Emmanuel Giner

List of Publications by Year
in descending order

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35	967	430843	434170
papers	citations	18	31
		h-index	g-index

35	35	35	677
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. Journal of Chemical Theory and Computation, 2019, 15, 3591-3609.	5.3	108
2	Using perturbatively selected configuration interaction in quantum Monte Carlo calculations. Canadian Journal of Chemistry, 2013, 91, 879-885.	1.1	105
3	Selected configuration interaction dressed by perturbation. Journal of Chemical Physics, 2018, 149, 064103.	3.0	92
4	Fixed-node diffusion Monte Carlo potential energy curve of the fluorine molecule F2 using selected configuration interaction trial wavefunctions. Journal of Chemical Physics, 2015, 142, 044115.	3.0	70
5	Communication: Toward an improved control of the fixed-node error in quantum Monte Carlo: The case of the water molecule. Journal of Chemical Physics, 2016, 144, 151103.	3.0	48
6	Almost exact energies for the Gaussian-2 set with the semistochastic heat-bath configuration interaction method. Journal of Chemical Physics, 2020, 153, 124117.	3.0	41
7	Spin Density Distribution in Open-Shell Transition Metal Systems: A Comparative Post-Hartreeâ€“Fock, Density Functional Theory, and Quantum Monte Carlo Study of the CuCl₂ Molecule. Journal of Chemical Theory and Computation, 2014, 10, 5286-5296.	5.3	39
8	Accurate nonrelativistic ground-state energies of 3d transition metal atoms. Journal of Chemical Physics, 2014, 141, 244110.	3.0	37
9	Range-separated multideterminant density-functional theory with a short-range correlation functional of the on-top pair density. Journal of Chemical Physics, 2019, 150, 084103.	3.0	34
10	Curing basis-set convergence of wave-function theory using density-functional theory: A systematically improvable approach. Journal of Chemical Physics, 2018, 149, 194301.	3.0	33
11	Quantum Monte Carlo with very large multideterminant wavefunctions. Journal of Computational Chemistry, 2016, 37, 1866-1875.	3.3	30
12	Using CIPSI Nodes in Diffusion Monte Carlo. ACS Symposium Series, 2016, , 15-46.	0.5	30
13	Chemically accurate excitation energies with small basis sets. Journal of Chemical Physics, 2019, 151, 144118.	3.0	30
14	A Density-Based Basis-Set Correction for Wave Function Theory. Journal of Physical Chemistry Letters, 2019, 10, 2931-2937.	4.6	26
15	A Jeziorski-Monkhorst fully uncontracted multi-reference perturbative treatment. I. Principles, second-order versions, and tests on ground state potential energy curves. Journal of Chemical Physics, 2017, 146, 224108.	3.0	25
16	Density-Based Basis-Set Incompleteness Correction for GW Methods. Journal of Chemical Theory and Computation, 2020, 16, 1018-1028.	5.3	24
17	Quantum Monte Carlo with reoptimised perturbatively selected configuration-interaction wave functions. Molecular Physics, 2016, 114, 910-920.	1.7	22
18	Metal-ligand delocalization and spin density in the CuCl2 and [CuCl4]2â^' molecules: Some insights from wave function theory. Journal of Chemical Physics, 2015, 143, 124305.	3.0	18

#	Article	IF	Citations
19	A basis-set error correction based on density-functional theory for strongly correlated molecular systems. Journal of Chemical Physics, 2020, 152, 174104.	3.0	16
20	Interplay between Electronic Correlation and Metalâ€“Ligand Delocalization in the Spectroscopy of Transition Metal Compounds: Case Study on a Series of Planar Cu²⁺ Complexes. Journal of Chemical Theory and Computation, 2018, 14, 6240-6252.	5.3	15
21	A simple approach to the state-specific MR-CC using the intermediate Hamiltonian formalism. Journal of Chemical Physics, 2016, 144, 064101.	3.0	14
22	A new form of transcorrelated Hamiltonian inspired by range-separated DFT. Journal of Chemical Physics, 2021, 154, 084119.	3.0	12
23	Taming the fixed-node error in diffusion Monte Carlo via range separation. Journal of Chemical Physics, 2020, 153, 174107.	3.0	11
24	Spin density and orbital optimization in open shell systems: A rational and computationally efficient proposal. Journal of Chemical Physics, 2016, 144, 104104.	3.0	9
25	Strongly localized approaches for delocalized systems. I. Ground state of linear polyenes. Computational and Theoretical Chemistry, 2017, 1116, 102-111.	2.5	9
26	Self-consistent density-based basis-set correction: How much do we lower total energies and improve dipole moments?. Journal of Chemical Physics, 2021, 155, 044109.	3.0	9
27	Accurate energies of transition metal atoms, ions, and monoxides using selected configuration interaction and density-based basis-set corrections. Journal of Chemical Physics, 2021, 155, 204104.	3.0	9
28	Alternative definition of excitation amplitudes in multi-reference state-specific coupled cluster. Journal of Chemical Physics, 2017, 146, 154107.	3.0	8
29	Relativistic short-range exchange energy functionals beyond the local-density approximation. Journal of Chemical Physics, 2020, 152, 214106.	3.0	8
30	Performance of a one-parameter correlation factor for transcorrelation: Study on a series of second row atomic and molecular systems. Journal of Chemical Physics, 2022, 156, .	3.0	8
31	The â€œFermi holeâ€•and the correlation introduced by the symmetrization or the anti-symmetrization of the wave function. Journal of Chemical Physics, 2016, 145, 124114.	3.0	6
32	Computation of the Isotropic Hyperfine Coupling Constant: Efficiency and Insights from a New Approach Based on Wave Function Theory. Journal of Chemical Theory and Computation, 2017, 13, 475-487.	5.3	6
33	Basis-set correction based on density-functional theory: Rigorous framework for a one-dimensional model. Journal of Chemical Physics, 2022, 156, 044113.	3.0	6
34	Orthogonal Valence Bond Hamiltonians incorporating dynamical correlation effects. Computational and Theoretical Chemistry, 2017, 1116, 134-140.	2.5	5
35	Basis-set correction for coupled-cluster estimation of dipole moments. Journal of Chemical Physics, 2022, 156, 174101.	3.0	4