

# Shiro Koseki

## List of Publications by Year in descending order

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55  
papers

20,860  
citations

411340

20  
h-index

198040

52  
g-index

55  
all docs

55  
docs citations

55  
times ranked

16364  
citing authors

#	ARTICLE	IF	CITATIONS
1	General atomic and molecular electronic structure system. <i>Journal of Computational Chemistry</i> , 1993, 14, 1347-1363.	1.5	19,020
2	Spin-orbit coupling in molecules: Chemistry beyond the adiabatic approximation. <i>International Reviews in Physical Chemistry</i> , 2003, 22, 551-592.	0.9	284
3	MCSCF/6-31G(d,p) calculations of one-electron spin-orbit coupling constants in diatomic molecules. <i>The Journal of Physical Chemistry</i> , 1992, 96, 10768-10772.	2.9	271
4	Main Group Effective Nuclear Charges for Spin-Orbit Calculations. <i>The Journal of Physical Chemistry</i> , 1995, 99, 12764-12772.	2.9	214
5	Effective Nuclear Charges for the First- through Third-Row Transition Metal Elements in Spin-Orbit Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10430-10435.	1.1	183
6	Relativistic potential energy surfaces of XH <sub>2</sub> (X=C, Si, Ge, Sn, and Pb) molecules: Coupling of 1A <sub>1</sub> and 3B <sub>1</sub> states. <i>Journal of Chemical Physics</i> , 1996, 104, 7988-7996.	1.2	77
7	Relativistic Study on Emission Mechanism in Tris(2-phenylpyridine)iridium. <i>Journal of Physical Chemistry C</i> , 2007, 111, 6897-6903.	1.5	68
8	Spin-Orbit Splittings in the Third-Row Transition Elements: A Comparison of Effective Nuclear Charge and Full Breit-Pauli Calculations. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8262-8268.	1.1	64
9	Benzannulation Effect on Eneidyne Cycloaromatization: An ab Initio Molecular Orbital Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7672-7675.	1.1	53
10	Spin-Orbit Coupling Constants in Atoms and Ions of Transition Elements: Comparison of Effective Core Potentials, Model Core Potentials, and All-Electron Methods. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2325-2339.	1.1	41
11	Potential energy surfaces and dynamical properties of three low-lying states of silylene. <i>Journal of Molecular Spectroscopy</i> , 1987, 123, 392-404.	0.4	36
12	Energy Component Analysis of the Pseudo-Jahn-Teller Effect in the Ground and Electronically Excited States of the Cyclic Conjugated Hydrocarbons: Cyclobutadiene, Benzene, and Cyclooctatetraene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5712-5718.	1.1	36
13	Dissociation Potential Curves of Low-Lying States in Transition Metal Hydrides. I. Hydrides of Group 4. <i>Journal of Physical Chemistry A</i> , 2002, 106, 785-794.	1.1	34
14	Dissociation Potential Curves of Low-Lying States in Transition Metal Hydrides. 2. Hydrides of Groups 3 and 5. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4707-4719.	1.1	34
15	Violation of Hund's multiplicity rule in the electronically excited states of conjugated hydrocarbons. <i>Canadian Journal of Chemistry</i> , 1985, 63, 1572-1579.	0.6	30
16	Dissociation Potential Curves of Low-Lying States in Transition Metal Hydrides. 3. Hydrides of Groups 6 and 7. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2560-2570.	1.1	28
17	Novel bis- and tris-cyclometalated iridium( $\text{III}$ ) complexes bearing a benzoyl group on each fluorinated 2-phenylpyridinate ligand aimed at development of blue phosphorescent materials for OLED. <i>RSC Advances</i> , 2016, 6, 51435-51445.	1.7	27
18	Relativistic Study on Emission Mechanism in Palladium and Platinum Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13295-13302.	1.1	26

