Toru Matsui

List of Publications by Year
in descending order

55 papers	888 citations	471509 17 h-index	501196 28 g-index
55 all docs	55 docs citations	55 times ranked	1046 citing authors

#	Article	IF	Citations
1	Factor analysis of error in oxidation potential calculation: A machine learning study. Journal of Computational Chemistry, 2022, 43, 1504-1512.	3.3	1
2	Unique Photophysical Properties of 1,8-Naphthalimide Derivatives: Generation of Semi-stable Radical Anion Species by Photo-Induced Electron Transfer from a Carboxy Group. ACS Omega, 2021, 6, 13456-13465.	3.5	6
3	A Practical Prediction of LogPo/w through Semiempirical Electronic Structure Calculations with Dielectric Continuum Model. Bulletin of the Chemical Society of Japan, 2021, 94, 1807-1814.	3.2	3
4	Recent Developments of Computational Methods for pKa Prediction Based on Electronic Structure Theory with Solvation Models. J, 2021, 4, 849-864.	0.9	7
5	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. Bulletin of the Chemical Society of Japan, 2020, 93, 621-629.	3.2	11
6	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
7	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
8	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
9	Theoretical study on naphthobischalcogenadiazole conjugated polymer systems and C61 derivative as organic photovoltaic semiconductors. Chemical Physics Letters, 2018, 693, 188-193.	2.6	5
10	A Theoretical Study on Redox Potential and pKa of [2Fe-2S] Cluster Model from Iron-Sulfur Proteins. Bulletin of the Chemical Society of Japan, 2018, 91, 1451-1456.	3.2	4
11	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
12	A computational scheme of pK_a values based on the three-dimensional reference interaction site model self-consistent field theory coupled with the linear fitting correction scheme. Physical Chemistry Chemical Physics, 2018, 20, 27272-27279.	2.8	11
13	Theoretical study on relationship between spin structure and electron conductivity of one-dimensional tri-nickel(II) complex. Polyhedron, 2017, 136, 125-131.	2.2	8
14	Assessment of Methodology and Chemical Group Dependences in the Calculation of the pK_a for Several Chemical Groups. Journal of Chemical Theory and Computation, 2017, 13, 4791-4803.	5.3	25
15	A Theoretical Guideline for Designing Effective Host Materials Based on 4,4â€²-Bis(9-carbazolyl)-1,1â€²-biphenyl Derivatives for Blue Phosphorescent Devices. Bulletin of the Chemical Society of Japan, 2017, 90, 195-204.	3.2	3
16	Analyses of Thiophene-Based Donorâ€“Acceptor Semiconducting Polymers toward Designing Optical and Conductive Properties: A Theoretical Perspective. Journal of Physical Chemistry C, 2016, 120, 8305-8314.	3.1	17
17	Theoretical Estimation of Effect of Conjugation Length and Side Chain in Charge Recombination Process in Poly(para-phenylenevinylene). Chemistry Letters, 2016, 45, 628-630.	1.3	2
18	Accurate Standard Hydrogen Electrode Potential and Applications to the Redox Potentials of Vitamin C and NAD/NADH. Journal of Physical Chemistry A, 2015, 119, 369-376.	2.5	102

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19	DFT and TD-DFT studies of electronic structures and one-electron excitation states of a cyanide-bridged molecular square complex. Inorganic Chemistry Frontiers, 2015, 2, 771-779.	6.0	18
20	How Can We Understand Au₈ Cores and Entangled Ligands of Selenolate- and Thiolate-Protected Gold Nanoclusters Au₂₄(ER)₂₀ and Au₂₀(ER)₁₆ (E = Se, S; R = Ph, Me)? A Theoretical Study. Journal of the American Chemical Society, 2015, 137, 8593-8602.	13.7	25
21	Theoretical Study on Reaction Mechanisms of Nitrite Reduction by Copper Nitrite Complexes: Toward Understanding and Controlling Possible Mechanisms of Copper Nitrite Reductase. Journal of Physical Chemistry B, 2015, 119, 5392-5403.	2.6	14
22	A density functional study on the pK_a of small polyprotic molecules. International Journal of Quantum Chemistry, 2014, 114, 1128-1134.	2.0	30
23	Nylon-Oligomer Hydrolase Promoting Cleavage Reactions in Unnatural Amide Compounds. Journal of Physical Chemistry Letters, 2014, 5, 1210-1216.	4.6	13
24	Theoretical studies of electronic structures, magnetic properties and electron conductivities of one-dimensional Nin (n = 3, 5, 7) complexes. Dalton Transactions, 2013, 42, 16200.	3.3	18
25	DFT calculations of effective exchange integrals at the complete basis set limit on oxo-vanadium ring complex. Polyhedron, 2013, 66, 97-101.	2.2	7
26	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. Journal of Chemical Theory and Computation, 2013, 9, 2974-2980.	5.3	36
27	Consistent scheme for computing standard hydrogen electrode and redox potentials. Journal of Computational Chemistry, 2013, 34, 21-26.	3.3	39
28	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
29	Theoretical Insight into Stereoselective Reaction Mechanisms of 2,4-Pentanediol-Tethered Ketene-Olefin [2 + 2] Cycloaddition. Journal of Physical Chemistry A, 2012, 116, 1168-1175.	2.5	7
30	An accurate density functional theory based estimation of pKa values of polar residues combined with experimental data: from amino acids to minimal proteins. Physical Chemistry Chemical Physics, 2012, 14, 4181.	2.8	67
31	Metal-Assisted Proton Transfer in Guanine-Cytosine Pair: An Approach from Quantum Chemistry. , 2012, , .		0
32	Theoretical Studies on Metal-Containing Artificial DNA Bases. Progress in Theoretical Chemistry and Physics, 2012, , 433-460.	0.2	0
33	Theoretical Study on Reaction Scheme of Silver(I) Containing 5-Substituted Uracils Bridge Formation. Journal of Physical Chemistry A, 2011, 115, 8504-8510.	2.5	18
34	Electron Conductivity in Modified Models of Artificial Metalâ€“DNA Using Greenâ€™s Function-Based Elastic Scattering Theory. Bulletin of the Chemical Society of Japan, 2011, 84, 366-375.	3.2	8
35	A Simple scheme for estimating the pKa values of 5-substituted uracils. Chemical Physics Letters, 2011, 502, 248-252.	2.6	32
36	Molecular dynamics studies on the mutational structures of a nylon-6 byproduct-degrading enzyme. Chemical Physics Letters, 2011, 507, 157-161.	2.6	12

