Ali Alavi

List of Publications by Year
in descending order

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88 papers	5,859 citations	76326 40 h-index	74163 75 g-index
90 all docs	90 docs citations	90 times ranked	3361 citing authors

#	Article	IF	Citations
1	Full configuration interaction quantum Monte Carlo treatment of fragments embedded in a periodic mean field. Journal of Chemical Physics, 2022, 156, 154107.	3.0	8
2	General embedded cluster protocol for accurate modeling of oxygen vacancies in metal-oxides. Journal of Chemical Physics, 2022, 156, 124704.	3.0	9
3	Spin Purification in Full-CI Quantum Monte Carlo via a First-Order Penalty Approach. Journal of Physical Chemistry A, 2022, 126, 2050-2060.	2.5	8
4	Enhancement of superexchange due to synergetic breathing and hopping in corner-sharing cuprates. Nature Physics, 2022, 18, 190-195.	16.7	10
5	FCIQMC-Tailored Distinguishable Cluster Approach: Open-Shell Systems. Journal of Chemical Theory and Computation, 2022, , .	5.3	4
6	Ab Initio Wavefunction Analysis of Electron Removal Quasi-Particle State of NdNiO2 With Fully Correlated Quantum Chemical Methods. Frontiers in Physics, 2022, 10, .	2.1	0
7	Combined unitary and symmetric group approach applied to low-dimensional Heisenberg spin systems. Physical Review B, 2022, 105, .	3.2	9
8	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
9	Chemical insights into the electronic structure of Fe(<scp>II</scp>) porphyrin using <scp>FCIQMC</scp>, <scp>DMRG</scp>, and generalized active spaces. International Journal of Quantum Chemistry, 2021, 121, e26454.	2.0	21
10	Population control bias and importance sampling in full configuration interaction quantum Monte Carlo. Physical Review B, 2021, 103, .	3.2	11
11	A full configuration interaction quantum Monte Carlo study of ScO, TiO, and VO molecules. Journal of Chemical Physics, 2021, 154, 164302.	3.0	11
12	Resolution of Low-Energy States in Spin-Exchange Transition-Metal Clusters: Case Study of Singlet States in [Fe(III)₄S₄] Cubanes. Journal of Physical Chemistry A, 2021, 125, 4727-4740.	2.5	22
13	Signatures of the BCS-BEC crossover in the yrast spectra of Fermi quantum rings. Physical Review Research, 2021, 3, .	3.6	5
14	Towards efficient and accurate ab initio solutions to periodic systems via transcorrelation and coupled cluster theory. Physical Review Research, 2021, 3, .	3.6	16
15	Binding curve of the beryllium dimer using similarity-transformed FCIQMC: Spectroscopic accuracy with triple-zeta basis sets. Journal of Chemical Physics, 2021, 155, 011102.	3.0	18
16	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Ironâ€“Sulfur Clusters. Journal of Chemical Theory and Computation, 2021, 17, 5684-5703.	5.3	25
17	Transcorrelated coupled cluster methods. Journal of Chemical Physics, 2021, 155, 191101.	3.0	17
18	Benchmark study of Nagaoka ferromagnetism by spin-adapted full configuration interaction quantum Monte Carlo. Physical Review B, 2021, 104, .	3.2	6

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19	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
20	The color center singlet state of oxygen vacancies in TiO2. Journal of Chemical Physics, 2020, 153, 204704.	3.0	13
21	FCIQMC-Tailored Distinguishable Cluster Approach. Journal of Chemical Theory and Computation, 2020, 16, 5621-5634.	5.3	22
22	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. Journal of Chemical Physics, 2020, 153, 034107.	3.0	55
23	Small polarons and the Janus nature of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mm (110). Physical Review B, 2020, 101, .	3.2	15
24	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
25	The adaptive shift method in full configuration interaction quantum Monte Carlo: Development and applications. Journal of Chemical Physics, 2020, 153, 224115.	3.0	33
26	Electronic correlations and magnetic interactions in infinite-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NdNiO</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2020, 102, .	3.2	38
27	Eliminating the wave-function singularity for ultracold atoms by a similarity transformation. Physical Review Research, 2020, 2, .	3.6	15
28	Similarity transformation of the electronic SchrÃ¶dinger equation via Jastrow factorization. Journal of Chemical Physics, 2019, 151, 061101.	3.0	40
29	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
30	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
31	Role of Valence and Semicore Electron Correlation on Spin Gaps in Fe(II)-Porphyrins. Journal of Chemical Theory and Computation, 2019, 15, 1492-1497.	5.3	51
32	Are smooth pseudopotentials a good choice for representing short-range interactions?. Physical Review A, 2019, 99, .	2.5	3
33	Compact numerical solutions to the two-dimensional repulsive Hubbard model obtained via nonunitary similarity transformations. Physical Review B, 2019, 99, .	3.2	43
34	A comparative study using state-of-the-art electronic structure theories on solid hydrogen phases under high pressures. Npj Computational Materials, 2019, 5, .	8.7	16
35	Unbiasing the initiator approximation in full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2019, 151, 224108.	3.0	56
36	Combining the Transcorrelated Method with Full Configuration Interaction Quantum Monte Carlo: Application to the Homogeneous Electron Gas. Journal of Chemical Theory and Computation, 2018, 14, 1403-1411.	5.3	52

