Iris Theophilou

List of Publications by Year
in descending order

21 papers	784 citations	933447 10 h-index	794594 19 g-index
21 all docs	21 docs citations	21 times ranked	1048 citing authors

#	Article	IF	Citations
1	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
2	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
3	Generalized Pauli constraints in reduced density matrix functional theory. Journal of Chemical Physics, 2015, 142, 154108.	3.0	39
4	Reduced Density-Matrix Approach to Strong Matter-Photon Interaction. ACS Photonics, 2019, 6, 2694-2711.	6.6	31
5	Hartree–Fock calculation for excited states. International Journal of Quantum Chemistry, 2013, 113, 690-693.	2.0	19
6	Light–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
7	Force balance approach for advanced approximations in density functional theories. Journal of Chemical Physics, 2019, 151, 154107.	3.0	17
8	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
9	Spin contamination for Hartree-Fock, optimized effective potential, and density functional approximations. Journal of Chemical Physics, 2007, 127, 234103.	3.0	13
10	Orbitals from local RDMFT: Are they Kohn-Sham or natural orbitals?. Journal of Chemical Physics, 2015, 143, 054106.	3.0	10
11	Conditions for Describing Triplet States in Reduced Density Matrix Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 2668-2678.	5.3	8
12	Kinetic-Energy Density-Functional Theory on a Lattice. Journal of Chemical Theory and Computation, 2018, 14, 4072-4087.	5.3	7
13	Virial Relations for Electrons Coupled to Quantum Field Modes. Journal of Chemical Theory and Computation, 2020, 16, 6236-6243.	5.3	6
14	Charge transfer excitations from excited state Hartree-Fock subsequent minimization scheme. Journal of Chemical Physics, 2014, 140, 164102.	3.0	5
15	Double excitations from modified Hartree Fock subsequent minimization scheme. Journal of Chemical Physics, 2013, 138, 124107.	3.0	4
16	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
17	Approximate spin symmetries in single determinantal approximations of many electron systems. Journal of Physics: Conference Series, 2008, 104, 012020.	0.4	1
18	Dissociation energies for small molecules from symmetry projected Hartree Fock states. Journal of Physics: Conference Series, 2010, 213, 012030.	0.4	1

#	Article	IF	Citations
19	Approximations based on density-matrix embedding theory for density-functional theories. Electronic Structure, 2021, 3, 035001.	2.8	1
20	Symmetry preserving and improved energy states derived from asymmetric Hartree-Fock. Journal of Physics: Conference Series, 2010, 213, 012024.	0.4	0
21	Spin projected and improved energy states from unrestricted Hartreeâ€"Fock. Molecular Physics, 2011, 109, 1495-1502.	1.7	0