studies on the Reaction of Dihydrogen with the Dinuclear Dinitrogen Complex of Zirconium [P2N2]Zr(μ2-N2)Zr[P2N2], P2N2 = PhP(CH2SiMe2NSiMe2CH2)2PPh. *Journal of the American Chemical Society*, **1999**, 121, 523-528	16.4	92
215	Critical Effect of Phosphane Ligands on the Mechanism of Carbon–Carbon Bond Formation Involving Palladium(II) Complexes: A Theoretical Investigation of Reductive Elimination from Square-Planar and T-Shaped Species. *European Journal of Inorganic Chemistry*, **2007**, 2007, 5390-5399	2.3	90
214	Molecular Orbital and IMOMM Studies of the Chain Transfer Mechanisms of the DiimineM(II)-Catalyzed (M = Ni, Pd) Ethylene Polymerization Reaction. *Organometallics*, **1998**, 17, 1850-1860	3.8	90
213	Metal-peroxo versus metal-oxo oxidants in non-heme iron-catalyzed olefin oxidations: computational and experimental studies on the effect of water. *Journal of the American Chemical Society*, **2005**, 127, 6548-9	16.4	88
212	Why Do Pt(PR3)2 Complexes Catalyze the Alkyne Diboration Reaction, but Their Palladium Analogues Do Not? A Density Functional Study. *Organometallics*, **1998**, 17, 742-751	3.8	88
211	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
210	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
209	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
208	Visible-light-driven hydrogen evolution from water using a noble-metal-free polyoxometalate catalyst. *Journal of Catalysis*, **2013**, 307, 48-54	7.3	83
207	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

206	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
205	Density Functional Study on Highly Ortho-Selective Addition of an Aromatic CH Bond to Olefins Catalyzed by a Ru(H)2(CO)(PR3)3 Complex. *Organometallics*, **2000**, 19, 2318-2329	3.8	80
204	Computational study of the aminolysis of esters. The reaction of methylformate with ammonia. *Journal of Organic Chemistry*, **2003**, 68, 1496-502	4.2	78
203	Theoretical Studies of the Factors Controlling Insertion Barriers for Olefin Polymerization by the Titanium-Chelating Bridged Catalysts. A Search for More Active New Catalysts. *Organometallics*, **1999**, 18, 373-379	3.8	78
202	Revisiting the polyoxometalate-based late-transition-metal-oxo complexes: the "oxo wall" stands. *Inorganic Chemistry*, **2012**, 51, 7025-31	5.1	77
201	Unusual 31P Chemical Shielding Tensors in Terminal Phosphido Complexes Containing a Phosphorus□Metal Triple Bond. *Journal of the American Chemical Society*, **1996**, 118, 10654-10655	16.4	76
200	A palladium-oxo complex. Stabilization of this proposed catalytic intermediate by an encapsulating polytungstate ligand. *Journal of the American Chemical Society*, **2005**, 127, 11948-9	16.4	75
199	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
198	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
197	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
196	Computational insights into the mechanism of radical generation in B12-dependent methylmalonyl-CoA mutase. *Journal of the American Chemical Society*, **2006**, 128, 1287-92	16.4	68
195	Terminal gold-oxo complexes. *Journal of the American Chemical Society*, **2007**, 129, 11118-33	16.4	66
194	Density Functional Study on the Mechanism of Palladium(0)-Catalyzed Thioboration Reaction of Alkynes. Differences between Pd(0) and Pt(0) Catalysts and between Thioboration and Diboration. *Organometallics*, **1998**, 17, 1383-1392	3.8	66
193	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
192	Desymmetrization of cyclohexanes by site- and stereoselective C-H functionalization. *Nature*, **2018**, 564, 395-399	50.4	61
191	Computational studies of reaction mechanisms of methane monooxygenase and ribonucleotide reductase. *Journal of Computational Chemistry*, **2002**, 23, 59-76	3.5	60
190	Water splitting with polyoxometalate-treated photoanodes: enhancing performance through sensitizer design. *Chemical Science*, **2015**, 6, 5531-5543	9.4	58
