Yu-ya Ohnishi

List of Publications by Year
in descending order

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27	950	623188	580395
papers	citations	14 h-index	25 g-index

28	28	28	1224
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ruthenium(II)-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Theoretical Study of Real Catalyst, Ligand Effects, and Solvation Effects. Journal of the American Chemical Society, 2005, 127, 4021-4032.	6.6	183
2	It Takes More Than an Imine: The Role of the Central Atom on the Electron-Accepting Ability of Benzotriazole and Benzothiadiazole Oligomers. Journal of the American Chemical Society, 2012, 134, 2599-2612.	6.6	135
3	Ruthenium(II)-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Theoretical Study of Significant Acceleration by Water Molecules. Organometallics, 2006, 25, 3352-3363.	1.1	96
4	Why Does Fluoride Anion Accelerate Transmetalation between Vinylsilane and Palladium(II)â^'Vinyl Complex? Theoretical Study. Journal of the American Chemical Society, 2008, 130, 12975-12985.	6.6	88
5	Orbital optimized unitary coupled cluster theory for quantum computer. Physical Review Research, 2020, 2, .	1.3	66
6	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. Organometallics, 2009, 28, 2583-2594.	1.1	60
7	Perspective: Explicitly correlated electronic structure theory for complex systems. Journal of Chemical Physics, 2017, 146, 080901.	1.2	51
8	Applications of quantum computing for investigations of electronic transitions in phenylsulfonyl-carbazole TADF emitters. Npj Computational Materials, 2021, 7, .	3.5	32
9	Theoretical and computational studies of organometallic reactions: successful or not?. Chemical Record, 2010, 10, 29-45.	2.9	31
10	Theoretical Study of Oxidative Additions of H₂ and MeCN to a Nickel(0) Complex:â€‰Significantly Large Correlation Effects and Characteristic Features of the Reaction. Journal of Physical Chemistry A, 2007, 111, 7915-7924.	1.1	27
11	Logarithm second-order many-body perturbation method for extended systems. Journal of Chemical Physics, 2010, 133, 034106.	1.2	23
12	Extensivity of Energy and Electronic and Vibrational Structure Methods for Crystals. Annual Review of Physical Chemistry, 2012, 63, 131-153.	4.8	21
13	Frontier Orbital Consistent Quantum Capping Potential (FOC-QCP) for Bulky Ligand of Transition Metal Complexes. Journal of Physical Chemistry A, 2008, 112, 1946-1955.	1.1	20
14	Explicitly correlated frequencyâ€independent secondâ€order green's function for accurate ionization energies. Journal of Computational Chemistry, 2016, 37, 2447-2453.	1.5	16
15	Variational quantum simulation for periodic materials. Physical Review Research, 2022, 4, .	1.3	15
16	Conjugated polymers for pure UV light emission: Poly(metaâ€phenylenes). Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 557-565.	2.4	13
17	Interaction Energy of Large Molecules from Restrained Denominator MP2-F12. Journal of Chemical Theory and Computation, 2014, 10, 4857-4861.	2.3	12
18	Hybrid coupled-cluster and perturbation method for extended systems of one-dimensional periodicity. Journal of Chemical Physics, 2011, 135, 094108.	1.2	11

#	Article	IF	Citations
19	Thermodynamic limit of the energy density in a crystal. Physical Chemistry Chemical Physics, 2012, 14, 7800.	1.3	10
20	Simulating time evolution with fully optimized single-qubit gates on parametrized quantum circuits. Physical Review A, 2022, 105, .	1.0	8
21	On the Validity of the Bornâ˜Oppenheimer Separation and the Accuracy of Diagonal Corrections in Anharmonic Molecular Vibrations. Journal of Physical Chemistry A, 2009, 113, 12461-12469.	1.1	6
22	Optimizing Parameterized Quantum Circuits with Free-Axis Selection. , 2021, , .		6
23	Charge-consistent redefinition of Fock integrals. Chemical Physics, 2012, 401, 152-156.	0.9	5
24	Massively parallel MP2â€F12 calculations on the <scp>K</scp> computer. International Journal of Quantum Chemistry, 2015, 115, 333-341.	1.0	5
25	Post-Hartreeâ€“Fock method in quantum chemistry for quantum computer. European Physical Journal: Special Topics, 2021, 230, 1037-1051.	1.2	5
26	Alternative formulation of explicitly correlated third-order MÃ¸llerâ€“Plesset perturbation theory. Molecular Physics, 2013, 111, 2516-2522.	0.8	4
27	HeterolyticÏ*f*-Bond Activation by Transition Metal Complexes. , 0, , 265-283.		1