Hirotoshi Mori

List of Publications by Citations

64 papers	728 citations	15 h-index	22 g-index
67 ext. papers	791 ext. citations	3.2 avg, IF	3.84 L-index

#	Paper	IF	Citations
64	Compact and efficient basis sets of s- and p-block elements for model core potential method. *Journal of Chemical Physics*, **2005**, 122, 074104	3.9	59
63	Excited-state intramolecular proton transfer in photochromic jet-cooled N-salicylideneaniline. *Journal of Photochemistry and Photobiology A: Chemistry*, **2002**, 154, 33-39	4.7	51
62	Fragment molecular orbital calculations on large scale systems containing heavy metal atom. *Chemical Physics Letters*, **2006**, 427, 159-165	2.5	48
61	Electronic band structure calculations on thin films of the L21 full Heusler alloys X2YSi (X, Y = Mn, Fe, and Co): Toward spintronic materials. *Thin Solid Films*, **2012**, 520, 4979-4983	2.2	34
60	Fragment molecular orbital-based molecular dynamics (FMO-MD) simulations on hydrated Zn(II) ion. *Chemical Physics Letters*, **2010**, 490, 41-45	2.5	31
59	Experimental and theoretical approaches toward anion-responsive tripod-lanthanide complexes: mixed-donor ligand effects on lanthanide complexation and luminescence sensing profiles. *Chemistry - A European Journal*, **2008**, 14, 5258-66	4.8	26
58	Revised model core potentials for third-row transition metal atoms from Lu to Hg. *Chemical Physics Letters*, **2009**, 476, 317-322	2.5	23
57	Origin of high oxygen reduction reaction activity of Pt and strategy to obtain better catalyst using sub-nanosized Pt-alloy clusters. *Scientific Reports*, **2017**, 7, 45381	4.9	22
56	Revised model core potentials for first-row transition-metal atoms from Sc to Zn. *Chemical Physics Letters*, **2008**, 452, 210-214	2.5	22
55	Theoretical study of hydration models of trivalent rare-earth ions using model core potentials. *Computational and Theoretical Chemistry*, **2010**, 949, 28-35		21
54	Theoretical study on vibrational circular dichroism spectra of tris(acetylacetonato)metal(III) complexes: anharmonic effects and low-lying excited states. *Journal of Chemical Physics*, **2011**, 135, 084506	3.9	20
53	Differences in hydration between cis- and trans-platin: Quantum insights by ab initio fragment molecular orbital-based molecular dynamics (FMO-MD). *Computational and Theoretical Chemistry*, **2012**, 986, 30-34	2	18
52	Structure and intermolecular hydrogen bond of jet-cooled p-aminophenol(H2O)1 studied by electronic and IR-dip spectroscopy and density functional theory calculations. *Chemical Physics*, **2002**, 277, 105-115	2.3	17
51	Density functional theory calculations of iodine cluster anions: Structures, chemical bonding nature, and vibrational spectra. *Computational and Theoretical Chemistry*, **2011**, 973, 69-75	2	16
50	CASSCF and CASPT2 calculations for lanthanide trihalides LnX3 using model core potentials. *Chemical Physics Letters*, **2009**, 474, 28-32	2.5	15
49	Revised model core potentials for second-row transition metal atoms from Y to Cd. *Chemical Physics Letters*, **2008**, 463, 230-234	2.5	15
48	Application of fragment molecular orbital scheme to silicon-containing systems. *Chemical Physics Letters*, **2006**, 430, 361-366	2.5	15