189	Molecular Orbital Study of H2and CH4Activation on Small Metal Clusters. 2. Pd3and Pt3. *Journal of Physical Chemistry A*, **1998**, 102, 6373-6384	2.8	58

188	Computational modeling of di-transition-metal-substituted gamma-keggin polyoxometalate anions. Structural refinement of the protonated divacant lacunary silicodecatungstate. *Inorganic Chemistry*, **2004**, 43, 7702-8	5.1	56
187	Ab initio molecular orbital study of the molecular and electronic structure of FeCH+2 and of the reaction mechanism of FeCH+2+H2. *Journal of Chemical Physics*, **1994**, 101, 10697-10707	3.9	56
186	Ab initio study of the molecular and electronic structure of CoCH2+ and of the reaction mechanism of methylenecobalt(1+) + hydrogen. *The Journal of Physical Chemistry*, **1993**, 97, 11435-11444		55
185	Ab initio molecular orbital study of the electronic and geometric structure of methylenerhodium(1+) and the reaction mechanism: RhCH2+ + H2 .fwdarw. Rh+ + CH4. *The Journal of Physical Chemistry*, **1993**, 97, 4064-4075		52
184	CH activation. *Nature Reviews Methods Primers*, **2021**, 1,		52
183	Flexible Reaction Pocket on Bulky Diphosphine Ir Complex Controls Regioselectivity in para-Selective CH Borylation of Arenes. *ACS Catalysis*, **2016**, 6, 7536-7546	13.1	52
182	Computational studies of tungsten-catalyzed endo-selective cycloisomerization of 4-pentyn-1-ol. *Journal of the American Chemical Society*, **2002**, 124, 4149-57	16.4	51
181	Molecular Orbital Study of the Reaction Mechanism of Sc+ with Methane. Comparison of the Reactivity of Early and Late First-Row Transition Metal Cations and Their Carbene Complexes. *The Journal of Physical Chemistry*, **1996**, 100, 11600-11609		50
180	Theoretical studies of the mechanism of ethylene polymerization reaction catalyzed by diimine-M(II) (M = Ni, Pd and Pt) and Ti- and Zr-chelating alkoxides. *Topics in Catalysis*, **1999**, 7, 107-123	2.3	50
179	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
178	Insights into the mechanism of selective olefin epoxidation catalyzed by [gamma-(SiO4)W10O32H4]4-. A computational study. *Inorganic Chemistry*, **2006**, 45, 5703-9	5.1	49
177	Tetracobalt-polyoxometalate catalysts for water oxidation: Key mechanistic details. *Journal of Catalysis*, **2017**, 350, 56-63	7.3	47
176	Factors Controlling Stability and Reactivity of Dimeric Pd(II) Complexes in CH Functionalization Catalysis. *ACS Catalysis*, **2016**, 6, 829-839	13.1	47
175	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
174	Theoretical Studies of Oxidative Addition of EH Bonds (E = S, Se, Te) to Palladium(0) and Platinum(0) Complexes. *Organometallics*, **2005**, 24, 4908-4914	3.8	47
173	Adsorption of Multiple H2 Molecules on Pd3 and Pd4 Clusters. A Density Functional Study. *Journal of Physical Chemistry A*, **2000**, 104, 11606-11614	2.8	47
172	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
171	Calculation of Nuclear Quadrupole Parameters in Imidazole Derivatives and Extrapolation to Coenzyme B12. A Theoretical Study. *Journal of Physical Chemistry B*, **1999**, 103, 8618-8627	3.4	45

170	Cu-Catalyzed aromatic C-H imidation with -fluorobenzenesulfonimide: mechanistic details and predictive models. *Chemical Science*, **2017**, 8, 988-1001	9.4	44
169	The Flexibility of Carboxylate Ligands in Methane Monooxygenase and Ribonucleotide Reductase: A Density Functional Study. *Journal of Physical Chemistry B*, **2001**, 105, 322-327	3.4	44
168	Iridium(III)-bis(oxazolinyl)phenyl catalysts for enantioselective C H functionalization. *Chemical Science*, **2013**, 4, 2590	9.4	43
167	Theoretical studies of biological nitrogen fixation. I. Density functional modeling of the Mo-site of the FeMo-cofactor. *Inorganic Chemistry*, **2001**, 40, 766-75	5.1	43
166	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
