

Yu-ya Ohnishi

List of Publications by Year in descending order

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27
papers

950
citations

623734

14
h-index

580821

25
g-index

28
all docs

28
docs citations

28
times ranked

1224
citing authors

#	ARTICLE	IF	CITATIONS
1	Variational quantum simulation for periodic materials. <i>Physical Review Research</i> , 2022, 4, .	3.6	15
2	Simulating time evolution with fully optimized single-qubit gates on parametrized quantum circuits. <i>Physical Review A</i> , 2022, 105, .	2.5	8
3	Post-Hartree-Fock method in quantum chemistry for quantum computer. <i>European Physical Journal: Special Topics</i> , 2021, 230, 1037-1051.	2.6	5
4	Applications of quantum computing for investigations of electronic transitions in phenylsulfonyl-carbazole TADF emitters. <i>Npj Computational Materials</i> , 2021, 7, .	8.7	32
5	Optimizing Parameterized Quantum Circuits with Free-Axis Selection. , 2021, , .		6
6	Orbital optimized unitary coupled cluster theory for quantum computer. <i>Physical Review Research</i> , 2020, 2, .	3.6	66
7	Perspective: Explicitly correlated electronic structure theory for complex systems. <i>Journal of Chemical Physics</i> , 2017, 146, 080901.	3.0	51
8	Explicitly correlated frequency-independent second-order green's function for accurate ionization energies. <i>Journal of Computational Chemistry</i> , 2016, 37, 2447-2453.	3.3	16
9	Massively parallel MP2-F12 calculations on the <sc>K</sc> computer. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 333-341.	2.0	5
10	Interaction Energy of Large Molecules from Restrained Denominator MP2-F12. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4857-4861.	5.3	12
11	Alternative formulation of explicitly correlated third-order Møller-Plesset perturbation theory. <i>Molecular Physics</i> , 2013, 111, 2516-2522.	1.7	4
12	Extensivity of Energy and Electronic and Vibrational Structure Methods for Crystals. <i>Annual Review of Physical Chemistry</i> , 2012, 63, 131-153.	10.8	21
13	Thermodynamic limit of the energy density in a crystal. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7800.	2.8	10
14	It Takes More Than an Imine: The Role of the Central Atom on the Electron-Accepting Ability of Benzotriazole and Benzothiadiazole Oligomers. <i>Journal of the American Chemical Society</i> , 2012, 134, 2599-2612.	13.7	135
15	Charge-consistent redefinition of Fock integrals. <i>Chemical Physics</i> , 2012, 401, 152-156.	1.9	5
16	Conjugated polymers for pure UV light emission: Poly(<i>meta</i> -phenylenes). <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2011, 49, 557-565.	2.1	13
17	Hybrid coupled-cluster and perturbation method for extended systems of one-dimensional periodicity. <i>Journal of Chemical Physics</i> , 2011, 135, 094108.	3.0	11
18	Theoretical and computational studies of organometallic reactions: successful or not?. <i>Chemical Record</i> , 2010, 10, 29-45.	5.8	31

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19	Logarithm second-order many-body perturbation method for extended systems. <i>Journal of Chemical Physics</i> , 2010, 133, 034106.	3.0	23
20	On the Validity of the Born-Oppenheimer Separation and the Accuracy of Diagonal Corrections in Anharmonic Molecular Vibrations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12461-12469.	2.5	6
21	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. <i>Organometallics</i> , 2009, 28, 2583-2594.	2.3	60
22	Frontier Orbital Consistent Quantum Capping Potential (FOC-QCP) for Bulky Ligand of Transition Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1946-1955.	2.5	20
23	Why Does Fluoride Anion Accelerate Transmetalation between Vinylsilane and Palladium(II)-Vinyl Complex? Theoretical Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 12975-12985.	13.7	88
24	Theoretical Study of Oxidative Additions of H ₂ and MeCN to a Nickel(0) Complex: Significant Large Correlation Effects and Characteristic Features of the Reaction. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7915-7924.	2.5	27
25	Ruthenium(II)-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Theoretical Study of Significant Acceleration by Water Molecules. <i>Organometallics</i> , 2006, 25, 3352-3363.	2.3	96
26	Ruthenium(II)-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Theoretical Study of Real Catalyst, Ligand Effects, and Solvation Effects. <i>Journal of the American Chemical Society</i> , 2005, 127, 4021-4032.	13.7	183
27	Heterolytic σ -Bond Activation by Transition Metal Complexes. , 0, , 265-283.		1