47	DFT studies of the electronic structure and geometry of 18-crown-6, hexaaza[18]annulene, and their complexes with cations of the heavier alkali and alkaline earth metals. *Inorganica Chimica Acta* , **2008**, 361, 2166-2171	2.7	14
46	Theoretical study of low-lying electronic states of Mn2 using a newly developed relativistic model core potential. *Chemical Physics Letters*, **2008**, 462, 23-26	2.5	12
45	The Hydrogen Bond of the One-Dimensional Assembled Complex [Ni(2,2?-biimidazole)2]: The Effect of Transition Metals on the Hydrogen Bond. *Bulletin of the Chemical Society of Japan*, **2004**, 77, 687-690	5.1	12
44	Assessment of chemical core potentials for the computation on enthalpies of formation of transition-metal complexes. *Chemical Physics Letters*, **2012**, 521, 150-156	2.5	11
43	Theoretical Study on the Hydration Structure of Divalent Radium Ion Using Fragment Molecular Orbital Molecular Dynamics (FMO MD) Simulation. *Journal of Solution Chemistry*, **2014**, 43, 1669-1675	1.8	11
42	Theoretical study of lanthanide mono cation-mediated C H bond activation. *Chemical Physics*, **2011**, 380, 48-53	2.3	11
41	A theoretical study of the physicochemical mechanisms associated with DNA recognition modulation in artificial zinc-finger proteins. *Journal of Physical Chemistry B*, **2011**, 115, 4774-80	3.4	10
40	Model core potential and all-electron studies of molecules containing rare gas atoms. *Journal of Physical Chemistry A*, **2010**, 114, 8786-92	2.8	10
39	4f-in-core model core potentials for trivalent lanthanides. *Chemical Physics Letters*, **2011**, 510, 261-266	2.5	10
38	Theoretical study of interactions between the Si(111) surface and metal atoms. *Surface Science*, **2002**, 514, 383-388	1.8	10
37	Recent Advances in Fragment Molecular Orbital-Based Molecular Dynamics (FMO-MD) Simulations		10
36	Electronic Structures of Platinum(II) Complexes with 2-Arylpyridine and 1,3-Diketonate Ligands: A Relativistic Density Functional Study on Photoexcitation and Phosphorescent Properties. *Journal of Physical Chemistry C*, **2014**, 118, 12443-12449	3.8	9
35	Computational research of the electronic structure of benzene trimer cation by ab initio method. *Chemical Physics Letters*, **2007**, 438, 157-161	2.5	9
34	Room-Temperature Phosphorescence Emitters Exhibiting Red to Near-Infrared Emission Derived from Intermolecular Charge-Transfer Triplet States of Naphthalenediimide-Halobenzoate Triad Molecules. *Chemistry - A European Journal*, **2021**, 27, 9535-9541	4.8	9
33	Effective Fragment Potential Version 2 - Molecular Dynamics (EFP2-MD) Simulation for Investigating Solution Structures of Ionic Liquids. *Chemistry Letters*, **2016**, 45, 1009-1011	1.7	8
32	Synthesis and Conformational Analysis of Alternately N-Alkylated Aromatic Amide Oligomers. *Journal of Organic Chemistry*, **2018**, 83, 14338-14349	4.2	8
31	Theoretical study on crystal-facet dependency of hydrogen storage rate for shape controlled Pd nano particles. *Chemical Physics Letters*, **2016**, 644, 255-260	2.5	7
30	Revised model core potentials of s-block elements. *Journal of Computational Chemistry*, **2007**, 28, 2424-30	3.5	7

29	LIF and IR Dip Spectra of Jet-Cooled p-Aminophenol-M (M = CO, N2): Hydrogen-Bonded or Van der Waals-Bonded Structure?. *Journal of Physical Chemistry A*, **2002**, 106, 4886-4890	2.8	7
28	Stereoselective interactions as manifested by vibrational circular dichroism spectra: the interplay between chiral metal complexes co-adsorbed in a montmorillonite clay. *Physical Chemistry Chemical Physics*, **2018**, 20, 25421-25427	3.6	7
27	Theoretical Design of a Molecular Switch with Controlled Hydrogen Bonds: Electronic and Vibrational Spectra of [Co(2,2?-biimidazole)(C6H4O2)(NH3)2]2. *Bulletin of the Chemical Society of Japan*, **2007**, 80, 1335-1340	5.1	6
26	Molecular orbital study for Na, Mg, and Al adsorption on the Si (111) surface. *Computational and Theoretical Chemistry*, **2003**, 630, 225-232		6
25	Effects of intermolecular interaction on proton tunneling: Theoretical study on two-dimensional potential energy surfaces for 9-hydroxyphenalenone-CO2/H2O complexes. *Journal of Chemical Physics*, **2003**, 119, 4159-4165	3.9	6
24	Theoretical Design of a New Optical Durable Molecular Switch. *Chemistry Letters*, **2004**, 33, 758-759	1.7	6
23	A Quantum Chemical Study on Hydration of Ra (II): Comparison with the Other Hydrated Divalent Alkaline Earth Metal Ions. *Journal of Computer Chemistry Japan*, **2014**, 13, 105-113	0.2	6
22	Development of Helical Aromatic Amide Foldamers with a Diphenylacetylene Backbone. *Journal of Organic Chemistry*, **2020**, 85, 2019-2039	4.2	6
21	Conformational Properties of Aromatic Oligoamides Bearing Pyrrole Rings. *Journal of Organic Chemistry*, **2018**, 83, 4606-4617	4.2	5
20	Comparison of Inhibitory Activities of Stereo-Isomers of Cyclic Phosphatidic Acid (cPA) on Autotaxin. *Cytologia*, **2011**, 76, 73-80	0.9	4
19	Calibration of new model core potentials for main group elements. *International Journal of Quantum Chemistry*, **2009**, 109, 3235-3245	2.1	4
18	POSSIBILITY OF MOLECULAR-SWITCH WITH CONTROLLED HYDROGEN BOND: UTILITY OF COMBINATION OF 2,2?-BIIMIDAZOLE AND REDOX-ACTIVE LIGAND. *Journal of Theoretical and Computational Chemistry*, **2005**, 04, 333-344	1.8	4
17	Fragment molecular orbital-based molecular dynamics (FMO-MD) simulations on hydrated Cu(II) ion. *Chem-Bio Informatics Journal*, **2014**, 14, 1-13	0.8	4
16	Theoretical Strategy for Improving CO2 Absorption of Mixed Ionic Liquids Focusing on the Anion Effect: A Comprehensive COSMO-RS Study. *Industrial & Engineering Chemistry Research*, **2020**, 59, 8848-8854	3.9	3
15	Importance of spin-orbit coupling effect and solvent effect in electronic transition assignments of PtII complexes: In the case of cis/trans-[PtIICl2(NH3)2]. *Journal of Molecular Structure*, **2013**, 1035, 218-223	3.4	3
14	Theoretical quest for photoconversion molecules having opposite directions of the electric dipole moment in S0 and S1 states. *Journal of Chemical Physics*, **2009**, 130, 184311	3.9	3
13	Cyclic Heterometallic Interactions formed from a Flexible Tripeptide Complex Showing Effective Antiferromagnetic Spin Coupling. *Angewandte Chemie - International Edition*, **2021**, 60, 5179-5183	16.4	3
12	Applicability of effective fragment potential version 2 Molecular dynamics (EFP2-MD) simulations for predicting excess properties of mixed solvents. *Chemical Physics Letters*, **2018**, 694, 82-85	2.5	2