165	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
164	The role of the central atom in structure and reactivity of polyoxometalates with adjacent d-electron metal sites. computational and experimental studies of gamma-[(Xn+O4)RuIII2(OH)2(MFM)10O32](8-n)-) for MFM = Mo and W, and X = AlIII, SiIV, PV, and SVI. *Journal of Physical Chemistry B*, **2006**, 110, 170-3	3.4	41
163	Electronic states of the triply charged molecular ion N23+ and laser-induced Coulomb explosion. *Physical Review A*, **1999**, 59, 4309-4315	2.6	41
162	Site-Selective Carbene-Induced C H Functionalization Catalyzed by Dirhodium Tetrakis(triarylcyclopropanecarboxylate) Complexes. *ACS Catalysis*, **2018**, 8, 678-682	13.1	40
161	Theoretical Studies on the Mechanism of the Methane -jMethanol Conversion Reaction Catalyzed by Methane Monooxygenase: O-Side vs N-Side Mechanisms. *Journal of Physical Chemistry A*, **2001**, 105, 3615-3622	2.8	40
160	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
159	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
158	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
157	Structure, stability, and electronic and NMR properties of various oxo- and nitrido-derivatives of [L(Salen)Mn(III)]+, where L = none and imidazole. A density functional study. *Inorganic Chemistry*, **2003**, 42, 2606-21	5.1	38
156	Does Reaction of Three-Coordinate Molybdenum(III) with N2O Proceed via the Same Mechanism as with N2? A Theoretical Study. *Organometallics*, **1999**, 18, 5653-5660	3.8	38
155	Spectroscopic Studies of Light-driven Water Oxidation Catalyzed by Polyoxometalates. *Industrial & Engineering Chemistry Research*, **2012**, 51, 11850-11859	3.9	36
154	Polyoxometalates in the Design of Effective and Tunable Water Oxidation Catalysts. *Israel Journal of Chemistry*, **2011**, 51, 238-246	3.4	36
153	Insights into the structure and reactivity of acylperoxo complexes in the Kochi-Jacobsen-Katsuki catalytic system. A density functional study. *Journal of the American Chemical Society*, **2003**, 125, 13879-89	16.4	36

152	Is the protein surrounding the active site critical for hydrogen peroxide reduction by selenoprotein glutathione peroxidase? An ONIOM study. *Journal of Physical Chemistry B*, **2006**, 110, 13608-13	3.4	35
151	Epoxidation of unfunctionalized olefins by Mn(salen) catalyst using organic peracids as oxygen source: a theoretical study. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 5743-8	11.5	35
150	Why Does the Reaction of the Dihydrogen Molecule with [P2N2]Zr(□2-N2)Zr[P2N2] Produce [P2N2]Zr(□2-N2H)Zr[P2N2](□H) but Not the Thermodynamically More Favorable [P2N2]Zr(□NH)2Zr[P2N2]? A Theoretical Study. *Journal of the American Chemical Society*, **1999**, 121, 5754-5761	16.4	35
149	Cu-based Polyoxometalate Catalyst for Efficient Catalytic Hydrogen Evolution. *Inorganic Chemistry*, **2016**, 55, 6750-8	5.1	34
148	Theoretical study of the mechanism of alkane hydroxylation and ethylene epoxidation reactions catalyzed by diiron bis-oxo complexes. The effect of substrate molecules. *Journal of the American Chemical Society*, **2002**, 124, 4135-48	16.4	34
147	Density Functional Study of Ethylene Polymerization Catalyzed by a Zirconium Non-Cyclopentadienyl Complex, L2ZrCH3+. Effects of Ligands and Bulky Substituents. *Organometallics*, **2001**, 20, 309-323	3.8	34
146	An ab initio molecular orbital study of the unimolecular dissociation reactions of di- and trichloroethylene. *Journal of Chemical Physics*, **1994**, 101, 5942-5956	3.9	34
145	Ab Initio Molecular Orbital Study of Electronic and Geometrical Structures of MCH2+ Complex and its Reactivity with H2, Where M = Co, Rh, and Ir. *Israel Journal of Chemistry*, **1993**, 33, 307-316	3.4	33
144	Does dinitrogen hydrogenation follow different mechanisms for [(eta5-C5Me4H)2Zr]2(mu2,eta2,eta2-N2) and {[PhP(CH2SiMe2NSiMe2CH2)PPh]Zr}2(mu2,eta2,eta2-N2) complexes? A computational study. *Journal of the American Chemical Society*, **2006**, 128, 11391-403	16.4	32