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37	Understanding the Mechanism Stabilizing Intermediate Spin States in Fe(II)-Porphyrin. Journal of Physical Chemistry A, 2018, 122, 4935-4947.	2.5	75
38	The Intricate Case of Tetramethyleneethane: A Full Configuration Interaction Quantum Monte Carlo Benchmark and Multireference Coupled Cluster Studies. Journal of Chemical Theory and Computation, 2018, 14, 2439-2445.	5.3	28
39	Accelerating the convergence of exact diagonalization with the transcorrelated method: Quantum gas in one dimension with contact interactions. Physical Review A, 2018, 98, .	2.5	18
40	Correlation energies of the high-density spin-polarized electron gas to meV accuracy. Physical Review B, 2018, 98, .	3.2	20
41	Nonlinear biases, stochastically sampled effective Hamiltonians, and spectral functions in quantum Monte Carlo methods. Physical Review B, 2018, 98, .	3.2	16
42	Time Propagation and Spectroscopy of Fermionic Systems Using a Stochastic Technique. Physical Review Letters, 2018, 121, 056401.	7.8	14
43	Combining Internally Contracted States and Matrix Product States To Perform Multireference Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 488-498.	5.3	55
44	Stochastic multi-reference perturbation theory with application to the linearized coupled cluster method. Journal of Chemical Physics, 2017, 146, 044107.	3.0	35
45	Semistochastic Heat-Bath Configuration Interaction Method: Selected Configuration Interaction with Semistochastic Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 1595-1604.	5.3	232
46	Density matrices in full configuration interaction quantum Monte Carlo: Excited states, transition dipole moments, and parallel distribution. Journal of Chemical Physics, 2017, 146, 244105.	3.0	47
47	Projector Quantum MonteÂCarlo Method for Nonlinear Wave Functions. Physical Review Letters, 2017, 118, 176403.	7.8	25
48	Assessment of multireference approaches to explicitly correlated full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2016, 145, 054117.	3.0	20
49	Synthesis and extensive characterisation of phosphorus doped graphite. RSC Advances, 2016, 6, 62140-62145.	3.6	4
50	Combining the Complete Active Space Self-Consistent Field Method and the Full Configuration Interaction Quantum Monte Carlo within a Super-CI Framework, with Application to Challenging Metal-Porphyrins. Journal of Chemical Theory and Computation, 2016, 12, 1245-1258.	5.3	156
51	Multireference linearized coupled cluster theory for strongly correlated systems using matrix product states. Journal of Chemical Physics, 2015, 143, 102815.	3.0	67
52	An excited-state approach within full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 134117.	3.0	77
53	Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces. Journal of Chemical Physics, 2015, 143, 102601.	3.0	10
54	Insights into the structure of many-electron wave functions of Mott-insulating antiferromagnets: The three-band Hubbard model in full configuration interaction quantum Monte Carlo. Physical Review B, 2015, 91, .	3.2	14

