# Kazuya Ishimura

List of Publications by Year
in descending order



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|---|---|---|---|
| 49 papers | 1,401 citations | 318942 23 h-index | 371746 37 g-index |
| 50 all docs | 50 docs citations | 50 times ranked | 1567 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | A new strategy for hyperconjugative antiaromatic compounds utilizing negative charges: a dibenzo[b,f]silepinyl dianion. Chemical Communications, 2021, 57, 11330-11333. | 2.2 | 1 |
| 2 | Theoretical analysis of the kinetic isotope effect on carboxylation in RubisCO. Journal of Computational Chemistry, 2020, 41, 1116-1123. | 1.5 | 1 |
| 3 | Reaction Behavior of the NO Molecule on the Surface of an M<sub>n</sub> Particle (M = Ru,) Tj ETQq1 1 0.784314 rgBT /Ove<br>Journal of Physical Chemistry A, 2019, 123, 7021-7033. | 1.1 | 24 |
| 4 | Ab initio quantum mechanics/molecular mechanics method with periodic boundaries employing Ewald summation technique to electron-charge interaction: Treatment of the surface-dipole term. Journal of Chemical Physics, 2019, 150, 124103. | 1.2 | 7 |
| 5 | Catalysis of Cu Cluster for NO Reduction by CO: Theoretical Insight into the Reaction Mechanism. ACS Omega, 2019, 4, 2596-2609. | 1.6 | 36 |
| 6 | SALMON: Scalable Ab-initio Lightâ€“Matter simulator for Optics and Nanoscience. Computer Physics Communications, 2019, 235, 356-365. | 3.0 | 114 |
| 7 | Electronic processes in NO dimerization on Ag and Cu clusters: DFT and MRMP2 studies. Journal of Computational Chemistry, 2019, 40, 181-190. | 1.5 | 9 |
| 8 | Large-Scale Quantum Chemical. , 2019, , 159-201. | | 0 |
| 9 | Theoretical Insight into Coreâ€“Shell Preference for Bimetallic Pt-M (M = Ru, Rh, Os, and Ir) Cluster and Its Electronic Structure. Journal of Physical Chemistry C, 2018, 122, 9081-9090. | 1.5 | 15 |
| 10 | Double aromaticity arising from Ïƒ- and Ï€-rings. Communications Chemistry, 2018, 1, . | 2.0 | 38 |
| 11 | First-Order Interacting Space Approach to Excited-State Molecular Interaction: Solvatochromic Shift of p-Coumaric Acid and Retinal Schiff Base. Journal of Chemical Theory and Computation, 2018, 14, 3643-3655. | 2.3 | 3 |
| 12 | Coreâ€“Shell versus Other Structures in Binary Cu<sub>38â€“n</sub>M<sub>n</sub> Nanoclusters (M = Ru, Rh, Pd, Ag, Os, Ir, Pt, and Au; n = 1, 2, and 6): Theoretical Insight into Determining Factors. Journal of Physical Chemistry C, 2017, 121, 10514-10528. | 1.5 | 16 |
| 13 | Performance Evaluations of Parallelized DFT Calculations with SMASH on Intel Xeon Phi Processor. Journal of Computer Chemistry Japan, 2016, 15, 92-96. | 0.0 | 1 |
| 14 | Electronic Polarization Effect of the Water Environment in Charge-Separated Donorâ€“Acceptor Systems: An Effective Fragment Potential Model Study. Journal of Physical Chemistry A, 2016, 120, 10273-10280. | 1.1 | 0 |
| 15 | On the hierarchical parallelization of ab initio simulations. Chemical Physics Letters, 2016, 646, 130-135. | 1.2 | 17 |
| 16 | Development of massively parallel quantum chemistry program SMASH. AIP Conference Proceedings, 2015, , . | 0.3 | 1 |
| 17 | Program Package of Photoinduced Electron Dynamics: GCEED (Grid-based Coupled Electron and) Tj ETQq1 1 0.784314 rgBT /Overloc<br>2 | | |
| 18 | Quantum Mechanical Molecular Interactions for Calculating the Excitation Energy in Molecular Environments: A Firstâ€Order Interacting Space Approach. ChemPhysChem, 2015, 16, 305-311. | 1.0 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | How Can We Understand Au<sub>8</sub> Cores and Entangled Ligands of Selenolate- and Thiolate-Protected Gold Nanoclusters Au<sub>24</sub>(ER)<sub>20</sub> and Au<sub>20</sub>(ER)<sub>16</sub> (E = Se, S; R = Ph, Me)? A Theoretical Study. Journal of the American Chemical Society, 2015, 137, 8593-8602. | 6.6 | 25 |
| 20 | Massively parallel MP2â€F12 calculations on the <scp>K</scp> computer. International Journal of Quantum Chemistry, 2015, 115, 333-341. | 1.0 | 5 |
| 21 | Facile Synthesis of Dibenzopentalene Dianions and Their Application as New Ï€â€Extended Ligands. Chemistry - A European Journal, 2014, 20, 7571-7575. | 1.7 | 14 |
| 22 | First-Principles Computational Visualization of Localized Surface Plasmon Resonance in Gold Nanoclusters. Journal of Physical Chemistry A, 2014, 118, 11317-11322. | 1.1 | 79 |
| 23 | Interaction Energy of Large Molecules from Restrained Denominator MP2-F12. Journal of Chemical Theory and Computation, 2014, 10, 4857-4861. | 2.3 | 12 |
| 24 | Massively-parallel electron dynamics calculations in real-time and real-space: Toward applications to nanostructures of more than ten-nanometers in size. Journal of Computational Physics, 2014, 265, 145-155. | 1.9 | 38 |
| 25 | Debromination of 1,2-Bis(phenylseleno)benzene Dibromide. Bulletin of the Chemical Society of Japan, 2013, 86, 990-992. | 2.0 | 2 |
| 26 | Molecular Structure and Electronic State of the Dibenzo[a,e]pentalene Anion Radical. Chemistry - an Asian Journal, 2012, 7, 480-483. | 1.7 | 21 |
| 27 | Analytic energy gradient for second-order MÃ¸ller-Plesset perturbation theory based on the fragment molecular orbital method. Journal of Chemical Physics, 2011, 135, 044110. | 1.2 | 48 |
| 28 | Synthesis of a Novel Lithocene that has Aromaticâ€Like Nature with Nonaromatic Rings. Chemistry - an Asian Journal, 2011, 6, 2907-2910. | 1.7 | 12 |
| 29 | MPI/OpenMP hybrid parallel implementation of second-order MÃ¸llerâ€“Plesset perturbation theory using numerical quadratures. Theoretical Chemistry Accounts, 2011, 130, 317-321. | 0.5 | 13 |
| 30 | Synthesis, Structure, and Reaction of Tetraethyldilithiostannole. Chemistry Letters, 2010, 39, 700-701. | 0.7 | 44 |
| 31 | Synthesis and Structures of Lithium Salts of Stannole Anions. Bulletin of the Chemical Society of Japan, 2010, 83, 825-827. | 2.0 | 20 |
| 32 | MPI/OpenMP Hybrid Parallel Algorithm for Hartreeâ^'Fock Calculations. Journal of Chemical Theory and Computation, 2010, 6, 1075-1080. | 2.3 | 23 |
| 33 | Synthesis, Structures, and Properties of Plumboles. Phosphorus, Sulfur and Silicon and the Related Elements, 2010, 185, 1068-1076. | 0.8 | 17 |
| 34 | Dilithioplumbole: A Lead-Bearing Aromatic Cyclopentadienyl Analog. Science, 2010, 328, 339-342. | 6.0 | 112 |
| 35 | Dichlorocarbene Addition to C<sub>60</sub> from the Trichloromethyl Anion: Carbene Mechanism or Bingel Mechanism?. Journal of Physical Chemistry A, 2009, 113, 3673-3676. | 1.1 | 24 |
| 36 | Mechanism and Dynamic Correlation Effects in Cycloaddition Reactions of Singlet Difluorocarbene to Alkenes and Disilene. Journal of Physical Chemistry A, 2009, 113, 9852-9860. | 1.1 | 12 |

