Iris Theophilou

List of Publications by Year
in descending order

21	784	933447 10	794594 19
papers	citations	h-index	g-index

21	21	21	1048
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Approximations based on density-matrix embedding theory for density-functional theories. Electronic Structure, 2021, 3, 035001.	2.8	1
2	Lightâ€“Matter Hybrid-Orbital-Based First-Principles Methods: The Influence of Polariton Statistics. Journal of Chemical Theory and Computation, 2020, 16, 5601-5620.	5.3	19
3	Virial Relations for Electrons Coupled to Quantum Field Modes. Journal of Chemical Theory and Computation, 2020, 16, 6236-6243.	5.3	6
4	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.	3.0	210
5	Force balance approach for advanced approximations in density functional theories. Journal of Chemical Physics, 2019, 151, 154107.	3.0	17
6	Self-Consistent Density-Functional Embedding: A Novel Approach for Density-Functional Approximations. Journal of Chemical Theory and Computation, 2019, 15, 5209-5220.	5.3	14
7	Reduced Density-Matrix Approach to Strong Matter-Photon Interaction. ACS Photonics, 2019, 6, 2694-2711.	6.6	31
8	Structure of the first order reduced density matrix in three electron systems: A generalized Pauli constraints assisted study. Journal of Chemical Physics, 2018, 148, 114108.	3.0	3
9	Kinetic-Energy Density-Functional Theory on a Lattice. Journal of Chemical Theory and Computation, 2018, 14, 4072-4087.	5.3	7
10	Conditions for Describing Triplet States in Reduced Density Matrix Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 2668-2678.	5.3	8
11	Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems. Physical Chemistry Chemical Physics, 2015, 17, 31371-31396.	2.8	376
12	Generalized Pauli constraints in reduced density matrix functional theory. Journal of Chemical Physics, 2015, 142, 154108.	3.0	39
13	Orbitals from local RDMFT: Are they Kohn-Sham or natural orbitals?. Journal of Chemical Physics, 2015, 143, 054106.	3.0	10
14	Charge transfer excitations from excited state Hartree-Fock subsequent minimization scheme. Journal of Chemical Physics, 2014, 140, 164102.	3.0	5
15	Hartreeâ€“Fock calculation for excited states. International Journal of Quantum Chemistry, 2013, 113, 690-693.	2.0	19
16	Double excitations from modified Hartree Fock subsequent minimization scheme. Journal of Chemical Physics, 2013, 138, 124107.	3.0	4
17	Spin projected and improved energy states from unrestricted Hartreeâ€“Fock. Molecular Physics, 2011, 109, 1495-1502.	1.7	0
18	Symmetry preserving and improved energy states derived from asymmetric Hartree-Fock. Journal of Physics: Conference Series, 2010, 213, 012024.	0.4	0

#	Article	IF	Citations
19	Dissociation energies for small molecules from symmetry projected Hartree Fock states. Journal of Physics: Conference Series, 2010, 213, 012030.	0.4	1
20	Approximate spin symmetries in single determinantal approximations of many electron systems. Journal of Physics: Conference Series, 2008, 104, 012020.	0.4	1
21	Spin contamination for Hartree-Fock, optimized effective potential, and density functional approximations. Journal of Chemical Physics, 2007, 127, 234103.	3.0	13