Atsushi Ishikawa

List of Publications by Year
in descending order

43	825	471509 17	501196 28
papers	citations	h-index	g-index

46	46	46	1021
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Onâ€Surface Synthesis of Porphyrinâ€Complex Multiâ€Block Coâ€Oligomers by Defluorinative Coupling. Angewandte Chemie, 2022, 134, .	2.0	3
2	Heterogeneous catalyst design by generative adversarial network and first-principles based microkinetics. Scientific Reports, 2022, 12, .	3.3	3
3	Hybrid Functional Study of H-Abstraction from Methane by Li-Doped, Pristine and Stepped MgO(100) and MgO(110) Surfaces. Catalysis Letters, 2021, 151, 627-633.	2.6	7
4	Theoretical prediction by DFT and experimental observation of heterocation-doping effects on hydrogen adsorption and migration over the CeO₂(111) surface. Physical Chemistry Chemical Physics, 2021, 23, 4509-4516.	2.8	7
5	Efficient Oxygen Evolution Electrocatalysis on CaFe₂O₄ and Its Reaction Mechanism. ACS Applied Energy Materials, 2021, 4, 3057-3066.	5.1	22
6	A First-Principles Microkinetics for Homogeneousâ€“Heterogeneous Reactions: Application to Oxidative Coupling of Methane Catalyzed by Magnesium Oxide. ACS Catalysis, 2021, 11, 2691-2700.	11.2	20
7	Manipulation of CO adsorption over Me1/CeO2 by heterocation doping: Key roles of single-atom adsorption energy. Journal of Chemical Physics, 2021, 154, 164705.	3.0	5
8	Câ€“H Bond Activation of Methane through Electronic Interaction with Pd(110). Journal of Physical Chemistry C, 2021, 125, 1368-1377.	3.1	8
9	Onâ€Surface Synthesis of Porphyrinâ€Complex Multiâ€Block Coâ€Oligomers by Defluorinative Coupling. Angewandte Chemie - International Edition, 2021, , .	13.8	9
10	The important role of N2H formation energy for low-temperature ammonia synthesis in an electric field. Catalysis Today, 2020, 351, 119-124.	4.4	29
11	Heteroatom doping effects on interaction of H2O and CeO2 (111) surfaces studied using density functional theory: Key roles of ionic radius and dispersion. Journal of Chemical Physics, 2020, 152, 014707.	3.0	13
12	What Is the Active Site for the Oxidative Coupling of Methane Catalyzed by MgO? A Metadynamics-Biased Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2020, 124, 6054-6062.	3.1	7
13	Surface Rashba-Edelstein Spin-Orbit Torque Revealed by Molecular Self-Assembly. Physical Review Applied, 2020, 13, .	3.8	9
14	Agglomeration Suppression of a Fe-Supported Catalyst and its Utilization for Low-Temperature Ammonia Synthesis in an Electric Field. ACS Omega, 2020, 5, 6846-6851.	3.5	21
15	Governing factors of supports of ammonia synthesis in an electric field found using density functional theory. Journal of Chemical Physics, 2019, 151, 064708.	3.0	13
16	Theoretical Analysis on Temperature- and Pressure-Dependences of NO-CO-O₂ Reaction on Rh(111) Surface. Journal of Computer Chemistry Japan, 2019, 18, 70-77.	0.1	1
17	Temperature- and pressure-dependent adsorption configuration of NO molecules on Rh(111) surface: A theoretical study. Surface Science, 2019, 686, 58-62.	1.9	6
18	Reaction energy benchmarks of hydrocarbon combustion by Gaussian basis and plane wave basis approaches. Journal of Computational Chemistry, 2019, 40, 1866-1873.	3.3	3