143	Synthesis, structure, and characterization of two polyoxometalate□photosensitizer hybrid materials. *Inorganica Chimica Acta*, **2010**, 363, 4381-4386	2.7	31
142	Diminishing □Stabilization of an Unsaturated Metal Center: Hydrogen Bonding to OsHCl(CO)(PtBu2Me)2. *Journal of the American Chemical Society*, **1998**, 120, 12553-12563	16.4	31
141	The mechanism of directed Ni(ii)-catalyzed C-H iodination with molecular iodine. *Chemical Science*, **2018**, 9, 1144-1154	9.4	31
140	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
139	Vicinal dinitridoruthenium-substituted polyoxometalates gamma-[XW10O38{RuN}2]6- (X = Si or Ge). *Chemistry - A European Journal*, **2009**, 15, 10233-43	4.8	30
138	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
137	Can Steric Effects Induce the Mechanism Switch in the Rhodium-Catalyzed Imine Boration Reaction? A Density Functional and ONIOM Study. *Organometallics*, **2005**, 24, 1938-1946	3.8	30
136	Activation and Adsorption of Multiple H2 Molecules on a Pd5 Cluster: A Density Functional Study. *Journal of Physical Chemistry A*, **2003**, 107, 4929-4939	2.8	30
135	Enhancing photo-reduction quantum efficiency using quasi-type II core/shell quantum dots. *Chemical Science*, **2016**, 7, 4125-4133	9.4	29

134	Extending metal-to-polyoxometalate charge transfer lifetimes: the effect of heterometal location. *Chemistry - A European Journal*, **2014**, 20, 4297-307	4.8	29
133	Theoretical studies of the complex [(BPMEN)Fe(II)(NCCH3)2](2+), precursor of non-heme iron catalysts for olefin epoxidation and cis-dihydroxylation. *Inorganic Chemistry*, **2003**, 42, 8449-55	5.1	29
132	Can the Binuclear Dinitrogen Complex [P2N2]Zr(μ2-N2)Zr[P2N2] Activate More Than One Hydrogen Molecule? A Theoretical Study. *Organometallics*, **2000**, 19, 3393-3403	3.8	29
131	Structure and Bonding Energy Analysis of Cobalt, Rhodium, and Iridium Borylene Complexes [(η5-C5H5)(CO)M(BNX2] (X = Me, SiH3, SiMe3) and [(η5-C5H5)(PMe3)M{BN(SiH3)2}] (M = Co, Rh, Ir). *Organometallics*, **2010**, 29, 142-148	3.8	28
130	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
129	Computational Studies of the Energetics and Reaction Pathways of Molecular Transformations of Benzoheterocycles on Triosmium Clusters. *Organometallics*, **2005**, 24, 5973-5982	3.8	28
128	Does the Active Site of Mammalian Glutathione Peroxidase (GPx) Contain Water Molecules? An ONIOM Study. *Journal of Physical Chemistry B*, **2004**, 108, 12643-12645	3.4	28
127	Rhodium-Stabilized Diarylcarbenes Behaving as Donor/Acceptor Carbenes. *ACS Catalysis*, **2020**, 10, 6240-6247	13.1	27
126	Understanding Regiodivergence in a Pd(II)-Mediated Site-Selective C–H Alkynylation. *ACS Catalysis*, **2018**, 8, 4516-4527	13.1	27
125	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
124	Insights into the mechanism of O–O formation and release from the Mn3O4Ca "cubane" cluster. *Journal of Physical Chemistry A*, **2010**, 114, 11417-24	2.8	27
123	Experimental and Computational Studies of Nucleophilic Attack, Tautomerization, and Hydride Migration in Benzoheterocycle Triosmium Clusters. *Organometallics*, **2006**, 25, 203-213	3.8	27
122	Can the ebselen derivatives catalyze the isomerization of peroxynitrite to nitrate?. *Journal of the American Chemical Society*, **2003**, 125, 3877-88	16.4	27
121	Sigma trans promotion effect in transition metal complexes: a manifestation of the composite nature of binding energy. *Molecular Physics*, **2002**, 100, 523-532	1.7	27
120	Ab initio molecular orbital study of electronic and geometrical structures of MCH+2 and MSiH+2 complexes (M=Co, Rh, and Ir). *Journal of Chemical Physics*, **1993**, 99, 7859-7872	3.9	27
119	C-C Cleavage Approach to C-H Functionalization of Saturated Aza-Cycles. *ACS Catalysis*, **2020**, 10, 2929-2941	13.1	26
