Ali Alavi

List of Publications by Year in Descending Order

85 papers	4,437 citations	35 h-index	66 g-index
90 ext. papers	5,135 ext. citations	4.9 avg, IF	6.03 L-index

#	Paper	IF	Citations
85	Full configuration interaction quantum Monte Carlo treatment of fragments embedded in a periodic mean field.. *Journal of Chemical Physics*, **2022**, 156, 154107	3.9	1
84	General embedded cluster protocol for accurate modeling of oxygen vacancies in metal-oxides.. *Journal of Chemical Physics*, **2022**, 156, 124704	3.9	0
83	Enhancement of superexchange due to synergetic breathing and hopping in corner-sharing cuprates. *Nature Physics*, **2022**, 18, 190-195	16.2	1
82	Benchmark study of Nagaoka ferromagnetism by spin-adapted full configuration interaction quantum Monte Carlo. *Physical Review B*, **2021**, 104,	3.3	2
81	Transcorrelated coupled cluster methods. *Journal of Chemical Physics*, **2021**, 155, 191101	3.9	3
80	Population control bias and importance sampling in full configuration interaction quantum Monte Carlo. *Physical Review B*, **2021**, 103,	3.3	6
79	A full configuration interaction quantum Monte Carlo study of ScO, TiO, and VO molecules. *Journal of Chemical Physics*, **2021**, 154, 164302	3.9	3
78	Resolution of Low-Energy States in Spin-Exchange Transition-Metal Clusters: Case Study of Singlet States in [Fe(III)S] Cubanes. *Journal of Physical Chemistry A*, **2021**, 125, 4727-4740	2.8	10
77	Signatures of the BCS-BEC crossover in the yrast spectra of Fermi quantum rings. *Physical Review Research*, **2021**, 3,	3.9	2
76	Towards efficient and accurate ab initio solutions to periodic systems via transcorrelation and coupled cluster theory. *Physical Review Research*, **2021**, 3,	3.9	3
75	Chemical insights into the electronic structure of Fe(II) porphyrin using FCIQMC, DMRG, and generalized active spaces. *International Journal of Quantum Chemistry*, **2021**, 121, e26454	2.1	11
74	Binding curve of the beryllium dimer using similarity-transformed FCIQMC: Spectroscopic accuracy with triple-zeta basis sets. *Journal of Chemical Physics*, **2021**, 155, 011102	3.9	4
73	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Iron-Sulfur Clusters. *Journal of Chemical Theory and Computation*, **2021**, 17, 5684-5703	6.4	9
72	Small polarons and the Janus nature of TiO2(110). *Physical Review B*, **2020**, 101,	3.3	7
71	Compression of Spin-Adapted Multiconfigurational Wave Functions in Exchange-Coupled Polynuclear Spin Systems. *Journal of Chemical Theory and Computation*, **2020**, 16, 2202-2215	6.4	16
70	Electronic correlations and magnetic interactions in infinite-layer NdNiO2. *Physical Review B*, **2020**, 102,	3.3	19
69	Eliminating the wave-function singularity for ultracold atoms by a similarity transformation. *Physical Review Research*, **2020**, 2,	3.9	4

