Lubos Mitas

List of Publications by Year in descending order

62 papers	3,973 citations	136740 32 h-index	123241 61 g-index
62 all docs	62 docs citations	62 times ranked	2653 citing authors

#	Article	IF	Citations
1	A quantum Monte Carlo study of systems with effective core potentials and node nonlinearities. Chemical Physics, 2022, 554, 111402.	0.9	2
2	High Accuracy Transition Metal Effective Cores for the Many-Body Diffusion Monte Carlo Method. Journal of Chemical Theory and Computation, 2022, 18, 828-839.	2.3	2
3	Weighted nodal domain averages of eigenstates for quantum Monte Carlo and beyond. Chemical Physics, 2022, 557, 111483.	0.9	3
4	Assessing the accuracy of compound formation energies with quantum Monte Carlo. Physical Review B, 2022, 105, .	1.1	2
5	Cohesion and excitations of diamond-structure silicon by quantum Monte Carlo: Benchmarks and control of systematic biases. Physical Review B, 2021, 103, .	1.1	12
6	Fundamental gap of fluorographene by many-body GW and fixed-node diffusion Monte Carlo methods. Journal of Chemical Physics, 2020, 153, 184706.	1.2	17
7	Binding and excitations in SixHy molecular systems using quantum Monte Carlo. Journal of Chemical Physics, 2020, 153, 144303.	1.2	8
8	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.	1.2	80
9	Many-body electronic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaScO</mml:mi><mml:mn>3</mml:mn></mml:msub><[illegible] by real-space quantum Monte Carlo. Physical Review B, 2020, 102, .	1.0	
10	Accurate Atomic Correlation and Total Energies for Correlation Consistent Effective Core Potentials. Journal of Chemical Theory and Computation, 2020, 16, 1482-1502.	2.3	14
11	A new generation of effective core potentials from correlated calculations: 4s and 4p main group elements and first row additions. Journal of Chemical Physics, 2019, 151, 144110.	1.2	32
12	Toward Accurate Hydrogen Bonds by Scalable Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 3552-3557.	2.3	12
13	A new generation of effective core potentials from correlated calculations: 2nd row elements. Journal of Chemical Physics, 2018, 149, 104108.	1.2	42
14	A new generation of effective core potentials from correlated calculations: 3d transition metal series. Journal of Chemical Physics, 2018, 149, 134108.	1.2	54
15	<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.	0.7	187
16	Quantum Monte Carlo with variable spins: Fixed-phase and fixed-node approximations. Physical Review E, 2017, 96, 043305.	0.8	7
17	A new generation of effective core potentials for correlated calculations. Journal of Chemical Physics, 2017, 147, 224106.	1.2	72
18	Globalâ€view coefficients: a data management solution for parallel quantum Monte Carlo applications. Concurrency Computation Practice and Experience, 2016, 28, 3655-3671.	1.4	3

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19	Noncovalent Interactions by Quantum Monte Carlo. Chemical Reviews, 2016, 116, 5188-5215.	23.0	114
20	Spin-orbit interactions in electronic structure quantum Monte Carlo methods. Physical Review A, 2016, 93, .	1.0	25
21	Quantum Monte Carlo with variable spins. Journal of Chemical Physics, 2016, 144, 244113.	1.2	17
22	Repulsive atomic Fermi gas with Rashba spin-orbit coupling: A quantum Monte Carlo study. Physical Review A, 2015, 91, .	1.0	7
23	Communication: Fixed-node errors in quantum Monte Carlo: Interplay of electron density and node nonlinearities. Journal of Chemical Physics, 2014, 140, 041102.	1.2	30
24	Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy. Physical Chemistry Chemical Physics, 2014, 16, 20915-20923.	1.3	46
25	Density dependence of fixed-node errors in diffusion quantum Monte Carlo: Triplet pair correlations. Chemical Physics Letters, 2014, 591, 170-174.	1.2	13
26	Study of dipole moments of LiSr and KRb molecules by quantum Monte Carlo methods. Molecular Physics, 2013, 111, 1744-1752.	0.8	8
27	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. Journal of Chemical Theory and Computation, 2013, 9, 4287-4292.	2.3	88
28	A global address space approach to automated data management for parallel Quantum Monte Carlo applications. , 2012, , .		4
29	Many-Body Nodal Hypersurface and Domain Averages for Correlated Wave Functions. ACS Symposium Series, 2012, , 77-87.	0.5	2
30	Applications of quantum Monte Carlo methods in condensed systems. Reports on Progress in Physics, 2011, 74, 026502.	8.1	169
31	Atomic Fermi gas in the unitary limit by quantum Monte Carlo methods: Effects of the interaction range. Physical Review A, 2011, 84, .	1.0	17
32	Precision benchmark calculations for four particles at unitarity. Physical Review A, 2011, 83, .	1.0	18
33	Wave functions for quantum Monte Carlo calculations in solids: Orbitals from density functional theory with hybrid exchange-correlation functionals. Physical Review B, 2010, 82, .	1.1	58
34	QWalk: A quantum Monte Carlo program for electronic structure. Journal of Computational Physics, 2009, 228, 3390-3404.	1.9	136
35	Quantum Monte Carlo for atoms, molecules and solids. Chemical Physics Letters, 2009, 478, 1-10.	1.2	60
36	Electronic structure quantum Monte Carlo. Acta Physica Slovaca, 2009, 59, .	1.4	26

