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	Variational quantum simulation for periodic materials. Physical Review Research, 2022, 4, .	1.3	15
2	Simulating time evolution with fully optimized single-qubit gates on parametrized quantum circuits. Physical Review A, 2022, 105, .	1.0	8
3	Post-Hartreeâ€“Fock method in quantum chemistry for quantum computer. European Physical Journal: Special Topics, 2021, 230, 1037-1051.	1.2	5
4	Applications of quantum computing for investigations of electronic transitions in phenylsulfonyl-carbazole TADF emitters. Npj Computational Materials, 2021, 7, .	3.5	32
5	Optimizing Parameterized Quantum Circuits with Free-Axis Selection. , 2021, , .		6
6	Orbital optimized unitary coupled cluster theory for quantum computer. Physical Review Research, 2020, 2, .	1.3	66
7	Perspective: Explicitly correlated electronic structure theory for complex systems. Journal of Chemical Physics, 2017, 146, 080901.	1.2	51
8	Explicitly correlated frequencyâ€independent secondâ€order green's function for accurate ionization energies. Journal of Computational Chemistry, 2016, 37, 2447-2453.	1.5	16
9	Massively parallel MP2â€F12 calculations on the <scp>K</scp> computer. International Journal of Quantum Chemistry, 2015, 115, 333-341.	1.0	5
10	Interaction Energy of Large Molecules from Restrained Denominator MP2-F12. Journal of Chemical Theory and Computation, 2014, 10, 4857-4861.	2.3	12
11	Alternative formulation of explicitly correlated third-order MÃ¸llerâ€“Plesset perturbation theory. Molecular Physics, 2013, 111, 2516-2522.	0.8	4
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	Thermodynamic limit of the energy density in a crystal. Physical Chemistry Chemical Physics, 2012, 14, 7800.	1.3	10
14	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
15	Charge-consistent redefinition of Fock integrals. Chemical Physics, 2012, 401, 152-156.	0.9	5
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	Hybrid coupled-cluster and perturbation method for extended systems of one-dimensional periodicity. Journal of Chemical Physics, 2011, 135, 094108.	1.2	11
18	Theoretical and computational studies of organometallic reactions: successful or not?. Chemical Record, 2010, 10, 29-45.	2.9	31

#	Article	IF	Citations
19	Logarithm second-order many-body perturbation method for extended systems. Journal of Chemical Physics, 2010, 133, 034106.	1.2	23
20	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
21	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. Organometallics, 2009, 28, 2583-2594.	1.1	60
22	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
23	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
24	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
25	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
26	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
27	HeterolyticÏ*f*-Bond Activation by Transition Metal Complexes. , 0, , 265-283.		1