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37	Theoretical Study on the Electronic Configurations and Nature of Chemical Bonds of Dirhodium Tetraacetato Complexes [Rh2(CH3COO)4(L)2] (L = H2O, Free): Broken Symmetry Approach. Bulletin of the Chemical Society of Japan, 2010, 83, 1481-1488.	3.2	11
38	Which hybrid GGA DFT is suitable for Cu2O2 systems if the spin contamination error is removed?. Chemical Physics, 2010, 368, 1-6.	1.9	25
39	Theoretical studies of the effect of orientation of ligands and spin contamination error on the chemical bonding in the FeO2 core in oxymyoglobin. Computational and Theoretical Chemistry, 2010, 954, 98-104.	1.5	3
40	Possibility of multi-conformational structure of mismatch DNA nucleobase in the presence of silver(I) ions. Chemical Physics Letters, 2010, 495, 125-130.	2.6	13
41	Sequenceâ€dependent protonâ€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
42	Effects of mercury(ii) on structural properties, electronic structure and UV absorption spectra of a duplex containing thymineâ€“mercury(ii)â€“thymine nucleobase pairs. Physical Chemistry Chemical Physics, 2010, 12, 909-917.	2.8	33
43	Quantum Theory in Terms of Cumulant Variables. Progress in Theoretical Chemistry and Physics, 2009, , 3-34.	0.2	4
44	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
45	Sequence dependent protonâ€transfer reaction in stacked GC pair I: The possibility of protonâ€transfer reactions. International Journal of Quantum Chemistry, 2009, 109, 2168-2177.	2.0	18
46	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
47	Theoretical studies on chemical bonding between Cu(II) and oxygen molecule in type 3 copper proteins. International Journal of Quantum Chemistry, 2009, 109, 3649-3658.	2.0	10
48	Sequence-dependent proton-transfer reaction in stacked GC pair II: The origin of stabilities of proton-transfer products. Chemical Physics Letters, 2009, 478, 238-242.	2.6	20
49	Theoretical Studies on Sulfur and Metal Cation (Cu(II), Ni(II), Pd(II), and Pt(II))-Containing Artificial DNA. Journal of Physical Chemistry B, 2009, 113, 12790-12795.	2.6	8
50	Spin Contamination Error in Optimized Geometry of Singlet Carbene (1A1) by Broken-Symmetry Method. Journal of Physical Chemistry A, 2009, 113, 15041-15046.	2.5	68
51	Structural Origin of Copper Ion Containing Artificial DNA: A Density Functional Study. Journal of Physical Chemistry B, 2008, 112, 16960-16965.	2.6	12
52	Dynamic Quantum Isotope Effects on Multiple Proton-Transfer Reactions. Bulletin of the Chemical Society of Japan, 2008, 81, 1230-1240.	3.2	14
53	Metal-assisted proton transfer reaction in base pairs. Nucleic Acids Symposium Series, 2007, 51, 225-226.	0.3	0
54	Multiple Proton-Transfer Reactions in DNA Base Pairs by Coordination of Pt Complex. Journal of Physical Chemistry B, 2007, 111, 1176-1181.	2.6	41

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55	Influence of Pt complex binding on the guanineâ€“cytosine pair: A theoretical study. Chemical Physics Letters, 2006, 423, 331-334.	2.6	34