Hirotoshi Mori

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6062669/publications.pdf

Version: 2024-02-01

66	861	516215 16	580395 25
papers	citations	h-index	g-index

67	67	67	883
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Compact and efficient basis sets of s- and p-block elements for model core potential method. Journal of Chemical Physics, 2005, 122, 074104.	1.2	65
2	Excited-state intramolecular proton transfer in photochromic jet-cooled N-salicylideneaniline. Journal of Photochemistry and Photobiology A: Chemistry, 2002, 154, 33-39.	2.0	54
3	Fragment molecular orbital calculations on large scale systems containing heavy metal atom. Chemical Physics Letters, 2006, 427, 159-165.	1.2	53
4	Electronic band structure calculations on thin films of the L21 full Heusler alloys X2YSi (X, Y = Mn,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.8	39
5	Fragment molecular orbital-based molecular dynamics (FMO-MD) simulations on hydrated Zn(II) ion. Chemical Physics Letters, 2010, 490, 41-45.	1.2	35
6	Revised model core potentials for third-row transitionâ€“metal atoms from Lu to Hg. Chemical Physics Letters, 2009, 476, 317-322.	1.2	31
7	Experimental and Theoretical Approaches Toward Anionâ€Responsive Tripodâ€“Lanthanide Complexes: Mixedâ€Donor Ligand Effects on Lanthanide Complexation and Luminescence Sensing Profiles. Chemistry - A European Journal, 2008, 14, 5258-5266.	1.7	28
8	Origin of high oxygen reduction reaction activity of Pt12 and strategy to obtain better catalyst using sub-nanosized Pt-alloy clusters. Scientific Reports, 2017, 7, 45381.	1.6	27
9	Theoretical study of hydration models of trivalent rare-earth ions using model core potentials. Computational and Theoretical Chemistry, 2010, 949, 28-35.	1.5	26
10	Revised model core potentials for first-row transition-metal atoms from Sc to Zn. Chemical Physics Letters, 2008, 452, 210-214.	1.2	23
11	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.	1.1	21
12	Roomâ€Temperature Phosphorescence Emitters Exhibiting Red to Nearâ€Infrared Emission Derived from Intermolecular Chargeâ€Transfer Triplet States of Naphthalenediimideâ˜Halobenzoate Triad Molecules. Chemistry - A European Journal, 2021, 27, 9535-9541.	1.7	21
13	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.	1.2	20
14	Structure and intermolecular hydrogen bond of jet-cooled p-aminophenolâ€“(H2O)1 studied by electronic and IR-dip spectroscopy and density functional theory calculations. Chemical Physics, 2002, 277, 105-115.	0.9	19
15	Revised model core potentials for second-row transition metal atoms from Y to Cd. Chemical Physics Letters, 2008, 463, 230-234.	1.2	17
16	Density functional theory calculations of iodine cluster anions: Structures, chemical bonding nature, and vibrational spectra. Computational and Theoretical Chemistry, 2011, 973, 69-75.	1.1	16
17	Application of fragment molecular orbital scheme to silicon-containing systems. Chemical Physics Letters, 2006, 430, 361-366.	1.2	15
18	CASSCF and CASPT2 calculations for lanthanide trihalides LnX3 using model core potentials. Chemical Physics Letters, 2009, 474, 28-32.	1.2	15

