Toshiaki Matsubara

List of Publications by Year
in descending order

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Version: 2024-02-01

		1684188	1372567
17	88	5	10
papers	citations	h-index	g-index

17	17	17	107
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The ONIOM molecular dynamics method for biochemical applications: Cytidine deaminase. Chemical Physics Letters, 2007, 437, 138-142.	2.6	23
2	Density Functional Study of the Mechanism of Câ‹®C, Oâˆ'H, and Nâˆ'H Bond Activation at the PdX (X = Sn, Si,) Tj ETQq0 0 0 rgBT /Overl	2.3	15
3	Density Functional Study of the Ïƒ and Ï€ Bond Activation at the PdX (X = Sn, Si, C) Bonds of the (H2PC2H4PH2)PdXH2 Complexes. Is the Bond Cleavage Homolytic or Heterolytic?. Journal of the American Chemical Society, 2002, 124, 679-689.	13.7	10
4	Computational Study of the Effects of Steric Hindrance on Amide Bond Cleavage. Journal of Physical Chemistry A, 2014, 118, 8664-8675.	2.5	8
5	ONIOM Study of the Mechanism of Olefin Hydrogenation by the Wilkinsonâ€™s Catalyst: Reaction Paths and Energy Surfaces of trans- and cis-Forms. Bulletin of the Chemical Society of Japan, 2013, 86, 243-254.	3.2	6
6	Quantum Mechanical and Molecular Dynamics Studies of the Reaction Mechanism of the Nucleophilic Substitution at the Si Atom. Journal of Physical Chemistry A, 2016, 120, 2636-2646.	2.5	6
7	Computational Study on the Mechanism of the Electron-Transfer-Induced Repair of the (6â€“4) Tâ€“T Photoproduct of DNA by Photolyase: Possibility of a Radical Cation Pathway. Bulletin of the Chemical Society of Japan, 2014, 87, 390-399.	3.2	5
8	Polyoxometalate-Assisted, One-Pot Synthesis of a Pentakis[(triphenylphosphane)gold]ammonium(2+) Cation Containing Regular Trigonal-Bipyramidal Geometries of Five Bonds to Nitrogen. Inorganic Chemistry, 2018, 57, 1504-1516.	4.0	5
9	Theoretical Study of the Heterolytic Ïƒ Bond Cleavage on the Geâ•Ο Bond of Germanone. An Insight into the Driving Force from Both Electronic and Dynamical Aspects. Journal of Physical Chemistry A, 2017, 121, 1768-1778.	2.5	3
10	Dynamic Effects on the Product Distribution of the Photoreaction of s-cis-1,3-Butadiene: A Nonadiabatic Molecular Dynamics Study. Bulletin of the Chemical Society of Japan, 2021, 94, 1720-1727.	3.2	3
11	Dynamic effects of the bridged structure on the quantum yield of the cis â†' trans photoisomerization of azobenzene. Physical Chemistry Chemical Physics, 2022, 24, 17303-17313.	2.8	2
12	Bâ‰¡B Triple Bond of Newly Synthesized Diboryne Can Take a Different Mechanism for the Ïƒ Bond Activation of Polar and Nonpolar Molecules. A Quantum Mechanical Study. Bulletin of the Chemical Society of Japan, 2018, 91, 1683-1690.	3.2	1
13	QM- and ONIOM-Molecular Dynamics Studies of the S_N2 Reaction. How Does the Rare Event Take Place?. Journal of Computer Chemistry Japan -International Edition, 2020, 6, n/a.	0.1	1
14	Computational Study of the Binding Mechanism of Complement C3b with Antigen. Bulletin of the Chemical Society of Japan, 2013, 86, 1426-1434.	3.2	0
15	Dataset of polyoxometalate-assisted N-heterocyclic carbene gold(I) complexes. Data in Brief, 2019, 25, 104002.	1.0	0
16	Density Functional Study of Ïƒ Bond Cleavage in Pâ€“P Multiple Bond of Phosphinophosphinidene. Journal of Computer Chemistry Japan -International Edition, 2021, 7, n/a.	0.1	0
17	Molecular Dynamics Study of the S_N2 Reaction. How Does the Rare Event Take Place?. Journal of Computer Chemistry Japan, 2019, 18, 145-146.	0.1	0