

Atsushi Ishikawa

List of Publications by Year in descending order

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papers

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1021
citing authors

#	ARTICLE	IF	CITATIONS
1	Solving the Schrödinger Equation of Atoms and Molecules without Analytical Integration Based on the Free Iterative-Complement-Interaction Wave Function. <i>Physical Review Letters</i> , 2007, 99, 240402.	7.8	79
2	Electrocatalytic synthesis of ammonia by surface proton hopping. <i>Chemical Science</i> , 2017, 8, 5434-5439.	7.4	72
3	Detection of optical trapping of CdTe quantum dots by two-photon-induced luminescence. <i>Physical Review B</i> , 2007, 75, .	3.2	68
4	Pd(ii)-promoted direct cross-coupling reaction of arenes via highly regioselective aromatic C-H activation: a theoretical study. <i>Dalton Transactions</i> , 2010, 39, 3279.	3.3	55
5	Catalytic performance of Ru, Os, and Rh nanoparticles for ammonia synthesis: A density functional theory analysis. <i>Journal of Catalysis</i> , 2018, 357, 213-222.	6.2	53
6	Machine learning prediction of coordination energies for alkali group elements in battery electrolyte solvents. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 26399-26405.	2.8	38
7	Oxygen Atom Transfer Reactions of Iridium and Osmium Complexes: Theoretical Study of Characteristic Features and Significantly Large Differences Between These Two Complexes. <i>Inorganic Chemistry</i> , 2009, 48, 8154-8163.	4.0	37
8	First-Principles Microkinetic Analysis of NO + CO Reactions on Rh(111) Surface toward Understanding NO _x Reduction Pathways. <i>Journal of Physical Chemistry C</i> , 2018, 122, 17378-17388.	3.1	29
9	The important role of N ₂ H formation energy for low-temperature ammonia synthesis in an electric field. <i>Catalysis Today</i> , 2020, 351, 119-124.	4.4	29
10	Solving the Schrödinger and Dirac equations of hydrogen molecular ion accurately by the free iterative complement interaction method. <i>Journal of Chemical Physics</i> , 2008, 128, 124103.	3.0	28
11	Accurate solutions of the Schrödinger and Dirac equations of H ⁺ , HD ⁺ , and HT ⁺ : With and without Born-Oppenheimer approximation and under magnetic field. <i>Chemical Physics</i> , 2012, 401, 62-72.	1.9	26
12	Electron-Hopping Brings Lattice Strain and High Catalytic Activity in the Low-Temperature Oxidative Coupling of Methane in an Electric Field. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2089-2096.	3.1	26
13	Quantum chemical approach for condensed-phase thermochemistry (III): Accurate evaluation of proton hydration energy and standard hydrogen electrode potential. <i>Chemical Physics Letters</i> , 2016, 650, 159-164.	2.6	24
14	Efficient Oxygen Evolution Electrocatalysis on CaFe ₂ O ₄ and Its Reaction Mechanism. <i>ACS Applied Energy Materials</i> , 2021, 4, 3057-3066.	5.1	22
15	Density Functional Theory Analysis of Elementary Reactions in NO _x Reduction on Rh Surfaces and Rh Clusters. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15272-15281.	3.1	21
16	Agglomeration Suppression of a Fe-Supported Catalyst and its Utilization for Low-Temperature Ammonia Synthesis in an Electric Field. <i>ACS Omega</i> , 2020, 5, 6846-6851.	3.5	21
17	Quantum chemical approach for condensed-phase thermochemistry: Proposal of a harmonic solvation model. <i>Journal of Chemical Physics</i> , 2014, 141, 174106.	3.0	20
18	A First-Principles Microkinetics for Homogeneous-Heterogeneous Reactions: Application to Oxidative Coupling of Methane Catalyzed by Magnesium Oxide. <i>ACS Catalysis</i> , 2021, 11, 2691-2700.	11.2	20