List of Publications

11	Electron affinities of heavier phosphoryl and thiophosphoryl halides APX3 (A = O, S and X = Br, I). *Journal of Computational Chemistry*, **2007**, 28, 2027-33	3.5	2
10	Adaptive Application Composition in Quantum Chemistry. *Lecture Notes in Computer Science*, **2009**, 194-211	2.9	2
9	Applicability of Effective Fragment Potential Version 2-Molecular Dynamics (EFP2-MD) Simulations for Predicting Dynamic Liquid Properties Including the Supercritical Fluid Phase. *Journal of Physical Chemistry B*, **2019**, 123, 194-200	3.4	2
8	The ABINIT-MP Program **2021**, 53-67		2
7	ELECTRONIC STRUCTURE AND PHOTOCHEMISTRY OF INORGANIC PHOTOCHROMIC COMPLEX [Cu(N,N?-DIETHYLETHYLENEDIAMINE)2]2+: PLANAR□TETRAHEDRAL GEOMETRY CHANGE ACCOMPANIED WITH d9□10 ELECTRONIC TRANSITION. *Journal of Theoretical and Computational Chemistry*, **2006**, 05, 887-894	1.8	1
6	Synthesis, X-ray structure, photophysical properties, and theoretical studies of six-membered cyclometalated iridium(iii) complexes: revisiting Ir(pnbi)(acac). *Dalton Transactions*, **2019**, 48, 15212-15219	4.3	1
5	Functional Group-Directed Photochemical Reactions of Aromatic Alcohols, Amines, and Thiols Triggered by Excited-State Hydrogen Detachment: Additive-free Oligomerization, Disulfidation, and C(sp)-H Carboxylation with CO. *Journal of Organic Chemistry*, **2021**, 86, 959-969	4.2	1
4	Room-Temperature Phosphorescence Emitters Exhibiting Red to Near-Infrared Emission Derived from Intermolecular Charge-Transfer Triplet States of Naphthalenediimide-Halobenzoate Triad Molecules. *Chemistry - A European Journal*, **2021**, 27, 9465	4.8	0
3	Photo-Induced State Conversion Mechanism of an Optically Durable Molecular Memory with Controlled Hydrogen Bonding: A Spin□Orbit CI Study of [{Co(2,2?-biimidazole)(C6H4O2)(NH3)2}2]. *Bulletin of the Chemical Society of Japan*, **2008**, 81, 235-240	5.1	
2	Computational Design of Proton-Electron Coupling System for Optically Durable Molecular Memory **2019**, 794-798		
1	Cyclic Heterometallic Interactions formed from a Flexible Tripeptide Complex Showing Effective Antiferromagnetic Spin Coupling. *Angewandte Chemie*, **2021**, 133, 5239-5243	3.6	