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|---|---|---|---|
| 37 | A new algorithm of two-electron repulsion integral calculations: a combination of Popleâ€“Hehre and McMurchieâ€“Davidson methods. Theoretical Chemistry Accounts, 2008, 120, 185-189. | 0.5 | 23 |
| 38 | Synthesis, structure and reactions of a trianion equivalent, trilithiostannane. Chemical Communications, 2008, , 6495. | 2.2 | 6 |
| 39 | Synthesis and Structure of Pentaorganostannate Having Five Carbon Substituents. Journal of the American Chemical Society, 2007, 129, 10974-10975. | 6.6 | 30 |
| 40 | Accuracy of the three-body fragment molecular orbital method applied to MÃ¸ller-Plesset perturbation theory. Journal of Computational Chemistry, 2007, 28, 1476-1484. | 1.5 | 79 |
| 41 | New parallel algorithm for MP2 energy gradient calculations. Journal of Computational Chemistry, 2007, 28, 2034-2042. | 1.5 | 38 |
| 42 | Synthesis of Stannaindenyl Anions and a Dianion. Organometallics, 2006, 25, 2967-2971. | 1.1 | 30 |
| 43 | Synthesis and Characterization of Dimetallostannafluorenes. Chemistry Letters, 2006, 35, 940-941. | 0.7 | 28 |
| 44 | Computations of the Energetics of C60F36Isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 57-65. | 1.0 | 1 |
| 45 | A new parallel algorithm of MP2 energy calculations. Journal of Computational Chemistry, 2006, 27, 407-413. | 1.5 | 67 |
| 46 | The Aromaticity of the Stannole Dianion. Angewandte Chemie - International Edition, 2005, 44, 6553-6556. | 7.2 | 90 |
| 47 | Synthesis and Characterization of Stable Hypervalent Carbon Compounds (10-C-5) Bearing a 2,6-Bis(p-substituted phenyloxymethyl)benzene Ligand. Journal of the American Chemical Society, 2005, 127, 5893-5901. | 6.6 | 70 |
| 48 | C72 isomers: the IPR-satisfying cage is disfavored by both energy and entropy. Chemical Physics Letters, 2004, 384, 114-118. | 1.2 | 64 |
| 49 | Ionized and excited states of ferrocene: Symmetry adapted clusterâ€“configurationâ€“interaction study. Journal of Chemical Physics, 2002, 117, 6533-6537. | 1.2 | 37 |