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19	Machine learning prediction of coordination energies for alkali group elements in battery electrolyte solvents. Physical Chemistry Chemical Physics, 2019, 21, 26399-26405.	2.8	38
20	Electron-Hopping Brings Lattice Strain and High Catalytic Activity in the Low-Temperature Oxidative Coupling of Methane in an Electric Field. Journal of Physical Chemistry C, 2018, 122, 2089-2096.	3.1	26
21	Catalytic performance of Ru, Os, and Rh nanoparticles for ammonia synthesis: A density functional theory analysis. Journal of Catalysis, 2018, 357, 213-222.	6.2	53
22	First-Principles Microkinetic Analysis of NO + CO Reactions on Rh(111) Surface toward Understanding NO_x Reduction Pathways. Journal of Physical Chemistry C, 2018, 122, 17378-17388.	3.1	29
23	Systematic Investigation of the Thermodynamic Properties of Amine Solvents for CO2 Chemical Absorption Using the Cluster-Continuum Model. Bulletin of the Chemical Society of Japan, 2017, 90, 451-460.	3.2	11
24	Density Functional Theory Analysis of Elementary Reactions in NO_x Reduction on Rh Surfaces and Rh Clusters. Journal of Physical Chemistry C, 2017, 121, 15272-15281.	3.1	21
25	Analysis on Si modified MMI-waveguide-type optical switch operated with carrier injection. , 2017, , .		0
26	Electrocatalytic synthesis of ammonia by surface proton hopping. Chemical Science, 2017, 8, 5434-5439.	7.4	72
27	Computational Chemistry Studies on CO₂ Chemical Absorption Technique: Challenge on Energy and Environmental Issue. Journal of Computer Chemistry Japan, 2016, 15, A15-A29.	0.1	4
28	Quantum chemical approach for condensed-phase thermochemistry (IV): Solubility of gaseous molecules. Chemical Physics Letters, 2016, 655-656, 103-109.	2.6	4
29	Quantum chemical approach for condensed-phase thermochemistry (III): Accurate evaluation of proton hydration energy and standard hydrogen electrode potential. Chemical Physics Letters, 2016, 650, 159-164.	2.6	24
30	Theoretical Analysis of the Oxidation Potentials of Organic Electrolyte Solvents. ECS Electrochemistry Letters, 2015, 4, A103-A105.	1.9	9
31	Quantum chemical approach for condensed-phase thermochemistry (II): Applications to formation and combustion reactions of liquid organic molecules. Chemical Physics Letters, 2015, 624, 6-11.	2.6	11
32	Theoretical Study on Excess-Electron Transfer in DNA Based on the Marcus Theory. Journal of Computer Chemistry Japan, 2014, 13, 242-249.	0.1	0
33	Quantum chemical approach for condensed-phase thermochemistry: Proposal of a harmonic solvation model. Journal of Chemical Physics, 2014, 141, 174106.	3.0	20
34	XPS of oxygen atoms on Ag(111) and Ag(110) surfaces: Accurate study with SAC/SACâ€CI combined with dipped adcluster model. Journal of Computational Chemistry, 2013, 34, 1828-1834.	3.3	3
35	Complicated Electronic Process of Câ€“C Ïƒ-Bond Activation of Cyclopropene by Ruthenium and Iridium Complexes: Theoretical Study. Organometallics, 2012, 31, 8189-8199.	2.3	5
36	Accurate solutions of the SchrÃ¶dinger and Dirac equations of , HD+, and HT+: With and without Bornâ€“Oppenheimer approximation and under magnetic field. Chemical Physics, 2012, 401, 62-72.	1.9	26

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37	Solving the SchrÃ¶dinger Equation for the Hydrogen Molecular Ion in a Magnetic Field Using the Free-Complement Method. Progress in Theoretical Chemistry and Physics, 2012, , 255-274.	0.2	0
38	Theoretical Study of Photoinduced Epoxidation of Olefins Catalyzed by Ruthenium Porphyrin. Journal of Physical Chemistry A, 2011, 115, 4774-4785.	2.5	16
39	Pd(ii)-promoted direct cross-coupling reaction of arenes via highly regioselective aromatic Câ€“H activation: a theoretical study. Dalton Transactions, 2010, 39, 3279.	3.3	55
40	Oxygen Atom Transfer Reactions of Iridium and Osmium Complexes: Theoretical Study of Characteristic Features and Significantly Large Differences Between These Two Complexes. Inorganic Chemistry, 2009, 48, 8154-8163.	4.0	37
41	Solving the SchrÃ¶dinger and Dirac equations of hydrogen molecular ion accurately by the free iterative complement interaction method. Journal of Chemical Physics, 2008, 128, 124103.	3.0	28
42	Detection of optical trapping of CdTe quantum dots by two-photon-induced luminescence. Physical Review B, 2007, 75, .	3.2	68
43	Solving the SchrÃ¶dinger Equation of Atoms and Molecules without Analytical Integration Based on the Free Iterative-Complement-Interaction Wave Function. Physical Review Letters, 2007, 99, 240402.	7.8	79