Shiro Koseki

List of Publications by Year
in descending order

55 papers	20,860 citations	361413 20 h-index	175258 52 g-index
55 all docs	55 docs citations	55 times ranked	14737 citing authors

#	Article	IF	Citations
1	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	3.3	19,020
2	Spin-orbit coupling in molecules: Chemistry beyond the adiabatic approximation. International Reviews in Physical Chemistry, 2003, 22, 551-592.	2.3	284
3	MCSCF/6-31G(d,p) calculations of one-electron spin-orbit coupling constants in diatomic molecules. The Journal of Physical Chemistry, 1992, 96, 10768-10772.	2.9	271
4	Main Group Effective Nuclear Charges for Spin-Orbit Calculations. The Journal of Physical Chemistry, 1995, 99, 12764-12772.	2.9	214
5	Effective Nuclear Charges for the First- through Third-Row Transition Metal Elements in Spinâ^'Orbit Calculations. Journal of Physical Chemistry A, 1998, 102, 10430-10435.	2.5	183
6	Relativistic potential energy surfaces of XH2 (X=C, Si, Ge, Sn, and Pb) molecules: Coupling of 1A1 and 3B1 states. Journal of Chemical Physics, 1996, 104, 7988-7996.	3.0	77
7	Relativistic Study on Emission Mechanism in Tris(2-phenylpyridine)iridium. Journal of Physical Chemistry C, 2007, 111, 6897-6903.	3.1	68
8	Spinâ^'Orbit Splittings in the Third-Row Transition Elements:Â Comparison of Effective Nuclear Charge and Full Breitâ^'Pauli Calculations. Journal of Physical Chemistry A, 2001, 105, 8262-8268.	2.5	64
9	Benzannelation Effect on Enediyne Cycloaromatization:Â An ab Initio Molecular Orbital Study. Journal of Physical Chemistry A, 1999, 103, 7672-7675.	2.5	53
10	Spinâ€“Orbit Coupling Constants in Atoms and Ions of Transition Elements: Comparison of Effective Core Potentials, Model Core Potentials, and All-Electron Methods. Journal of Physical Chemistry A, 2019, 123, 2325-2339.	2.5	41
11	Potential energy surfaces and dynamical properties of three low-lying states of silylene. Journal of Molecular Spectroscopy, 1987, 123, 392-404.	1.2	36
12	Energy Component Analysis of the Pseudo-Jahnâ^'Teller Effect in the Ground and Electronically Excited States of the Cyclic Conjugated Hydrocarbons:Â Cyclobutadiene, Benzene, and Cyclooctatetraene. Journal of Physical Chemistry A, 1997, 101, 5712-5718.	2.5	36
13	Dissociation Potential Curves of Low-Lying States in Transition Metal Hydrides. I. Hydrides of Group 4. Journal of Physical Chemistry A, 2002, 106, 785-794.	2.5	34
14	Dissociation Potential Curves of Low-Lying States in Transition Metal Hydrides. 2. Hydrides of Groups 3 and 5. Journal of Physical Chemistry A, 2004, 108, 4707-4719.	2.5	34
15	Violation of Hund's multiplicity rule in the electronically excited states of conjugated hydrocarbons. Canadian Journal of Chemistry, 1985, 63, 1572-1579.	1.1	30
16	Dissociation Potential Curves of Low-Lying States in Transition Metal Hydrides. 3. Hydrides of Groups 6 and 7. Journal of Physical Chemistry A, 2006, 110, 2560-2570.	2.5	28
17	Novel bis- and tris-cyclometalated iridium(<scp>iii</scp>) complexes bearing a benzoyl group on each fluorinated 2-phenylpyridinate ligand aimed at development of blue phosphorescent materials for OLED. RSC Advances, 2016, 6, 51435-51445.	3.6	27
18	Relativistic Study on Emission Mechanism in Palladium and Platinum Complexes. Journal of Physical Chemistry A, 2006, 110, 13295-13302.	2.5	26