118	Computational study of the aminolysis of 2-benzoxazolinone. *Journal of Organic Chemistry*, **2003**, 68, 3406-12	4.2	26
117	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

116	Density Functional Study of Mo-Carbonyl-Catalyzed Alkynol Cycloisomerization: Comparison with W-Catalyzed Reaction. *Organometallics*, **2005**, 24, 2921-2929	3.8	25
115	Versatile and cooperative reactivity of a triruthenium polyhydride cluster. A computational study. *Journal of the American Chemical Society*, **2003**, 125, 9910-1	16.4	25
114	Differences and Similarities in the Reactivity of Peroxynitrite Anion and Peroxynitrous Acid with Ebselen. A Theoretical Study *Journal of Physical Chemistry A*, **2003**, 107, 1563-1573	2.8	25
113	Enantioselectivity Model for Pd-Catalyzed CH Functionalization Mediated by the Mono-N-protected Amino Acid (MPAA) Family of Ligands. *ACS Catalysis*, **2017**, 7, 4344-4354	13.1	24
112	A Density Functional Study of the Completion of the Methane Monooxygenase Catalytic Cycle. Methanol Complex to MMOH Resting State. *Journal of Physical Chemistry B*, **2001**, 105, 8452-8460	3.4	24
111	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
110	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
109	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
108	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
107	Insight into Mechanistic Features of Ruthenium(II) Pybox-Catalyzed CH Amination. *Organometallics*, **2012**, 31, 4950-4961	3.8	23
106	Internal degrees of freedom, structural motifs, and conformational energetics of the 5'-deoxyadenosyl radical: implications for function in adenosylcobalamin-dependent enzymes. A computational study. *Journal of the American Chemical Society*, **2003**, 125, 570-9	16.4	23
105	Skeletal Rearrangement in the Trinuclear nido-Ruthenacyclopentadiene Complexes: Theoretical and Experimental Studies. *Organometallics*, **2003**, 22, 1718-1727	3.8	23
104	Catalytic Triple Bond Activation and Vinyl Vinyl Reductive Coupling by Pt(IV) Complexes. A Density Functional Study. *Organometallics*, **2001**, 20, 1652-1667	3.8	23
103	A Density Functional Study of Possible Intermediates of the Reaction of Dioxygen Molecule with Nonheme Iron Complexes. 2. Water-Assisted Model Studies. *Journal of Physical Chemistry B*, **2001**, 105, 4453-4463	3.4	23
102	Buffer-Induced Acceleration and Inhibition in Polyoxometalate-Catalyzed Organophosphorus Ester Hydrolysis. *ACS Catalysis*, **2018**, 8, 7068-7076	13.1	22
101	Can bis(imino)pyridine iron, (PDI)FeL1L2, complexes catalyze CH bond functionalization?. *Chemical Science*, **2013**, 4, 3758	9.4	22
100	A DFT study of the mechanism of Ni superoxide dismutase (NiSOD): role of the active site cysteine-6 residue in the oxidative half-reaction. *Journal of Computational Chemistry*, **2006**, 27, 1438-45	3.5	22
99	Ditantalum dinitrogen complex: reaction of H2 molecule with "end-on-bridged" [Ta(IV)]2((1): (1)-N2) and Bis(hitrido) [Ta(V)]2(N)2 complexes. *Inorganic Chemistry*, **2011**, 50, 9481-90	5.1	21

98	Mechanistic Aspects of Dinitrogen Hydrogenation Catalyzed by the Geometry-Constrained Zirconium and Titanium Complexes: Computational Studies. *Organometallics*, **2007**, 26, 5978-5986	3.8	21
97	Cooperative pull and push effects on the O-O bond cleavage in acylperoxo complexes of [(Salen)MnIIIL]: ensuring formation of manganese(V) oxo species. *Inorganic Chemistry*, **2005**, 44, 306-15	5.1	21
96	New complexes and materials for O2-based oxidations. *Journal of Molecular Catalysis A*, **2006**, 251, 234-238		21
95	Protein effects on the O2 binding to the active site of the methane monooxygenase: ONIOM studies. *International Journal of Quantum Chemistry*, **2004**, 99, 972-980	2.1	21
