Eric Neuscamman

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4674700/publications.pdf

Version: 2024-02-01

44	4,105	304743	233421
papers	citations	22 h-index	45 g-index

45	45	45	4592
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	<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.	1.8	187
3	Optimizing large parameter sets in variational quantum Monte Carlo. Physical Review B, 2012, 85, .	3.2	91
4	A review of canonical transformation theory. International Reviews in Physical Chemistry, 2010, 29, 231-271.	2.3	86
5	Size Consistency Error in the Antisymmetric Geminal Power Wave Function can be Completely Removed. Physical Review Letters, 2012, 109, 203001.	7.8	83
6	Quadratic canonical transformation theory and higher order density matrices. Journal of Chemical Physics, 2009, 130, 124102.	3.0	81
7	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. Journal of Chemical Physics, 2020, 152, 174105.	3.0	80
8	Strongly contracted canonical transformation theory. Journal of Chemical Physics, 2010, 132, 024106.	3.0	75
9	A study of cumulant approximations to n-electron valence multireference perturbation theory. Journal of Chemical Physics, 2009, 130, 194107.	3.0	70
10	The Jastrow antisymmetric geminal power in Hilbert space: Theory, benchmarking, and application to a novel transition state. Journal of Chemical Physics, 2013, 139, 194105.	3.0	64
11	An Efficient Variational Principle for the Direct Optimization of Excited States. Journal of Chemical Theory and Computation, 2016, 12, 3436-3440.	5.3	48
12	Communication: A Jastrow factor coupled cluster theory for weak and strong electron correlation. Journal of Chemical Physics, 2013, 139, 181101.	3.0	46
13	Communication: A mean field platform for excited state quantum chemistry. Journal of Chemical Physics, 2018, 149, 081101.	3.0	46
14	A Generalized Variational Principle with Applications to Excited State Mean Field Theory. Journal of Chemical Theory and Computation, 2020, 16, 1526-1540.	5.3	36
15	Striped Spin Liquid Crystal Ground State Instability of Kagome Antiferromagnets. Physical Review Letters, 2013, 111, 187205.	7.8	34
16	Size Consistent Excited States via Algorithmic Transformations between Variational Principles. Journal of Chemical Theory and Computation, 2017, 13, 6078-6088.	5.3	31
17	Tracking Excited States in Wave Function Optimization Using Density Matrices and Variational Principles. Journal of Chemical Theory and Computation, 2019, 15, 4790-4803.	5.3	31
18	Extended implementation of canonical transformation theory: parallelization and a new level-shifted condition. Physical Chemistry Chemical Physics, 2012, 14, 7809.	2.8	29

#	Article	IF	Citations
19	Improved Optimization for the Cluster Jastrow Antisymmetric Geminal Power and Tests on Triple-Bond Dissociations. Journal of Chemical Theory and Computation, 2016, 12, 3149-3159.	5.3	29
20	Excited State Specific Multi-Slater Jastrow Wave Functions. Journal of Physical Chemistry A, 2019, 123, 1487-1497.	2.5	27
21	Nonstochastic algorithms for Jastrow-Slater and correlator product state wave functions. Physical Review B, 2011, 84, .	3.2	26
22	Subtractive manufacturing with geminal powers:making good use of a bad wave function. Molecular Physics, 2016, 114, 577-583.	1.7	23
23	Density Functional Extension to Excited-State Mean-Field Theory. Journal of Chemical Theory and Computation, 2020, 16, 164-178.	5.3	22
24	Excitation variance matching with limited configuration interaction expansions in variational Monte Carlo. Journal of Chemical Physics, 2017, 147, 164114.	3.0	21
25	A Blocked Linear Method for Optimizing Large Parameter Sets in Variational Monte Carlo. Journal of Chemical Theory and Computation, 2017, 13, 2604-2611.	5.3	20
26	Excited-State Diffusion Monte Carlo Calculations: A Simple and Efficient Two-Determinant Ansatz. Journal of Chemical Theory and Computation, 2019, 15, 178-189.	5.3	20
27	Improving Excited-State Potential Energy Surfaces via Optimal Orbital Shapes. Journal of Physical Chemistry A, 2020, 124, 8273-8279.	2.5	18
28	Communication: Variation after response in quantum Monte Carlo. Journal of Chemical Physics, 2016, 145, 081103.	3.0	17
29	Complementary first and second derivative methods for ansatz optimization in variational Monte Carlo. Physical Chemistry Chemical Physics, 2019, 21, 14491-14510.	2.8	17
30	A self-consistent field formulation of excited state mean field theory. Journal of Chemical Physics, 2020, 153, 164108.	3.0	16
31	Correlator product state study of molecular magnetism in the giant Keplerate Mo<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>72</mml:mn></mml:msub></mml:math>Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>30</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	3.2	15
32	Equation of Motion Theory for Excited States in Variational Monte Carlo and the Jastrow Antisymmetric Geminal Power in Hilbert Space. Journal of Chemical Theory and Computation, 2016, 12, 3719-3726.	5.3	15
33	A hybrid approach to excited-state-specific variational Monte Carlo and doubly excited states. Journal of Chemical Physics, 2020, 153, 234105.	3.0	15
34	Variational Excitations in Real Solids: Optical Gaps and Insights into Many-Body Perturbation Theory. Physical Review Letters, 2019, 123, 036402.	7.8	14
35	N⁵-Scaling Excited-State-Specific Perturbation Theory. Journal of Chemical Theory and Computation, 2020, 16, 6132-6141.	5.3	14
36	Suppressing Ionic Terms with Number-Counting Jastrow Factors in Real Space. Journal of Chemical Theory and Computation, 2017, 13, 2035-2042.	5.3	13

#	Article	IF	Citations
37	Charge-transfer excited states: Seeking a balanced and efficient wave function ansatz in variational Monte Carlo. Journal of Chemical Physics, 2017, 147, 194101.	3.0	13
38	Core excitations with excited state mean field and perturbation theory. Journal of Chemical Physics, 2020, 153, 154102.	3.0	13
39	Amplitude Determinant Coupled Cluster with Pairwise Doubles. Journal of Chemical Theory and Computation, 2016, 12, 5841-5850.	5.3	12
40	Excited state mean-field theory without automatic differentiation. Journal of Chemical Physics, 2020, 152, 204112.	3.0	12
41	A variational Monte Carlo approach for core excitations. Journal of Chemical Physics, 2020, 153, 144108.	3.0	10
42	Reduced scaling Hilbert space variational Monte Carlo. Journal of Chemical Physics, 2018, 149, 184106.	3.0	6
43	Clean and Convenient Tessellations for Number Counting Jastrow Factors. Journal of Chemical Theory and Computation, 2019, 15, 1102-1121.	5.3	4
44	Starting-point-independent quantum Monte Carlo calculations of iron oxide. Physical Review B, 2020, 102, .	3.2	4