68	The adaptive shift method in full configuration interaction quantum Monte Carlo: Development and applications. *Journal of Chemical Physics*, **2020**, 153, 224115	3.9	15
67	The Ground State Electronic Energy of Benzene. *Journal of Physical Chemistry Letters*, **2020**, 11, 8922-8929	6.4	52
66	The color center singlet state of oxygen vacancies in TiO. *Journal of Chemical Physics*, **2020**, 153, 204704	3.9	7
65	FCIQMC-Tailored Distinguishable Cluster Approach. *Journal of Chemical Theory and Computation*, **2020**, 16, 5621-5634	6.4	14
64	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. *Journal of Chemical Physics*, **2020**, 153, 034107	3.9	28
63	Similarity transformation of the electronic Schrödinger equation via Jastrow factorization. *Journal of Chemical Physics*, **2019**, 151, 061101	3.9	22
62	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	6.4	310
61	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	3.9	30
60	Role of Valence and Semicore Electron Correlation on Spin Gaps in Fe(II)-Porphyrins. *Journal of Chemical Theory and Computation*, **2019**, 15, 1492-1497	6.4	32
59	Are smooth pseudopotentials a good choice for representing short-range interactions?. *Physical Review A*, **2019**, 99,	2.6	2
58	Compact numerical solutions to the two-dimensional repulsive Hubbard model obtained via nonunitary similarity transformations. *Physical Review B*, **2019**, 99,	3.3	25
57	A comparative study using state-of-the-art electronic structure theories on solid hydrogen phases under high pressures. *Npj Computational Materials*, **2019**, 5,	10.9	10
56	Unbiasing the initiator approximation in full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2019**, 151, 224108	3.9	38
55	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	6.4	30
54	Understanding the Mechanism Stabilizing Intermediate Spin States in Fe(II)-Porphyrin. *Journal of Physical Chemistry A*, **2018**, 122, 4935-4947	2.8	53
53	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	6.4	24
52	Time Propagation and Spectroscopy of Fermionic Systems Using a Stochastic Technique. *Physical Review Letters*, **2018**, 121, 056401	7.4	10
51	Accelerating the convergence of exact diagonalization with the transcorrelated method: Quantum gas in one dimension with contact interactions. *Physical Review A*, **2018**, 98,	2.6	8

50	Correlation energies of the high-density spin-polarized electron gas to meV accuracy. *Physical Review B*, **2018**, 98,	3.3	13
49	Nonlinear biases, stochastically sampled effective Hamiltonians, and spectral functions in quantum Monte Carlo methods. *Physical Review B*, **2018**, 98,	3.3	10
48	Combining Internally Contracted States and Matrix Product States To Perform Multireference Perturbation Theory. *Journal of Chemical Theory and Computation*, **2017**, 13, 488-498	6.4	46
47	Stochastic multi-reference perturbation theory with application to the linearized coupled cluster method. *Journal of Chemical Physics*, **2017**, 146, 044107	3.9	31
46	Semistochastic Heat-Bath Configuration Interaction Method: Selected Configuration Interaction with Semistochastic Perturbation Theory. *Journal of Chemical Theory and Computation*, **2017**, 13, 1595-1604	6.4	178
45	Density matrices in full configuration interaction quantum Monte Carlo: Excited states, transition dipole moments, and parallel distribution. *Journal of Chemical Physics*, **2017**, 146, 244105	3.9	34
44	Projector Quantum Monte Carlo Method for Nonlinear Wave Functions. *Physical Review Letters*, **2017**, 118, 176403	7.4	19
43	Synthesis and extensive characterisation of phosphorus doped graphite. *RSC Advances*, **2016**, 6, 62140-62145	3.7	4
42	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, 1245-58	6.4	134
41	Assessment of multireference approaches to explicitly correlated full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2016**, 145, 054117	3.9	14
40	Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application. *Journal of Chemical Physics*, **2015**, 142, 184107	3.9	71
39	Krylov-Projected Quantum Monte Carlo Method. *Physical Review Letters*, **2015**, 115, 050603	7.4	44
38	Stochastic Multiconfigurational Self-Consistent Field Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 5316-25	6.4	78
37	Analytic nuclear forces and molecular properties from full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2015**, 143, 054108	3.9	18
36	Multireference linearized coupled cluster theory for strongly correlated systems using matrix product states. *Journal of Chemical Physics*, **2015**, 143, 102815	3.9	60
35	An excited-state approach within full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2015**, 143, 134117	3.9	60
34	Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces. *Journal of Chemical Physics*, **2015**, 143, 102601	3.9	10
33	Theory and Practice: Bulk Synthesis of C3B and its H2- and Li-Storage Capacity. *Angewandte Chemie*, **2015**, 127, 6017-6021	3.6	2