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55	AccurateAbÂInitioCalculation of Ionization Potentials of the First-Row Transition Metals with the Configuration-Interaction Quantum MonteÂCarlo Technique. Physical Review Letters, 2015, 114, 033001.	7.8	42
56	Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application. Journal of Chemical Physics, 2015, 142, 184107.	3.0	83
57	Krylov-Projected Quantum MonteÂCarlo Method. Physical Review Letters, 2015, 115, 050603.	7.8	53
58	Stochastic Multiconfigurational Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2015, 11, 5316-5325.	5.3	86
59	Analytic nuclear forces and molecular properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 054108.	3.0	24
60	Unbiased reduced density matrices and electronic properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2014, 141, 244117.	3.0	90
61	Linear-scaling and parallelisable algorithms for stochastic quantum chemistry. Molecular Physics, 2014, 112, 1855-1869.	1.7	92
62	Explicitly correlated plane waves: Accelerating convergence in periodic wavefunction expansions. Journal of Chemical Physics, 2013, 139, 084112.	3.0	62
63	Towards an exact description of electronic wavefunctions in real solids. Nature, 2013, 493, 365-370.	27.8	440
64	Full configuration interaction perspective on the homogeneous electron gas. Physical Review B, 2012, 85, .	3.2	99
65	An explicitly correlated approach to basis set incompleteness in full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2012, 137, 164112.	3.0	49
66	Investigation of the full configuration interaction quantum Monte Carlo method using homogeneous electron gas models. Journal of Chemical Physics, 2012, 136, 244101.	3.0	86
67	Taming the First-Row Diatomics: A Full Configuration Interaction Quantum Monte Carlo Study. Journal of Chemical Theory and Computation, 2012, 8, 4138-4152.	5.3	77
68	Full Configuration Interaction Excitations of Ethene and Butadiene: Resolution of an Ancient Question. Journal of Chemical Theory and Computation, 2012, 8, 4441-4451.	5.3	57
69	Convergence of many-body wave-function expansions using a plane-wave basis: From homogeneous electron gas to solid state systems. Physical Review B, 2012, 86, .	3.2	101
70	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. Journal of Chemical Theory and Computation, 2011, 7, 2780-2785.	5.3	117
71	Breaking the carbon dimer: The challenges of multiple bond dissociation with full configuration interaction quantum Monte Carlo methods. Journal of Chemical Physics, 2011, 135, 084104.	3.0	134
72	A study of electron affinities using the initiator approach to full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2011, 134, 024112.	3.0	89

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73	Approaching chemical accuracy using full configuration-interaction quantum Monte Carlo: A study of ionization potentials. Journal of Chemical Physics, 2010, 132, 174104.	3.0	110
74	Dynamics of quantum tunneling: Effects on the rate and transition path of OH on Cu(110). Physical Review B, 2010, 81, .	3.2	14
75	Communications: Survival of the fittest: Accelerating convergence in full configuration-interaction quantum Monte Carlo. Journal of Chemical Physics, 2010, 132, 041103.	3.0	308
76	Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in Slater determinant space. Journal of Chemical Physics, 2009, 131, 054106.	3.0	567
77	Ammonium cyanate: a DFT study of crystal structure, rotational barriers and vibrational spectrum. Molecular Physics, 2004, 102, 869-876.	1.7	5
78	Entropy of H2O Wetting Layersâ€. Journal of Physical Chemistry B, 2004, 108, 14362-14367.	2.6	24
79	Reconstruction of charged surfaces: General trends and a case study of Pt(110) and Au(110). Physical Review B, 2003, 68, .	3.2	125
80	Where do the H atoms reside in PdHxsystems?. Molecular Physics, 2003, 101, 1781-1787.	1.7	71
81	Two interacting electrons in a spherical box:â€, An exact diagonalization study. Physical Review B, 2002, 66, .	3.2	36
82	The use of XANES and ELNES for the Characterisation of Stabilised Zirconia. Materials Research Society Symposia Proceedings, 2001, 699, 821.	0.1	1
83	Mechanism for the high reactivity of CO oxidation on a rutheniumâ€“oxide. Journal of Chemical Physics, 2001, 114, 5956-5957.	3.0	51
84	Two interacting electrons in a box: An exact diagonalization study. Journal of Chemical Physics, 2000, 113, 7735-7745.	3.0	39
85	Ab InitioMolecular Dynamics with Excited Electrons. Physical Review Letters, 1994, 73, 2599-2602.	7.8	227
86	Charge-transfer molecular dynamics. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1992, 65, 489-500.	0.6	45
87	Molecular-dynamics simulation of argon physisorbed on magnesium oxide. Molecular Physics, 1990, 69, 703-713.	1.7	18
88	Molecular-dynamics simulation of methane adsorbed on MgO: Evidence for a Kosterlitz-Thouless transition. Molecular Physics, 1990, 71, 1173-1191.	1.7	27