Nick Blunt

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3489299/publications.pdf

Version: 2024-02-01

28 papers	2,654 citations	394286 19 h-index	501076 28 g-index
28 all docs	28 docs citations	28 times ranked	1609 citing authors

#	Article	IF	Citations
1	P<scp>y</scp>SCF: the Pythonâ€based simulations of chemistry framework. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1340.	6.2	894
2	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	1.2	388
3	<tt>QMCPACK</tt>: an open sourceab initioquantum Monte Carlo package for the electronic structure of atoms, molecules and solids. Journal of Physics Condensed Matter, 2018, 30, 195901.	0.7	187
4	Multi-qubit entanglement and algorithms on a neutral-atom quantum computer. Nature, 2022, 604, 457-462.	13.7	180
5	Unbiased reduced density matrices and electronic properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2014, 141, 244117.	1.2	90
6	The sign problem and population dynamics in the full configuration interaction quantum Monte Carlo method. Journal of Chemical Physics, 2012, 136, 054110.	1.2	88
7	Accurate Exchange-Correlation Energies for the Warm Dense Electron Gas. Physical Review Letters, 2016, 117, 115701.	2.9	88
8	Density-matrix quantum Monte Carlo method. Physical Review B, 2014, 89, .	1.1	84
9	Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application. Journal of Chemical Physics, 2015, 142, 184107.	1.2	83
10	An excited-state approach within full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 134117.	1.2	77
11	Interaction picture density matrix quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 044116.	1.2	69
12	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. Journal of Chemical Physics, 2020, 153, 034107.	1.2	55
13	Krylov-Projected Quantum MonteÂCarlo Method. Physical Review Letters, 2015, 115, 050603.	2.9	53
14	A new mechanism for oceanâ€“atmosphere coupling in midlatitudes. Quarterly Journal of the Royal Meteorological Society, 2011, 137, 1095-1101.	1.0	48
15	Density matrices in full configuration interaction quantum Monte Carlo: Excited states, transition dipole moments, and parallel distribution. Journal of Chemical Physics, 2017, 146, 244105.	1.2	47
16	Communication: An efficient and accurate perturbative correction to initiator full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2018, 148, 221101.	1.2	35
17	The HANDE-QMC Project: Open-Source Stochastic Quantum Chemistry from the Ground State Up. Journal of Chemical Theory and Computation, 2019, 15, 1728-1742.	2.3	33
18	Open-Source Development Experiences in Scientific Software: The HANDE Quantum Monte Carlo Project. Journal of Open Research Software, 2015, 3, 9.	2.7	21

#	Article	IF	Citations
19	Preconditioning and Perturbative Estimators in Full Configuration Interaction Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 3537-3551.	2.3	20
20	Excited-State Diffusion Monte Carlo Calculations: A Simple and Efficient Two-Determinant Ansatz. Journal of Chemical Theory and Computation, 2019, 15, 178-189.	2.3	20
21	Nonlinear biases, stochastically sampled effective Hamiltonians, and spectral functions in quantum Monte Carlo methods. Physical Review B, 2018, 98, .	1.1	16
22	Multireference configuration interaction and perturbation theory without reduced density matrices. Journal of Chemical Physics, 2019, 151, 211102.	1.2	16
23	Efficient multireference perturbation theory without high-order reduced density matrices. Journal of Chemical Physics, 2020, 153, 164120.	1.2	16
24	Charge-transfer excited states: Seeking a balanced and efficient wave function ansatz in variational Monte Carlo. Journal of Chemical Physics, 2017, 147, 194101.	1.2	13
25	A hybrid approach to extending selected configuration interaction and full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2019, 151, 174103.	1.2	13
26	Response Formalism within Full Configuration Interaction Quantum Monte Carlo: Static Properties and Electrical Response. Journal of Chemical Theory and Computation, 2018, 14, 3532-3546.	2.3	9
27	Quantum computing in pharma: A multilayer embedding approach for near future applications. Journal of Computational Chemistry, 2023, 44, 406-421.	1.5	7
28	Fixed- and Partial-Node Approximations in Slater Determinant Space for Molecules. Journal of Chemical Theory and Computation, 2021, 17, 6092-6104.	2.3	4