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19	Energy Component Analysis of the Pseudo-Jahnâ^'Teller Effect in the Bicyclic Nonalternant Hydrocarbons:Â The Pentalenoid and Heptalenoid Systems. The Journal of Physical Chemistry, 1996, 100, 2100-2106.	2.9	23
20	Spinâ€"Orbit Coupling Analyses of the Geometrical Effects on Phosphorescence in Ir(ppy)3 and Its Derivatives. Journal of Physical Chemistry C, 2013, 117, 5314-5327.	3.1	21
21	Strong Nuclear Ring Currents and Magnetic Fields in Pseudorotating OsH₄ Molecules Induced by Circularly Polarized Laser Pulses. Chemistry - an Asian Journal, 2012, 7, 1261-1295.	3.3	20
22	Theoretical study on the absorption spectra of fac-Ir(ppy)3 in the amorphous phase of organic electro-luminescent devices. Research on Chemical Intermediates, 2009, 35, 851-863.	2.7	17
23	Parallelization of multireference perturbation calculations with GAMESS. Journal of Computational Chemistry, 2001, 22, 1243-1251.	3.3	16
24	Characterization of multielectron dynamics in molecules: A multiconfiguration time-dependent Hartree-Fock picture. Journal of Chemical Physics, 2014, 141, 114105.	3.0	16
25	Photochemistry of Phenyl Azides Bearing 2â€Hydroxy and 2â€Amino Groups Studied by Matrixâ€Isolation Spectroscopy: Generation and Characterization of Reactive oâ€Quinoid Compounds. Liebigs Annalen, 1996, 1996, 1971-1980.	0.8	15
26	Pseudo-Jahnâ^'Teller Distortion from Planarity in Heterocyclic Seven- and Eight-Membered Ring Systems with Eight Ï€ Electrons. Journal of Physical Chemistry A, 2003, 107, 2749-2756.	2.5	14
27	Ab Initio MCSCF Study on the Pseudo-Jahnâ^'Teller Distortion from Planarity in Cycloheptatriene, Heptalene, and Heptafulvalene. Journal of Physical Chemistry A, 2000, 104, 5343-5350.	2.5	11
28	Tetra-hydrides of the third-row transition elements: spinâ€"orbit coupling effects on geometrical deformation in WH4 and OsH4. Theoretical Chemistry Accounts, 2008, 120, 85-94.	1.4	11
29	Theoretical Study on Phosphorescent Materials for Organic Electro-Luminescent Devices. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1352-1360.	0.4	11
30	Tetrahydrides of third-row transition elements: Spin-orbit coupling effects on the stability of rhenium tetrahydride. Journal of Chemical Physics, 2010, 133, 174112.	3.0	11
31	Energy Component Analysis of the Pseudo Jahn-Teller Effect in Pentalene and Heptalene. Chemistry Letters, 1992, 21, 791-794.	1.3	10
32	Theoretical study of environmental effects on proton transfer reaction through the peptide bond in a model system. Theoretical Chemistry Accounts, 2008, 120, 263-271.	1.4	10
33	QM/MM investigation of the degradation mechanism of the electron-transporting layer. Theoretical Chemistry Accounts, 2011, 130, 439-448.	1.4	10
34	Time-Dependent Multiconfiguration Theory and Its Application to Ultrafast Electronic Dynamics of Molecules in an Intense Laser Field. Progress of Theoretical Physics Supplement, 2012, 196, 16-38.	0.1	10
35	Efficient approach to include molecular polarizations using charge and atom dipole response kernels to calculate free energy gradients in the QM/MM scheme. Physical Chemistry Chemical Physics, 2015, 17, 26955-26968.	2.8	10
36	Ab Initio MCSCF Study on Electronically Excited Singlet States of Fulvalene Systems:â€‰ Energy Component Analysis of the Pseudo-Jahnâ^'Teller Effect. Journal of Physical Chemistry A, 1998, 102, 6668-6675.	2.5	9

