Takashi Kamachi

List of Publications by Year
in descending order

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49 papers	1,996 citations	257450 24 h-index	243625 44 g-index

52 all docs	52 docs citations	52 times ranked	2897 citing authors

#	Article	IF	Citations
1	Machine Learning for Catalysis Informatics: Recent Applications and Prospects. ACS Catalysis, 2020, 10, 2260-2297.	11.2	309
2	Theoretical Study of the Direct Synthesis of H₂O₂ on Pd and Pd/Au Surfaces. Journal of Physical Chemistry C, 2008, 112, 19501-19505.	3.1	121
3	Molecular motor-driven abrupt anisotropic shape change in a single crystal of a Ni complex. Nature Chemistry, 2014, 6, 1079-1083.	13.6	111
4	Density Functional Theory Calculations of Oxygen Vacancy Formation and Subsequent Molecular Adsorption on Oxide Surfaces. Journal of Physical Chemistry C, 2018, 122, 29435-29444.	3.1	103
5	Computational Exploration of the Catalytic Mechanism of Dopamine Î²-Monooxygenase:Â Modeling of Its Mononuclear Copper Active Sites. Inorganic Chemistry, 2005, 44, 4226-4236.	4.0	82
6	Mechanistic Study on the Production of Hydrogen Peroxide in the Anthraquinone Process. European Journal of Organic Chemistry, 2011, 2011, 4113-4120.	2.4	76
7	Participation of Multioxidants in the pH Dependence of the Reactivity of Ferrate(VI). Journal of Organic Chemistry, 2005, 70, 4380-4388.	3.2	71
8	Assembling an alkyl rotor to access abrupt and reversible crystalline deformation of a cobalt(II) complex. Nature Communications, 2015, 6, 8810.	12.8	69
9	Superior thermoelasticity and shape-memory nanopores in a porous supramolecular organic framework. Nature Communications, 2016, 7, 11564.	12.8	58
10	Water-Assisted Oxo Mechanism for Heme Metabolism. Journal of the American Chemical Society, 2005, 127, 10686-10692.	13.7	54
11	How axial ligands control the reactivity of high-valent iron(IV)â€“oxo porphyrin Ï€-cation radicals in alkane hydroxylation: A computational study. Journal of Inorganic Biochemistry, 2006, 100, 751-754.	3.5	41
12	Catalytic Roles of Active-Site Amino Acid Residues of Coenzyme B12-Dependent Diol Dehydratase:Â Protonation State of Histidine and Pull Effect of Glutamate. Journal of the American Chemical Society, 2004, 126, 16207-16216.	13.7	40
13	Hydrolytic Enantioselective Protonation of Cyclic Dienyl Esters and a Î²-Diketone with Chiral Phase-Transfer Catalysts. Organic Letters, 2012, 14, 6178-6181.	4.6	40
14	Computational Exploration of the Mechanism of the Hydrogenation Step of the Anthraquinone Process for Hydrogen Peroxide Production. Journal of Physical Chemistry C, 2015, 119, 8748-8754.	3.1	40
15	Computational Mutation Analysis of Hydrogen Abstraction and Radical Rearrangement Steps in the Catalysis of Coenzyme B₁₂â€Dependent Diol Dehydratase. Chemistry - A European Journal, 2007, 13, 7864-7873.	3.3	39
16	Selective carbon dioxide adsorption of Îµ-Keggin-type zincomolybdate-based purely inorganic 3D frameworks. Journal of Materials Chemistry A, 2015, 3, 746-755.	10.3	39
17	How Heme Metabolism Occurs in Heme Oxygenase:Â Computational Study of Oxygen-Donation Ability of the Oxo and Hydroperoxo Species. Journal of the American Chemical Society, 2004, 126, 3672-3673.	13.7	38
18	Mechanistic Proposals for Direct Benzene Hydroxylation over Feâ^'ZSM-5 Zeolite. Journal of Physical Chemistry B, 2003, 107, 11404-11410.	2.6	37

