

Werner Dobrautz

List of Publications by Year in descending order

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papers

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1163117

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docs citations

12
times ranked

138
citing authors

#	ARTICLE	IF	CITATIONS
1	Combined unitary and symmetric group approach applied to low-dimensional Heisenberg spin systems. <i>Physical Review B</i> , 2022, 105, .	3.2	9
2	Performance of a one-parameter correlation factor for transcorrelation: Study on a series of second row atomic and molecular systems. <i>Journal of Chemical Physics</i> , 2022, 156, .	3.0	8
3	Resolution of Low-Energy States in Spin-Exchange Transition-Metal Clusters: Case Study of Singlet States in $[\text{Fe}(\text{III})_4\text{S}_4]$ Cubanes. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4727-4740.	2.5	22
4	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Iron-Sulfur Clusters. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5684-5703.	5.3	25
5	Benchmark study of Nagaoka ferromagnetism by spin-adapted full configuration interaction quantum Monte Carlo. <i>Physical Review B</i> , 2021, 104, .	3.2	6
6	NECI: <i>N</i> -Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. <i>Journal of Chemical Physics</i> , 2020, 153, 034107.	3.0	55
7	Compression of Spin-Adapted Multiconfigurational Wave Functions in Exchange-Coupled Polynuclear Spin Systems. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2202-2215.	5.3	28
8	Similarity transformation of the electronic Schrödinger equation via Jastrow factorization. <i>Journal of Chemical Physics</i> , 2019, 151, 061101.	3.0	40
9	Efficient formulation of full configuration interaction quantum Monte Carlo in a spin eigenbasis via the graphical unitary group approach. <i>Journal of Chemical Physics</i> , 2019, 151, 094104.	3.0	49
10	Compact numerical solutions to the two-dimensional repulsive Hubbard model obtained via nonunitary similarity transformations. <i>Physical Review B</i> , 2019, 99, .	3.2	43
11	Time Propagation and Spectroscopy of Fermionic Systems Using a Stochastic Technique. <i>Physical Review Letters</i> , 2018, 121, 056401.	7.8	14