

Toru Matsui

List of Publications by Year in descending order

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55
papers

888
citations

471509

17
h-index

501196

28
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55
all docs

55
docs citations

55
times ranked

1046
citing authors

#	ARTICLE	IF	CITATIONS
1	Accurate Standard Hydrogen Electrode Potential and Applications to the Redox Potentials of Vitamin C and NAD/NADH. <i>Journal of Physical Chemistry A</i> , 2015, 119, 369-376.	2.5	102
2	Spin Contamination Error in Optimized Geometry of Singlet Carbene (1A1) by Broken-Symmetry Method. <i>Journal of Physical Chemistry A</i> , 2009, 113, 15041-15046.	2.5	68
3	An accurate density functional theory based estimation of pKa values of polar residues combined with experimental data: from amino acids to minimal proteins. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4181.	2.8	67
4	Multiple Proton-Transfer Reactions in DNA Base Pairs by Coordination of Pt Complex. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1176-1181.	2.6	41
5	Consistent scheme for computing standard hydrogen electrode and redox potentials. <i>Journal of Computational Chemistry</i> , 2013, 34, 21-26.	3.3	39
6	A Density Functional Theory Based Protocol to Compute the Redox Potential of Transition Metal Complex with the Correction of Pseudo-Counterion: General Theory and Applications. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2974-2980.	5.3	36
7	Influence of Pt complex binding on the guanine-cytosine pair: A theoretical study. <i>Chemical Physics Letters</i> , 2006, 423, 331-334.	2.6	34
8	Effects of mercury(II) on structural properties, electronic structure and UV absorption spectra of a duplex containing thymine-mercury(II)-thymine nucleobase pairs. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 909-917.	2.8	33
9	A Simple scheme for estimating the pKa values of 5-substituted uracils. <i>Chemical Physics Letters</i> , 2011, 502, 248-252.	2.6	32
10	A density functional study on the pK_a of small polyprotic molecules. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1128-1134.	2.0	30
11	Which hybrid GGA DFT is suitable for Cu ₂ O ₂ systems if the spin contamination error is removed?. <i>Chemical Physics</i> , 2010, 368, 1-6.	1.9	25
12	How Can We Understand Au ₈ Cores and Entangled Ligands of Selenolate- and Thiolate-Protected Gold Nanoclusters Au ₂₄ (ER) ₂₀ and Au ₂₀ (ER) ₁₆ (E = Se, S; R = Ph, Me)? A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2015, 137, 8593-8602.	13.7	25
13	Assessment of Methodology and Chemical Group Dependences in the Calculation of the pK_a for Several Chemical Groups. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4791-4803.	5.3	25
14	Sequence-dependent proton-transfer reaction in stacked GC pair II: The origin of stabilities of proton-transfer products. <i>Chemical Physics Letters</i> , 2009, 478, 238-242.	2.6	20
15	Sequence dependent proton-transfer reaction in stacked GC pair I: The possibility of proton-transfer reactions. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2168-2177.	2.0	18
16	Theoretical Study on Reaction Scheme of Silver(I) Containing 5-Substituted Uracils Bridge Formation. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8504-8510.	2.5	18
17	Theoretical studies of electronic structures, magnetic properties and electron conductivities of one-dimensional Ni _n (n = 3, 5, 7) complexes. <i>Dalton Transactions</i> , 2013, 42, 16200.	3.3	18
18	DFT and TD-DFT studies of electronic structures and one-electron excitation states of a cyanide-bridged molecular square complex. <i>Inorganic Chemistry Frontiers</i> , 2015, 2, 771-779.	6.0	18

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19	Analyses of Thiophene-Based Donor–Acceptor Semiconducting Polymers toward Designing Optical and Conductive Properties: A Theoretical Perspective. <i>Journal of Physical Chemistry C</i> , 2016, 120, 8305-8314.	3.1	17
20	Dynamic Quantum Isotope Effects on Multiple Proton-Transfer Reactions. <i>Bulletin of the Chemical Society of Japan</i> , 2008, 81, 1230-1240.	3.2	14
21	Theoretical Study on Reaction Mechanisms of Nitrite Reduction by Copper Nitrite Complexes: Toward Understanding and Controlling Possible Mechanisms of Copper Nitrite Reductase. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5392-5403.	2.6	14
22	Possibility of multi-conformational structure of mismatch DNA nucleobase in the presence of silver(I) ions. <i>Chemical Physics Letters</i> , 2010, 495, 125-130.	2.6	13
23	Nylon-Oligomer Hydrolase Promoting Cleavage Reactions in Unnatural Amide Compounds. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1210-1216.	4.6	13
24	Structural Origin of Copper Ion Containing Artificial DNA: A Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16960-16965.	2.6	12
25	Molecular dynamics studies on the mutational structures of a nylon-6 byproduct-degrading enzyme. <i>Chemical Physics Letters</i> , 2011, 507, 157-161.	2.6	12
26	Theoretical Study on the Electronic Configurations and Nature of Chemical Bonds of Dirhodium Tetraacetato Complexes [Rh ₂ (CH ₃ COO) ₄ (L) ₂] (L = H ₂ O, Free): Broken Symmetry Approach. <i>Bulletin of the Chemical Society of Japan</i> , 2010, 83, 1481-1488.	3.2	11
27	A computational scheme of $\langle K \rangle$ values based on the three-dimensional reference interaction site model self-consistent field theory coupled with the linear fitting correction scheme. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27272-27279.	2.8	11
28	Characterization of Structure and Catalytic Activity of a Complex between Heme and an All Parallel-Stranded Tetrameric G-Quadruplex Formed from DNA/RNA Chimera Sequence d(TTA)r(GGG)dT. <i>Bulletin of the Chemical Society of Japan</i> , 2020, 93, 621-629.	3.2	11
29	Theoretical studies on chemical bonding between Cu(II) and oxygen molecule in type 3 copper proteins. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3649-3658.	2.0	10
30	Theoretical Studies on Sulfur and Metal Cation (Cu(II), Ni(II), Pd(II), and Pt(II))-Containing Artificial DNA. <i>Journal of Physical Chemistry B</i> , 2009, 113, 12790-12795.	2.6	8
31	Electron Conductivity in Modified Models of Artificial Metal–DNA Using Green's Function-Based Elastic Scattering Theory. <i>Bulletin of the Chemical Society of Japan</i> , 2011, 84, 366-375.	3.2	8
32	Theoretical study on relationship between spin structure and electron conductivity of one-dimensional tri-nickel(II) complex. <i>Polyhedron</i> , 2017, 136, 125-131.	2.2	8
33	Theoretical Insight into Stereoselective Reaction Mechanisms of 2,4-Pentanediol-Tethered Ketene-Olefin [2 + 2] Cycloaddition. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1168-1175.	2.5	7
34	DFT calculations of effective exchange integrals at the complete basis set limit on oxo-vanadium ring complex. <i>Polyhedron</i> , 2013, 66, 97-101.	2.2	7
35	Recent Developments of Computational Methods for pK _a Prediction Based on Electronic Structure Theory with Solvation Models. <i>J.</i> , 2021, 4, 849-864.	0.9	7
36	Unique Photophysical Properties of 1,8-Naphthalimide Derivatives: Generation of Semi-stable Radical Anion Species by Photo-Induced Electron Transfer from a Carboxy Group. <i>ACS Omega</i> , 2021, 6, 13456-13465.	3.5	6