#	Article	IF	Citations
19	Theoretical Study on the Hydration Structure of Divalent Radium Ion Using Fragment Molecular Orbitalâ€“Molecular Dynamics (FMOâ€“MD) Simulation. Journal of Solution Chemistry, 2014, 43, 1669-1675.	0.6	15
20	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.	1.2	14
21	The Hydrogen Bond of the One-Dimensional Assembled Complex [Ni(2,2â€²-biimidazole)2]: The Effect of Transition Metals on the Hydrogen Bond. Bulletin of the Chemical Society of Japan, 2004, 77, 687-690.	2.0	13
22	4f-in-core model core potentials for trivalent lanthanides. Chemical Physics Letters, 2011, 510, 261-266.	1.2	13
23	Theoretical study of low-lying electronic states of Mn2 using a newly developed relativistic model core potential. Chemical Physics Letters, 2008, 462, 23-26.	1.2	12
24	Assessment of chemical core potentials for the computation on enthalpies of formation of transition-metal complexes. Chemical Physics Letters, 2012, 521, 150-156.	1.2	12
25	Model Core Potential and All-Electron Studies of Molecules Containing Rare Gas Atoms^{â€}. Journal of Physical Chemistry A, 2010, 114, 8786-8792.	1.1	11
26	Theoretical study of lanthanide mono cation-mediated Câ€“F bond activation. Chemical Physics, 2011, 380, 48-53.	0.9	11
27	Synthesis and Conformational Analysis of AlternatelyN-Alkylated Aromatic Amide Oligomers. Journal of Organic Chemistry, 2018, 83, 14338-14349.	1.7	11
28	Recent Advances in Fragment Molecular Orbital-Based Molecular Dynamics (FMO-MD) Simulations. , 0, , .		11
29	Theoretical study of interactions between the Si surface and metal atoms. Surface Science, 2002, 514, 383-388.	0.8	10
30	A Theoretical Study of the Physicochemical Mechanisms Associated with DNA Recognition Modulation in Artificial Zinc-Finger Proteins. Journal of Physical Chemistry B, 2011, 115, 4774-4780.	1.2	10
31	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.	1.5	10
32	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.	1.3	10
33	The ABINIT-MP Program. , 2021, , 53-67.		10
34	LIF and IR Dip Spectra of Jet-Cooled p-Aminophenolâ^'M (M = CO, N2): Hydrogen-Bonded or Van der Waals-Bonded Structure?. Journal of Physical Chemistry A, 2002, 106, 4886-4890.	1.1	9
35	Computational research of the electronic structure of benzene trimer cation by ab initio method. Chemical Physics Letters, 2007, 438, 157-161.	1.2	9
36	Effective Fragment Potential Version 2 - Molecular Dynamics (EFP2-MD) Simulation for Investigating Solution Structures of Ionic Liquids. Chemistry Letters, 2016, 45, 1009-1011.	0.7	9

#	Article	IF	Citations
37	Theoretical study on crystal-facet dependency of hydrogen storage rate for shape controlled Pd nano particles. Chemical Physics Letters, 2016, 644, 255-260.	1.2	9
38	Development of Helical Aromatic Amide Foldamers with a Diphenylacetylene Backbone. Journal of Organic Chemistry, 2020, 85, 2019-2039.	1.7	9
39	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.	0.0	9
40	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.	1.2	8
41	Revised model core potentials of sâ€block elements. Journal of Computational Chemistry, 2007, 28, 2424-2430.	1.5	8
42	Conformational Properties of Aromatic Oligoamides Bearing Pyrrole Rings. Journal of Organic Chemistry, 2018, 83, 4606-4617.	1.7	8
43	Theoretical Design of a Molecular Switch with Controlled Hydrogen Bonds: Electronic and Vibrational Spectra of [Co(2,2â€²-biimidazole)(C6H4O2)(NH3)2]2. Bulletin of the Chemical Society of Japan, 2007, 80, 1335-1340.	2.0	7
44	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.	1.8	7
45	Molecular orbital study for Na, Mg, and Al adsorption on the Si (111) surface. Computational and Theoretical Chemistry, 2003, 630, 225-232.	1.5	6
46	Theoretical Design of a New Optical Durable Molecular Switch. Chemistry Letters, 2004, 33, 758-759.	0.7	6
47	Cyclic Heterometallic Interactions formed from a Flexible Tripeptide Complex Showing Effective Antiferromagnetic Spin Coupling. Angewandte Chemie - International Edition, 2021, 60, 5179-5183.	7.2	6
48	Comprehensive Physical Chemistry Learning Based on Blended Learning: A New Laboratory Course. Journal of Chemical Education, 2021, 98, 3864-3870.	1.1	6
49	Fragment molecular orbitalâˆ’based molecular dynamics (FMO-MD) simulations on hydrated Cu(II) ion. Chem-Bio Informatics Journal, 2014, 14, 1-13.	0.1	5
50	Adaptive Application Composition in Quantum Chemistry. Lecture Notes in Computer Science, 2009, , 194-211.	1.0	5
51	POSSIBILITY OF MOLECULAR-SWITCH WITH CONTROLLED HYDROGEN BOND: UTILITY OF COMBINATION OF 2,2â€²-BIIMIDAZOLE AND REDOX-ACTIVE LIGAND. Journal of Theoretical and Computational Chemistry, 2005, 04, 333-344.	1.8	4
52	Calibration of new model core potentials for main group elements. International Journal of Quantum Chemistry, 2009, 109, 3235-3245.	1.0	4
53	Comparison of Inhibitory Activities of Stereo-Isomers of Cyclic Phosphatidic Acid (cPA) on Autotaxin. Cytologia, 2011, 76, 73-80.	0.2	4
54	Importance of spinâ€“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.	1.8	4