94	A Density Functional Study of Possible Intermediates of the Reaction of Dioxygen Molecule with Non-Heme Iron Complexes. 1. N-Side versus O-Side Mechanism with Water-Free Model. *Journal of Physical Chemistry B*, **2001**, 105, 8616-8628	3.4	21
93	[12]Annulene gemini surfactants: structure and self-assembly. *Angewandte Chemie - International Edition*, **2007**, 46, 5889-91	16.4	20
92	Complex catalysts from self-repairing ensembles to highly reactive air-based oxidation systems. *Comptes Rendus Chimie*, **2007**, 10, 305-312	2.7	20
91	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
90	Axial Ligand and Solvent Effects on the O□D Bond Activation in Acylperoxo Complexes of [(Salen)MnIIIL]: MnIV versus MnV Oxo Species. *Journal of Physical Chemistry B*, **2004**, 108, 3845-3854	3.4	19
89	Transition Metal Substitution Effects on Metal-to-Polyoxometalate Charge Transfer. *Inorganic Chemistry*, **2016**, 55, 4308-19	5.1	19
88	Unveiling the Role of Base and Additive in the Ullmann-Type of Arene-Aryl C□ Coupling Reaction. *ACS Catalysis*, **2018**, 8, 4829-4837	13.1	18
87	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
86	Theoretical Studies of the Reaction Mechanisms of Dimethylsulfide and Dimethylselenide with Peroxynitrite. *Journal of Physical Chemistry A*, **2003**, 107, 5862-5873	2.8	18
85	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
84	Reaction Mechanism of Nerve-Agent Hydrolysis with the Cs8Nb6O19 Lindqvist Hexaniobate Catalyst. *Journal of Physical Chemistry C*, **2016**, 120, 16822-16830	3.8	17
83	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
82	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
81	Theoretical Study of the Mechanism of Oxidative Addition of Allyl□Ammonium and □minium Salts to Low-Valent Metal Complexes. Rationalization of Selective C□N and N□H Bond Activation. *Organometallics*, **2000**, 19, 4402-4415	3.8	17

80	Ab initio molecular orbital study of oxidative addition of H2 and CH4 to the RhCl(CO)(PH3)2 complex. *Journal of Organometallic Chemistry*, **1995**, 504, 93-105	2.3	17
79	Impact of ambient gases on the mechanism of [CsNbO]-promoted nerve-agent decomposition. *Chemical Science*, **2018**, 9, 2147-2158	9.4	16
78	Multi-Tasking POM Systems. *Frontiers in Chemistry*, **2018**, 6, 365	5	16
77	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
76	Computational studies of nucleophilic attack and protonation of electron-deficient benzoheterocycle triosmium clusters. *Inorganic Chemistry*, **2006**, 45, 4963-73	5.1	16
75	Tailored quinones support high-turnover Pd catalysts for oxidative C-H arylation with O. *Science*, **2020**, 370, 1454-1460	33.3	16
74	Di-Palladium Complexes are Active Catalysts for Mono-N-Protected Amino Acid-Accelerated Enantioselective C□H Functionalization. *ACS Catalysis*, **2019**, 9, 11386-11397	13.1	15
73	Reaction of H2 with a Binuclear Zirconium Dinitrogen Complex - Evaluation of Theoretical Models and Hybrid Approaches. *Journal of Chemical Theory and Computation*, **2006**, 2, 1298-316	6.4	15
72	Density functional study of the roles of chemical composition of di-transition-metal-substituted gamma-Keggin polyoxometalate anions. *Journal of Physical Chemistry B*, **2006**, 110, 5230-7	3.4	15
71	Theoretical Prediction of a New Dinitrogen Reduction Process: Utilization of Four Dihydrogen Molecules and a Zr2Pt2 Cluster. *Journal of Physical Chemistry B*, **2004**, 108, 10012-10018	3.4	15
70	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
69	Does the Tetrahydroborate Species AuBH4 Exist? Ab Initio MO Study of the Structure and Stability of CuBH4, AgBH4, and AuBH4. *Organometallics*, **1995**, 14, 3327-3334	3.8	14
68	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
67	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
66	Potential Energy Surfaces of Transition-Metal-Catalyzed Chemical Reactions. *Advances in Chemical Physics*, **2007**, 61-128		13
65	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
