Werner Dobrautz

List of Publications by Year in descending order

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1163117 1281871 11 308 8 11 citations h-index g-index papers 12 12 12 138 all docs docs citations times ranked citing authors

#	Article	IF	CITATIONS
1	NECI: $\langle i \rangle N \langle i \rangle$ -Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. Journal of Chemical Physics, 2020, 153, 034107.	3.0	55
2	Efficient formulation of full configuration interaction quantum Monte Carlo in a spin eigenbasis via the graphical unitary group approach. Journal of Chemical Physics, 2019, 151, 094104.	3.0	49
3	Compact numerical solutions to the two-dimensional repulsive Hubbard model obtained via nonunitary similarity transformations. Physical Review B, 2019, 99, .	3.2	43
4	Similarity transformation of the electronic Schr $\tilde{A}\P$ dinger equation via Jastrow factorization. Journal of Chemical Physics, 2019, 151, 061101.	3.0	40
5	Compression of Spin-Adapted Multiconfigurational Wave Functions in Exchange-Coupled Polynuclear Spin Systems. Journal of Chemical Theory and Computation, 2020, 16, 2202-2215.	5.3	28
6	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Iron–Sulfur Clusters. Journal of Chemical Theory and Computation, 2021, 17, 5684-5703.	5.3	25
7	Resolution of Low-Energy States in Spin-Exchange Transition-Metal Clusters: Case Study of Singlet States in [Fe(III) ₄ S ₄] Cubanes. Journal of Physical Chemistry A, 2021, 125, 4727-4740.	2.5	22
8	Time Propagation and Spectroscopy of Fermionic Systems Using a Stochastic Technique. Physical Review Letters, 2018, 121, 056401.	7.8	14
9	Combined unitary and symmetric group approach applied to low-dimensional Heisenberg spin systems. Physical Review B, 2022, 105, .	3.2	9
10	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
11	Benchmark study of Nagaoka ferromagnetism by spin-adapted full configuration interaction quantum Monte Carlo. Physical Review B, 2021, 104, .	3.2	6