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19	Theoretical Study of Photoinduced Epoxidation of Olefins Catalyzed by Ruthenium Porphyrin. Journal of Physical Chemistry A, 2011, 115, 4774-4785.	2.5	16
20	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
21	Heteroatom doping effects on interaction of H ₂ O and CeO ₂ (111) surfaces studied using density functional theory: Key roles of ionic radius and dispersion. Journal of Chemical Physics, 2020, 152, 014707.	3.0	13
22	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
23	Systematic Investigation of the Thermodynamic Properties of Amine Solvents for CO ₂ Chemical Absorption Using the Cluster-Continuum Model. Bulletin of the Chemical Society of Japan, 2017, 90, 451-460.	3.2	11
24	Theoretical Analysis of the Oxidation Potentials of Organic Electrolyte Solvents. ECS Electrochemistry Letters, 2015, 4, A103-A105.	1.9	9
25	Surface Rashba-Edelstein Spin-Orbit Torque Revealed by Molecular Self-Assembly. Physical Review Applied, 2020, 13, .	3.8	9
26	Onâ€‘Surface Synthesis of Porphyrinâ€‘Complex Multiâ€‘Block Coâ€‘Oligomers by Defluorinative Coupling. Angewandte Chemie - International Edition, 2021, , .	13.8	9
27	Câ€‘H Bond Activation of Methane through Electronic Interaction with Pd(110). Journal of Physical Chemistry C, 2021, 125, 1368-1377.	3.1	8
28	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
29	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
30	Theoretical prediction by DFT and experimental observation of heterocation-doping effects on hydrogen adsorption and migration over the CeO ₂ (111) surface. Physical Chemistry Chemical Physics, 2021, 23, 4509-4516.	2.8	7
31	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
32	Complicated Electronic Process of Câ€‘C Ĩf-Bond Activation of Cyclopropene by Ruthenium and Iridium Complexes: Theoretical Study. Organometallics, 2012, 31, 8189-8199.	2.3	5
33	Manipulation of CO adsorption over MeI/CeO ₂ by heterocation doping: Key roles of single-atom adsorption energy. Journal of Chemical Physics, 2021, 154, 164705.	3.0	5
34	Computational Chemistry Studies on CO ₂ Chemical Absorption Technique: Challenge on Energy and Environmental Issue. Journal of Computer Chemistry Japan, 2016, 15, A15-A29.	0.1	4
35	Quantum chemical approach for condensed-phase thermochemistry (IV): Solubility of gaseous molecules. Chemical Physics Letters, 2016, 655-656, 103-109.	2.6	4
36	XPS of oxygen atoms on Ag(111) and Ag(110) surfaces: Accurate study with SAC/SACâ€‘I combined with dipped adcluster model. Journal of Computational Chemistry, 2013, 34, 1828-1834.	3.3	3

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37	Reaction energy benchmarks of hydrocarbon combustion by Gaussian basis and plane wave basis approaches. <i>Journal of Computational Chemistry</i> , 2019, 40, 1866-1873.	3.3	3
38	On-Surface Synthesis of Porphyrin-Complex Multi-Block Co-Oligomers by Defluorinative Coupling. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	3
39	Heterogeneous catalyst design by generative adversarial network and first-principles based microkinetics. <i>Scientific Reports</i> , 2022, 12, .	3.3	3
40	Theoretical Analysis on Temperature- and Pressure-Dependences of NO-CO-O ₂ Reaction on Rh(111) Surface. <i>Journal of Computer Chemistry Japan</i> , 2019, 18, 70-77.	0.1	1
41	Theoretical Study on Excess-Electron Transfer in DNA Based on the Marcus Theory. <i>Journal of Computer Chemistry Japan</i> , 2014, 13, 242-249.	0.1	0
42	Analysis on Si modified MMI-waveguide-type optical switch operated with carrier injection. , 2017, , .		0
43	Solving the Schrödinger Equation for the Hydrogen Molecular Ion in a Magnetic Field Using the Free-Complement Method. <i>Progress in Theoretical Chemistry and Physics</i> , 2012, , 255-274.	0.2	0