32	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,	3.3	13
31	Accurate Ab initio calculation of ionization potentials of the first-row transition metals with the configuration-interaction quantum Monte Carlo technique. *Physical Review Letters*, **2015**, 114, 033001	7.4	37
30	Unbiased reduced density matrices and electronic properties from full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2014**, 141, 244117	3.9	74
29	Linear-scaling and parallelisable algorithms for stochastic quantum chemistry. *Molecular Physics*, **2014**, 112, 1855-1869	1.7	82
28	Explicitly correlated plane waves: accelerating convergence in periodic wavefunction expansions. *Journal of Chemical Physics*, **2013**, 139, 084112	3.9	55
27	Towards an exact description of electronic wavefunctions in real solids. *Nature*, **2013**, 493, 365-70	50.4	375
26	Taming the First-Row Diatomics: A Full Configuration Interaction Quantum Monte Carlo Study. *Journal of Chemical Theory and Computation*, **2012**, 8, 4138-52	6.4	68
25	Full Configuration Interaction Excitations of Ethene and Butadiene: Resolution of an Ancient Question. *Journal of Chemical Theory and Computation*, **2012**, 8, 4441-51	6.4	56
24	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,	3.3	87
23	Full configuration interaction perspective on the homogeneous electron gas. *Physical Review B*, **2012**, 85,	3.3	86
22	An explicitly correlated approach to basis set incompleteness in full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2012**, 137, 164112	3.9	44
21	Investigation of the full configuration interaction quantum Monte Carlo method using homogeneous electron gas models. *Journal of Chemical Physics*, **2012**, 136, 244101	3.9	73
20	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. *Journal of Chemical Theory and Computation*, **2011**, 7, 2780-5	6.4	95
19	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	3.9	120
18	A study of electron affinities using the initiator approach to full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2011**, 134, 024112	3.9	75
17	Approaching chemical accuracy using full configuration-interaction quantum Monte Carlo: a study of ionization potentials. *Journal of Chemical Physics*, **2010**, 132, 174104	3.9	98
16	Dynamics of quantum tunneling: Effects on the rate and transition path of OH on Cu(110). *Physical Review B*, **2010**, 81,	3.3	12
15	Communications: Survival of the fittest: accelerating convergence in full configuration-interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2010**, 132, 041103	3.9	256

14	Fermion Monte Carlo without fixed nodes: a game of life, death, and annihilation in Slater determinant space. *Journal of Chemical Physics*, **2009**, 131, 054106	3.9	469
13	Dipole Amplification: A Principle for the Self-Assembly of Asymmetric Monomers on Metal Surfaces. *Angewandte Chemie*, **2008**, 120, 2456-2460	3.6	3
12	Ammonium cyanate: a DFT study of crystal structure, rotational barriers and vibrational spectrum. *Molecular Physics*, **2004**, 102, 869-876	1.7	5
11	Entropy of H2O Wetting Layers *Journal of Physical Chemistry B*, **2004**, 108, 14362-14367	3.4	24
10	Where do the H atoms reside in PdH x systems?. *Molecular Physics*, **2003**, 101, 1781-1787	1.7	63
9	Reconstruction of charged surfaces: General trends and a case study of Pt(110) and Au(110). *Physical Review B*, **2003**, 68,	3.3	113
8	Two interacting electrons in a spherical box: An exact diagonalization study. *Physical Review B*, **2002**, 66,	3.3	32
7	Mechanism for the high reactivity of CO oxidation on a ruthenium oxide. *Journal of Chemical Physics*, **2001**, 114, 5956-5957	3.9	47
6	The use of XANES and ELNES for the Characterisation of Stabilised Zirconia. *Materials Research Society Symposia Proceedings*, **2001**, 699, 821		1
5	Two interacting electrons in a box: An exact diagonalization study. *Journal of Chemical Physics*, **2000**, 113, 7735-7745	3.9	35
4	Ab initio molecular dynamics with excited electrons. *Physical Review Letters*, **1994**, 73, 2599-2602	7.4	213
3	Charge-transfer molecular dynamics. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1992**, 65, 489-500		43
2	Molecular-dynamics simulation of argon physisorbed on magnesium oxide. *Molecular Physics*, **1990**, 69, 703-713	1.7	16
1	Molecular-dynamics simulation of methane adsorbed on MgO: Evidence for a Kosterlitz-Thouless transition. *Molecular Physics*, **1990**, 71, 1173-1191	1.7	26