64	Broad-Spectrum Liquid- and Gas-Phase Decontamination of Chemical Warfare Agents by One-Dimensional Heteropolyniobates. *Angewandte Chemie*, **2016**, 128, 7529-7533	3.6	13
63	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

62	Peroxynitrite Reactions with Dimethylsulfide and Dimethylselenide: An Experimental Study. *Journal of Physical Chemistry A*, **2004**, 108, 289-294	2.8	12
61	Multimodal Characterization of Materials and Decontamination Processes for Chemical Warfare Protection. *ACS Applied Materials & Interfaces*, **2020**, 12, 14721-14738	9.5	12
60	Biologically Inspired Total Synthesis of Ulbactin F, an Iron-Binding Natural Product. *Organic Letters*, **2018**, 20, 5922-5926	6.2	12
59	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
58	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
57	Zeolite-supported palladium tetramer and its reactivity toward H2 molecules: computational studies. *Journal of Physical Chemistry A*, **2008**, 112, 5973-83	2.8	11
56	Generality and Strength of Transition Metal Effects. *Journal of the American Chemical Society*, **2018**, 140, 10612-10618	16.4	10
55	Density Functional Study of Platinum(II)-Mediated Bicyclization of 1,6-Dienylphenols. *Organometallics*, **2007**, 26, 2540-2549	3.8	10
54	Electronic reorganization: origin of sigma trans promotion effect. *Journal of Computational Chemistry*, **2007**, 28, 423-41	3.5	10
53	A density functional study of geometry and electronic structures of [(SiO4)(MIII)2(OH)2W10O32]4 M=Mo, Ru and Rh. *Journal of Molecular Catalysis A*, **2007**, 262, 227-235		10
52	Hydrogen Scrambling in [(C5Me5)Os(dmpm)(CH3)H]+. A Density Functional and ONIOM Study. *Organometallics*, **2002**, 21, 555-564	3.8	10
51	Metallaboranes with Group 8 and 9 Transition Metals. Is Accurateab initioMolecular Orbital Calculation of Structure, Stability, and NMR Chemical Shifts Possible?. *Bulletin of the Chemical Society of Japan*, **1993**, 66, 3259-3270	5.1	10
50	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
49	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
48	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
47	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
46	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
45	Reactivity of Ebtellur Derivatives with the Peroxynitrite Anion: Comparison with Their Ebselen Analogues. *Journal of Physical Chemistry A*, **2003**, 107, 5631-5639	2.8	9

44	Ab initio molecular orbital study of structure and NMR 11B chemical shifts of Lewis base adducts of CO, NH3, PF3, and PH3 with small nido-boranes, B3H7 and B4H8. *Chemical Physics Letters*, **1993**, 214, 69-76	2.5	9
43	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
42	Reactivity of [1,2-Benzisotellurazol-3(2H)-one] with Peroxynitrous Acid: Comparison with Ebselen Analogues. *Journal of Physical Chemistry A*, **2003**, 107, 9984-9990	2.8	8
41	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
40	Mechanistic details of the cobalt-mediated dehydrogenative dimerization of aminoquinoline-directed benzamides. *Chemical Science*, **2020**, 11, 6085-6096	9.4	7
39	Roles of Base in the Pd-Catalyzed Annulative Chlorophenylene Dimerization. *ACS Catalysis*, **2020**, 10, 3059-3073	13.1	7
38	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
37	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
36	How Many Methyl Groups in [{(η5-C5MenH5−n)2Zr}2(μ,η2,η2-N2)] Are Needed for Dinitrogen Hydrogenation? A Theoretical Study. *Angewandte Chemie*, **2005**, 117, 7263-7265	3.6	7
35	Key mechanistic details of paraoxon decomposition by polyoxometalates: Critical role of para-nitro substitution. *Chemical Physics*, **2019**, 518, 30-37	2.3	7
34	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
33	Density functional studies of the electronic and geometric structures of Pt3+, Pt3O+, Pt3O2+ and Pt3CH4+. *Computational and Theoretical Chemistry*, **2002**, 586, 35-46		6