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37	Theoretical Study of Electronic and Atomic Structures of (MnO)_{<I>n</I>}. Journal of Computational and Theoretical Nanoscience, 2009, 6, 2583-2588.	0.4	5
38	Quantum Monte Carlo Calculations of Structural Properties of FeO Under Pressure. Physical Review Letters, 2008, 101, 185502.	2.9	62
39	Real-time landscape model interaction using a tangible geospatial modeling environment. IEEE Computer Graphics and Applications, 2006, 26, 55-63.	1.0	30
40	Hartreeâ€“Fock versus quantum Monte Carlo study of persistent current in a one-dimensional ring with single scatterer. Physica E: Low-Dimensional Systems and Nanostructures, 2006, 32, 350-353.	1.3	4
41	Structure of Fermion Nodes and Nodal Cells. Physical Review Letters, 2006, 96, 240402.	2.9	53
42	Path sampling method for modeling overland water flow, sediment transport, and short term terrain evolution in Open Source GIS. Developments in Water Science, 2004, 55, 1479-1490.	0.1	23
43	A quantum Monte Carlo study of electron correlation in transition metal oxygen molecules. Chemical Physics Letters, 2003, 370, 412-417.	1.2	69
44	Quantum monte carlo methods for electronic structure of nanosystems. Israel Journal of Chemistry, 2002, 42, 261-268.	1.0	1
45	Multivariate Interpolation of Precipitation Using Regularized Spline with Tension. Transactions in GIS, 2002, 6, 135-150.	1.0	107
46	High Accuracy Many-Body Calculational Approaches for Excitations in Molecules. Physical Review Letters, 2001, 86, 472-475.	2.9	169
47	Electron Correlation inC4N+2Carbon Rings: Aromatic versus Dimerized Structures. Physical Review Letters, 2000, 85, 1702-1705.	2.9	112
48	Silicon Clusters of Intermediate Size: Energetics, Dynamics, and Thermal Effects. Physical Review Letters, 2000, 84, 1479-1482.	2.9	143
49	Distributed soil erosion simulation for effective erosion prevention. Water Resources Research, 1998, 34, 505-516.	1.7	147
50	High Accuracy Molecular Heats of Formation and Reaction Barriers: Essential Role of Electron Correlation. Physical Review Letters, 1997, 79, 4353-4356.	2.9	51
51	Quantum Monte Carlo. Current Opinion in Solid State and Materials Science, 1997, 2, 696-700.	5.6	5
52	Role of dynamic cartography in simulations of landscape processes based on multivariate fields. Computers and Geosciences, 1997, 23, 437-446.	2.0	45
53	Electronic structure by quantum Monte Carlo: atoms, molecules and solids. Computer Physics Communications, 1996, 96, 107-117.	3.0	45
54	Family of low-energy elongatedSin(nâ‰50) clusters. Physical Review B, 1995, 52, 16735-16738.	1.1	132

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55	Quantum Monte Carlo Determination of Electronic and Structural Properties of SinClusters (nâ‰20). Physical Review Letters, 1995, 74, 1323-1326.	2.9	253
56	Structure and Stability of Molecular Carbon: Importance of Electron Correlation. Physical Review Letters, 1995, 75, 3870-3873.	2.9	216
57	Modelling spatially and temporally distributed phenomena: new methods and tools for GRASS GIS. International Journal of Geographical Information Science, 1995, 9, 433-446.	2.2	100
58	Quantum Monte Carlo calculation of the Fe atom. Physical Review A, 1994, 49, 4411-4414.	1.0	51
59	Quantum Monte Carlo of nitrogen: Atom, dimer, atomic, and molecular solids. Physical Review Letters, 1994, 72, 2438-2441.	2.9	129
60	Interpolation by regularized spline with tension: I. Theory and implementation. Mathematical Geosciences, 1993, 25, 641-655.	0.9	333
61	Nonlocal pseudopotentials and diffusion Monte Carlo. Journal of Chemical Physics, 1991, 95, 3467-3475.	1.2	267
62	Core-valence partitioning and quasiparticle pseudopotentials. Physical Review B, 1991, 44, 3395-3398.	1.1	24