#	Article	IF	Citations
19	Enantioselective Alkylation by Binaphthyl Chiral Phase-Transfer Catalysts: A DFT-Based Conformational Analysis. Organic Letters, 2014, 16, 472-475.	4.6	36
20	The Catalytic Mechanism of Fluoroacetate Dehalogenase: A Computational Exploration of Biological Dehalogenation. Chemistry - A European Journal, 2009, 15, 7394-7403.	3.3	35
21	Intraprotein transmethylation via a CH₃â€“Co(<scp>iii</scp>) species in myoglobin reconstituted with a cobalt corrinoid complex. Dalton Transactions, 2016, 45, 3277-3284.	3.3	31
22	Possible Peroxo State of the Dicopper Site of Particulate Methane Monooxygenase from Combined Quantum Mechanics and Molecular Mechanics Calculations. Inorganic Chemistry, 2016, 55, 2771-2775.	4.0	28
23	Combined Experimental and Theoretical Approach To Understand the Reactivity of a Mononuclear Cu(II)â^'Hydroperoxo Complex in Oxygenation Reactions. Journal of Physical Chemistry A, 2008, 112, 13102-13108.	2.5	25
24	Thermally Induced Intraâ€Carboxyl Proton Shuttle in a Molecular Rackâ€andâ€Pinion Cascade Achieving Macroscopic Crystal Deformation. Angewandte Chemie - International Edition, 2016, 55, 14628-14632.	13.8	25
25	Low-Mode Conformational Search Method with Semiempirical Quantum Mechanical Calculations: Application to Enantioselective Organocatalysis. Journal of Chemical Information and Modeling, 2016, 56, 347-353.	5.4	23
26	Linear Correlations between Adsorption Energies and HOMO Levels for the Adsorption of Small Molecules on TiO₂ Surfaces. Journal of Physical Chemistry C, 2019, 123, 20988-20997.	3.1	23
27	Redox Potentials of Cobalt Corrinoids with Axial Ligands Correlate with Heterolytic Coâ€“C Bond Dissociation Energies. Inorganic Chemistry, 2017, 56, 1950-1955.	4.0	22
28	Changes in Surface Oxygen Vacancy Formation Energy at Metal/Oxide Perimeter Sites: A Systematic Study on Metal Nanoparticles Deposited on an In₂O₃(111) Support. Journal of Physical Chemistry C, 2020, 124, 27621-27630.	3.1	22
29	Frontier Molecular Orbital Based Analysis of Solidâ€“Adsorbate Interactions over Group 13 Metal Oxide Surfaces. Journal of Physical Chemistry C, 2020, 124, 15355-15365.	3.1	22
30	Esterification of Tertiary Amides by Alcohols Through Câ^'N Bond Cleavage over CeO₂. ChemCatChem, 2019, 11, 449-456.	3.7	21
31	Generation of adenosyl radical from S-adenosylmethionine (SAM) in biotin synthase. Journal of Inorganic Biochemistry, 2011, 105, 850-857.	3.5	20
32	Dynamic Kinetic Resolution of N-Protected Amino Acid Esters via Phase-Transfer Catalytic Base Hydrolysis. ACS Catalysis, 2018, 8, 5708-5713.	11.2	20
33	Surface Oxygen Vacancy Formation Energy Calculations in 34 Orientations of Î²-Ga₂O₃ and Î¸-Al₂O₃. Journal of Physical Chemistry C, 2020, 124, 10509-10522.	3.1	19
34	Effect of Oxygen Vacancies on Adsorption of Small Molecules on Anatase and Rutile TiO₂ Surfaces: A Frontier Orbital Approach. Journal of Physical Chemistry C, 2021, 125, 3827-3844.	3.1	18
35	Catalytic Roles of the Metal Ion in the Substrate-Binding Site of Coenzyme B₁₂-Dependent Diol Dehydratase. Inorganic Chemistry, 2011, 50, 2944-2952.	4.0	17
36	Crystal Structures and Coordination Behavior of Aqua- and Cyano-Co(III) Tetradehydrocorrins in the Heme Pocket of Myoglobin. Inorganic Chemistry, 2016, 55, 1287-1295.	4.0	16

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37	Combined theoretical and experimental study on alcoholysis of amides on CeO2 surface: A catalytic interplay between Lewis acid and base sites. Catalysis Today, 2018, 303, 256-262.	4.4	13
38	Factors determining surface oxygen vacancy formation energy in ternary spinel structure oxides with zinc. Physical Chemistry Chemical Physics, 2021, 23, 23768-23777.	2.8	12
39	Auto-Generation of Corrugated Nonpolar Stoichiometric Slab Models. Materials Transactions, 2020, 61, 78-87.	1.2	10
40	Computational Mutation Design of Diol Dehydratase: Catalytic Ability toward Glycerol beyond the Wild-Type Enzyme. Bulletin of the Chemical Society of Japan, 2014, 87, 950-959.	3.2	7
41	Dynamic Kinetic Resolution of Azlactones via Phase-Transfer Catalytic Alcoholysis. ACS Catalysis, 2021, 11, 14067-14075.	11.2	7
42	A new understanding on how heme metabolism occurs in heme oxygenase: water-assisted oxo mechanism. Dalton Transactions, 2012, 41, 11642.	3.3	6
43	Algorithm for Automatic Detection of Surface Atoms. Transactions of the Materials Research Society of Japan, 2020, 45, 115-120.	0.2	6
44	DFT Study on the pH Dependence of the Reactivity of Ferrate(VI). ACS Symposium Series, 2016, , 473-487.	0.5	5
45	Automated Identification of Facet Pair Orientations. Materials Transactions, 2020, 61, 1430-1433.	1.2	5
46	Synthesis and Structure of a Water-soluble Âµ-Î·¹:Î·¹-N₂ Dinuclear Ru^{II} Complex with a Polyamine Ligand. Chemistry Letters, 2016, 45, 149-151.	1.3	4
47	TiO2 -Supported Re as a General and Chemoselective Heterogeneous Catalyst for Hydrogenation of Carboxylic Acids to Alcohols. Chemistry - A European Journal, 2017, 23, 980-980.	3.3	3
48	Thermally Induced Intraâ€Carboxyl Proton Shuttle in a Molecular Rackâ€andâ€Pinion Cascade Achieving Macroscopic Crystal Deformation. Angewandte Chemie, 2016, 128, 14848-14852.	2.0	2
49	Esterification of Tertiary Amides by Alcohols Through Câ^'N Bond Cleavage over CeO 2. ChemCatChem, 2019, 11, 15-15.	3.7	0