32	Ab Initio MO Study of Cluster Rearrangements in Pentagonal Pyramidal Clusters: B6H10 Borane and [(IrB5H8)(CO)(PH3)2] Metallaborane. *Journal of the American Chemical Society*, **1994**, 116, 3932-3942	16.4	6
31	A solvent-free solid catalyst for the selective and color-indicating ambient-air removal of sulfur mustard. *Communications Chemistry*, **2021**, 4,	6.3	6
30	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
29	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
28	Theoretical Study of the Structure and Properties of [(η(5)-C5Me4H)2Zr]2(μ(2),η(2),η(2)-N2). *Journal of Chemical Theory and Computation*, **2006**, 2, 336-41	6.4	5
27	The roles of steric and electronic effects in the 2-hydroxy-2?-nitrodiphenyl sulfones to 2-(o-nitrophenoxy)-benzene-sulfinic acids rearrangement (Smiles). Computational study. *Computational and Theoretical Chemistry*, **2004**, 679, 45-52		5

26	A comparative study of various computational approaches in calculating the structure of pyridoxal 5'-phosphate (PLP)-dependent beta-lyase protein. The importance of protein environment. *Journal of Computational Chemistry*, **2005**, 26, 443-6	3.5	5
25	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
24	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
23	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
22	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
21	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
20	Unified Mechanistic Concept of the Copper-Catalyzed and Amide-Oxazoline-Directed C(sp2)□H Bond Functionalization. *ACS Catalysis*,12620-12631	13.1	4
19	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
18	Unconventional mechanism and selectivity of the Pd-catalyzed C-H bond lactonization in aromatic carboxylic acid.. *Nature Communications*, **2022**, 13, 315	17.4	3
17	Enhanced intersystem crossing of boron dipyrromethene by TEMPO radical. *Journal of Chemical Physics*, **2020**, 153, 154201	3.9	3
16	Pyochelin Biosynthetic Metabolites Bind Iron and Promote Growth in Demonstrating Siderophore-like Activity. *ACS Infectious Diseases*, **2021**, 7, 544-551	5.5	3
15	Modulating electronic coupling at the quantum dot/molecule interface by wavefunction engineering. *Journal of Chemical Physics*, **2019**, 150, 124704	3.9	2
14	Theoretical Studies of the N2 Cleavage by Three-Coordinate Group 6 Complexes ML3. *ACS Symposium Series*, **1999**, 198-207	0.4	2
13	An alternative mechanism of BH2SH formation in the reaction of B2H6 with SH2: concerted elimination of BH3 and H2 from H2S□B2H6. Ab initio MO study. *Chemical Physics Letters*, **1993**, 216, 313-318	2.5	2
12	Light-Promoted Dearomative Cross-Coupling of Heteroarenium Salts and Aryl Iodides via Nickel Catalysis. *ACS Catalysis*, **2022**, 12, 1818-1829	13.1	2
11	A bulk adjusted linear combination of atomic orbitals (BA-LCAO) approach for nanoparticles. *Journal of Computational Chemistry*, **2019**, 40, 212-221	3.5	2
10	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
9	Roles of Ligand and Oxidant in Pd(II)-Catalyzed and Ligand-Enabled C(sp3)□H Lactonization in Aliphatic Carboxylic Acid: Mechanistic Studies. *ACS Catalysis*,4848-4858	13.1	2

8	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
7	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
6	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
5	Tafel Slope Analyses for Homogeneous Catalytic Reactions. *Catalysts*, **2021**, 11, 87	4	1
4	Hydrogen-Bonding as a Factor to Determine the Regioselectivity for Pd-mediated CH Activation of Pyridine. *ChemCatChem*, **2021**, 13, 1201-1206	5.2	0
3	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
2	Polyniobate Nanothreads for Decomposition of the Nerve Agent Simulant Dimethyl Chlorophosphate. *ACS Applied Nano Materials*, **2021**, 4, 5649-5654	5.6	0
1	Keiji Morokuma. *Journal of Physical Chemistry A*, **2018**, 122, 880-881	2.8	