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37	Spin-orbit coupling effects in dihydrides of third-row transition elements. II. Interplay of nonadiabatic coupling in the dissociation path of rhenium dihydride. Journal of Chemical Physics, 2009, 131, 044122.	3.0	9
38	Theoretical Analyses on Phosphorescent Processes in Pt(thpy)2 and Its Derivatives. Journal of Physical Chemistry C, 2014, 118, 15412-15421.	3.1	9
39	Modeling of Spin-Forbidden Reactions. Reviews in Computational Chemistry, 2004, , 101-152.	1.5	8
40	Energy Component Analysis of the Pseudo-Jahnâ^Teller Effect in the Ground State of the Triafulvalene Anion, Pentafulvalene Cation, and Heptafulvalene Anion Radicals. Journal of Physical Chemistry A, 1998, 102, 490-495.	2.5	7
41	Ab Initio MCSCF Study on Eight Ï€-Electron Heterocyclic Conjugated Systems:â€‰ Energy Component Analysis of the Pseudo-Jahnâ^Teller Distortion from Planarity. Journal of Physical Chemistry A, 2001, 105, 1334-1342.	2.5	7
42	Neutral-Fragmentation Paths of Methane Induced by Intense Ultrashort IR Laser Pulses: Ab Initio Molecular Orbital Approach. Journal of Physical Chemistry A, 2013, 117, 333-341.	2.5	7
43	Spinâ€“orbit coupling analyses of phosphorescent processes in Ir(Zppy)3 (Z = NH2, NO2 and CN). RSC Advances, 2015, 5, 35760-35772.	3.6	7
44	Spinâ€“orbit coupling analyses of phosphorescence: the effects of cyclometalated ligand replacement in fac-Ir(ppy)₃with various bpy ligands on blue phosphorescence. RSC Advances, 2016, 6, 65020-65030.	3.6	7
45	Free Energy Contribution Analysis Using Response Kernel Approximation: Insights into the Acylation Reaction of a Beta-Lactamase. Journal of Physical Chemistry B, 2016, 120, 9338-9346.	2.6	6
46	Effect of phenyl substitution on the lifetime and product distribution of cyclobutylidene: preference change in the rearrangements via 1,2-carbon shift and 1,2-hydrogen shift. Tetrahedron Letters, 2006, 47, 3995-3999.	1.4	5
47	Ab initio MCSCF study on several azide molecules: energy component analysis of the pseudo-Jahnâ€“Teller effect. RSC Advances, 2013, 3, 10775.	3.6	5
48	Numerical Estimation of the Pseudo-Jahnâ€“Teller Effect Using Nonadiabatic Coupling Integrals in Monocyclic and Bicyclic Conjugated Molecules. Journal of Physical Chemistry A, 2016, 120, 10207-10215.	2.5	3
49	Multiconfiguration Self-Consistent Field Study on Formonitrile Imine and N-Substituted Nitrile Imines HCN₂â€“R: Energy Component Analysis of the Pseudo-Jahnâ€“Teller Effect. Journal of Physical Chemistry A, 2017, 121, 2298-2310.	2.5	3
50	Full-Optimized Reaction Space MCSCF+MP2 Study on Reactions of Diradical Systems:â€‰ o-C6H4(CH)2, o-C6H4CHN, and o-C6H4N2. Journal of Physical Chemistry A, 1997, 101, 3377-3381.	2.5	2
51	Exploring the Reaction Paths on the Potential Energy Surfaces of the S₁ and T₁ States in Methylenecyclopropane. Photochemistry and Photobiology, 2021, 97, 126-135.	2.5	2
52	Molecular Orbital Analysis of High Harmonic Generation. , 2014, , .		1
53	Computational approach for molecular design using free energy contribution analysis. AIP Conference Proceedings, 2018, , .	0.4	1
54	Spin-Orbit Coupling Effects in Di-Hydrides of Third-Row Transition Elements. AIP Conference Proceedings, 2007, , .	0.4	0

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55	Theoretical Design of Blue-Color Phosphorescent Complexes for Organic Light-Emitting Diodes: Emission Intensities and Nonradiative Transition Rate Constants in Ir(ppy)₂(acac) Derivatives. Journal of Physical Chemistry A, 2021, 125, 10604-10614.	2.5	0