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37	Estimation of effective exchange integral value of polyradical systems based on the band calculation. International Journal of Quantum Chemistry, 2009, 109, 3632-3640.	2.0	5
38	Sequence-dependent proton-transfer reaction in stacked GC pair III: The influence of proton transfer to conductivity. International Journal of Quantum Chemistry, 2010, 110, 2221-2230.	2.0	5
39	Theoretical study on naphthobis(chalcogen)diazole conjugated polymer systems and C61 derivative as organic photovoltaic semiconductors. Chemical Physics Letters, 2018, 693, 188-193.	2.6	5
40	Estimation of Acid Dissociation Constants (pK_a) of N-Containing Heterocycles in DMSO and Transferability of Gibbs Free Energy in Different Solvent Conditions. Chemistry Letters, 2020, 49, 307-310.	1.3	5
41	Quantum Theory in Terms of Cumulant Variables. Progress in Theoretical Chemistry and Physics, 2009, 3-34.	0.2	4
42	A Theoretical Study on Redox Potential and pK_a of [2Fe-2S] Cluster Model from Iron-Sulfur Proteins. Bulletin of the Chemical Society of Japan, 2018, 91, 1451-1456.	3.2	4
43	A Density Functional Theory-Based Scheme to Compute the Redox Potential of a Transition Metal Complex: Applications to Heme Compound. Molecules, 2019, 24, 819.	3.8	4
44	Theoretical studies of the effect of orientation of ligands and spin contamination error on the chemical bonding in the FeO ₂ core in oxyhemoglobin. Computational and Theoretical Chemistry, 2010, 954, 98-104.	1.5	3
45	A Theoretical Guideline for Designing Effective Host Materials Based on 4,4'-Bis(9-carbazolyl)-1,1'-biphenyl Derivatives for Blue Phosphorescent Devices. Bulletin of the Chemical Society of Japan, 2017, 90, 195-204.	3.2	3
46	Molecular Dynamics and Quantum Chemical Approach for the Estimation of an Intramolecular Hydrogen Bond Strength in Okadaic Acid. Journal of Physical Chemistry B, 2018, 122, 7233-7242.	2.6	3
47	A Practical Prediction of $\log P_{ow}$ through Semiempirical Electronic Structure Calculations with Dielectric Continuum Model. Bulletin of the Chemical Society of Japan, 2021, 94, 1807-1814.	3.2	3
48	Temperature-Independent Stereoselectivity in Intramolecular Cycloaddition of Ketene Generated from Diazoester in Solution and in Vapor Phase: How Entropy Term Governs the Selectivity. Bulletin of the Chemical Society of Japan, 2012, 85, 504-510.	3.2	2
49	Theoretical Estimation of Effect of Conjugation Length and Side Chain in Charge Recombination Process in Poly(<i>para</i> -phenylenevinylene). Chemistry Letters, 2016, 45, 628-630.	1.3	2
50	The Study of the Octanol-Water Partition Coefficient by the Computational Chemistry Method. Journal of Computer Chemistry Japan, 2019, 18, 241-243.	0.1	1
51	Factor analysis of error in oxidation potential calculation: A machine learning study. Journal of Computational Chemistry, 2022, 43, 1504-1512.	3.3	1
52	Metal-assisted proton transfer reaction in base pairs. Nucleic Acids Symposium Series, 2007, 51, 225-226.	0.3	0
53	Electronic structure and UV absorption spectra of metal-mediate DNA: an approach from theoretical chemistry. Nucleic Acids Symposium Series, 2009, 53, 181-182.	0.3	0
54	Metal-Assisted Proton Transfer in Guanine-Cytosine Pair: An Approach from Quantum Chemistry. , 2012, , .		0

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55	Theoretical Studies on Metal-Containing Artificial DNA Bases. Progress in Theoretical Chemistry and Physics, 2012, , 433-460.	0.2	0