#	Article	IF	Citations
55	Applicability of effective fragment potential version 2 â€“ Molecular dynamics (EFP2-MD) simulations for predicting excess properties of mixed solvents. Chemical Physics Letters, 2018, 694, 82-85.	1.2	4
56	Synthesis, X-ray structure, photophysical properties, and theoretical studies of six-membered cyclometalated iridium(<scp>iii</scp>) complexes: revisiting Ir(pnbi)₂(acac). Dalton Transactions, 2019, 48, 15212-15219.	1.6	4
57	Theoretical quest for photoconversion molecules having opposite directions of the electric dipole moment in S[sub 0] and S[sub 1] states. Journal of Chemical Physics, 2009, 130, 184311.	1.2	3
58	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.	1.2	3
59	Electron affinities of heavier phosphoryl and thiophosphoryl halides APX3 (A = O, S and X = Br, I). Journal of Computational Chemistry, 2007, 28, 2027-2033.	1.5	2
60	Functional Group-Directed Photochemical Reactions of Aromatic Alcohols, Amines, and Thiols Triggered by Excited-State Hydrogen Detachment: Additive-free Oligomerization, Disulfidation, and C(sp²)â€“H Carboxylation with CO₂. Journal of Organic Chemistry, 2021, 86, 959-969.	1.7	2
61	Roomâ€Temperature Phosphorescence Emitters Exhibiting Red to Nearâ€Infrared Emission Derived from Intermolecular Chargeâ€Transfer Triplet States of Naphthalenediimideâ€“Halobenzoate Triad Molecules. Chemistry - A European Journal, 2021, 27, 9465-9465.	1.7	2
62	ELECTRONIC STRUCTURE AND PHOTOCHEMISTRY OF INORGANIC PHOTOCHROMIC COMPLEX [Cu(N,Nâ€²-DIETHYLETHYLENEDIAMINE)2]2+: PLANARâ€“TETRAHEDRAL GEOMETRY CHANGE ACCOMPANIED WITH d9â€“d10 ELECTRONIC TRANSITION. Journal of Theoretical and Computational Chemistry, 2006, 05, 887-894.	1.8	1
63	Photo-Induced State Conversion Mechanism of an Optically Durable Molecular Memory with Controlled Hydrogen Bonding: A Spinâ€“Orbit CI Study of [{Co(2,2â€²-biimidazole)(C6H4O2)(NH3)2}2]. Bulletin of the Chemical Society of Japan, 2008, 81, 235-240.	2.0	0
64	Fragment Molecular Orbital-Based Molecular Dynamics Study on Hydrated Ln(III) Ions. , 2015, , .		0
65	Cyclic Heterometallic Interactions formed from a Flexible Tripeptide Complex Showing Effective Antiferromagnetic Spin Coupling. Angewandte Chemie, 2021, 133, 5239-5243.	1.6	0
66	Computational Design of Proton-Electron Coupling System for Optically Durable Molecular Memory. , 2019, , 794-798.		0