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19	Energy Component Analysis of the Pseudo-Jahn-Teller Effect in the Bicyclic Nonalternant Hydrocarbons: The Pentalenoid and Heptalenoid Systems. <i>The Journal of Physical Chemistry</i> , 1996, 100, 2100-2106.	2.9	23
20	Spin-Orbit Coupling Analyses of the Geometrical Effects on Phosphorescence in Ir(ppy) <sub>3</sub> and Its Derivatives. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5314-5327.	1.5	21
21	Strong Nuclear Ring Currents and Magnetic Fields in Pseudorotating OsH <sub>4</sub> Molecules Induced by Circularly Polarized Laser Pulses. <i>Chemistry - an Asian Journal</i> , 2012, 7, 1261-1295.	1.7	20
22	Theoretical study on the absorption spectra of fac-Ir(ppy) <sub>3</sub> in the amorphous phase of organic electro-luminescent devices. <i>Research on Chemical Intermediates</i> , 2009, 35, 851-863.	1.3	17
23	Parallelization of multireference perturbation calculations with GAMESS. <i>Journal of Computational Chemistry</i> , 2001, 22, 1243-1251.	1.5	16
24	Characterization of multielectron dynamics in molecules: A multiconfiguration time-dependent Hartree-Fock picture. <i>Journal of Chemical Physics</i> , 2014, 141, 114105.	1.2	16
25	Photochemistry of Phenyl Azides Bearing 2-Hydroxy and 2-Amino Groups Studied by Matrix Isolation Spectroscopy: Generation and Characterization of Reactive Quinoid Compounds. <i>Liebigs Annalen</i> , 1996, 1996, 1971-1980.	0.8	15
26	Pseudo-Jahn-Teller Distortion from Planarity in Heterocyclic Seven- and Eight-Membered Ring Systems with Eight $\pi$ Electrons. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2749-2756.	1.1	14
27	Ab Initio MCSCF Study on the Pseudo-Jahn-Teller Distortion from Planarity in Cycloheptatriene, Heptalene, and Heptafulvalene. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5343-5350.	1.1	11
28	Tetra-hydrides of the third-row transition elements: spin-orbit coupling effects on geometrical deformation in WH <sub>4</sub> and OsH <sub>4</sub> . <i>Theoretical Chemistry Accounts</i> , 2008, 120, 85-94.	0.5	11
29	Theoretical Study on Phosphorescent Materials for Organic Electro-Luminescent Devices. <i>Journal of Computational and Theoretical Nanoscience</i> , 2009, 6, 1352-1360.	0.4	11
30	Tetrahydrides of third-row transition elements: Spin-orbit coupling effects on the stability of rhenium tetrahydride. <i>Journal of Chemical Physics</i> , 2010, 133, 174112.	1.2	11
31	Energy Component Analysis of the Pseudo Jahn-Teller Effect in Pentalene and Heptalene. <i>Chemistry Letters</i> , 1992, 21, 791-794.	0.7	10
32	Theoretical study of environmental effects on proton transfer reaction through the peptide bond in a model system. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 263-271.	0.5	10
33	QM/MM investigation of the degradation mechanism of the electron-transporting layer. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 439-448.	0.5	10
34	Time-Dependent Multiconfiguration Theory and Its Application to Ultrafast Electronic Dynamics of Molecules in an Intense Laser Field. <i>Progress of Theoretical Physics Supplement</i> , 2012, 196, 16-38.	0.2	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. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26955-26968.	1.3	10
36	Ab Initio MCSCF Study on Electronically Excited Singlet States of Fulvalene Systems: Energy Component Analysis of the Pseudo-Jahn-Teller Effect. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6668-6675.	1.1	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. <i>Journal of Chemical Physics</i> , 2009, 131, 044122.	1.2	9
38	Theoretical Analyses on Phosphorescent Processes in Pt(thpy) <sub>2</sub> and Its Derivatives. <i>Journal of Physical Chemistry C</i> , 2014, 118, 15412-15421.	1.5	9
39	Modeling of Spin-Forbidden Reactions. <i>Reviews in Computational Chemistry</i> , 2004, , 101-152.	1.5	8
40	Energy Component Analysis of the Pseudo-Jahn-Teller Effect in the Ground State of the Triafulvalene Anion, Pentafulvalene Cation, and Heptafulvalene Anion Radicals. <i>Journal of Physical Chemistry A</i> , 1998, 102, 490-495.	1.1	7
41	Ab Initio MCSCF Study on Eight $\pi$ -Electron Heterocyclic Conjugated Systems: Energy Component Analysis of the Pseudo-Jahn-Teller Distortion from Planarity. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1334-1342.	1.1	7
42	Neutral-Fragmentation Paths of Methane Induced by Intense Ultrashort IR Laser Pulses: Ab Initio Molecular Orbital Approach. <i>Journal of Physical Chemistry A</i> , 2013, 117, 333-341.	1.1	7
43	Spin-orbit coupling analyses of phosphorescent processes in Ir(Zppy) <sub>3</sub> (Z = NH <sub>2</sub> , NO <sub>2</sub> and CN). <i>RSC Advances</i> , 2015, 5, 35760-35772.	1.7	7
44	Spin-orbit coupling analyses of phosphorescence: the effects of cyclometalated ligand replacement in fac-Ir(ppy) <sub>3</sub> with various bpy ligands on blue phosphorescence. <i>RSC Advances</i> , 2016, 6, 65020-65030.	1.7	7
45	Free Energy Contribution Analysis Using Response Kernel Approximation: Insights into the Acylation Reaction of a Beta-Lactamase. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9338-9346.	1.2	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. <i>Tetrahedron Letters</i> , 2006, 47, 3995-3999.	0.7	5
47	Ab initio MCSCF study on several azide molecules: energy component analysis of the pseudo-Jahn-Teller effect. <i>RSC Advances</i> , 2013, 3, 10775.	1.7	5
48	Numerical Estimation of the Pseudo-Jahn-Teller Effect Using Nonadiabatic Coupling Integrals in Monocyclic and Bicyclic Conjugated Molecules. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10207-10215.	1.1	3
49	Multiconfiguration Self-Consistent Field Study on Formonitrile Imine and N-Substituted Nitrile Imines HCN <sub>2</sub> : Energy Component Analysis of the Pseudo-Jahn-Teller Effect. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2298-2310.	1.1	3
50	Full-Optimized Reaction Space MCSCF+MP2 Study on Reactions of Diradical Systems: o-C <sub>6</sub> H <sub>4</sub> (CH) <sub>2</sub> , o-C <sub>6</sub> H <sub>4</sub> CHN, and o-C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 1997, 101, 3377-3381.	1.1	2
51	Exploring the Reaction Paths on the Potential Energy Surfaces of the S <sub>1</sub> and T <sub>1</sub> States in Methylene-cyclopropane. <i>Photochemistry and Photobiology</i> , 2021, 97, 126-135.	1.3	2
52	Molecular Orbital Analysis of High Harmonic Generation. , 2014, , .		1
53	Computational approach for molecular design using free energy contribution analysis. <i>AIP Conference Proceedings</i> , 2018, , .	0.3	1
54	Spin-Orbit Coupling Effects in Di-Hydrides of Third-Row Transition Elements. <i>AIP Conference Proceedings</i> , 2007, , .	0.3	0

#	ARTICLE	IF	CITATIONS
55	Theoretical Design of Blue-Color Phosphorescent Complexes for Organic Light-Emitting Diodes: Emission Intensities and Nonradiative Transition Rate Constants in Ir(ppy) <sub>2</sub> (acac) Derivatives. Journal of Physical Chemistry A, 2021, 125, 10604-10614.	1.1	0