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	Interpolation by regularized spline with tension: I. Theory and implementation. Mathematical Geosciences, 1993, 25, 641-655.	0.9	333
2	Nonlocal pseudopotentials and diffusion Monte Carlo. Journal of Chemical Physics, 1991, 95, 3467-3475.	1.2	267
3	Quantum Monte Carlo Determination of Electronic and Structural Properties of SinClusters (nâ‰20). Physical Review Letters, 1995, 74, 1323-1326.	2.9	253
4	Structure and Stability of Molecular Carbon: Importance of Electron Correlation. Physical Review Letters, 1995, 75, 3870-3873.	2.9	216
5	<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
6	High Accuracy Many-Body Calculational Approaches for Excitations in Molecules. Physical Review Letters, 2001, 86, 472-475.	2.9	169
7	Applications of quantum Monte Carlo methods in condensed systems. Reports on Progress in Physics, 2011, 74, 026502.	8.1	169
8	Distributed soil erosion simulation for effective erosion prevention. Water Resources Research, 1998, 34, 505-516.	1.7	147
9	Silicon Clusters of Intermediate Size: Energetics, Dynamics, and Thermal Effects. Physical Review Letters, 2000, 84, 1479-1482.	2.9	143
10	QWalk: A quantum Monte Carlo program for electronic structure. Journal of Computational Physics, 2009, 228, 3390-3404.	1.9	136
11	Family of low-energy elongatedSin(nâ‰50) clusters. Physical Review B, 1995, 52, 16735-16738.	1.1	132
12	Quantum Monte Carlo of nitrogen: Atom, dimer, atomic, and molecular solids. Physical Review Letters, 1994, 72, 2438-2441.	2.9	129
13	Noncovalent Interactions by Quantum Monte Carlo. Chemical Reviews, 2016, 116, 5188-5215.	23.0	114
14	Electron Correlation inC4N+2Carbon Rings: Aromatic versus Dimerized Structures. Physical Review Letters, 2000, 85, 1702-1705.	2.9	112
15	Multivariate Interpolation of Precipitation Using Regularized Spline with Tension. Transactions in GIS, 2002, 6, 135-150.	1.0	107
16	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
17	Quantum Monte Carlo Methods Describe Noncovalent Interactions with Subchemical Accuracy. Journal of Chemical Theory and Computation, 2013, 9, 4287-4292.	2.3	88
18	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

#	Article	IF	Citations
19	A new generation of effective core potentials for correlated calculations. Journal of Chemical Physics, 2017, 147, 224106.	1.2	72
20	A quantum Monte Carlo study of electron correlation in transition metal oxygen molecules. Chemical Physics Letters, 2003, 370, 412-417.	1.2	69
21	Quantum Monte Carlo Calculations of Structural Properties of FeO Under Pressure. Physical Review Letters, 2008, 101, 185502.	2.9	62
22	Quantum Monte Carlo for atoms, molecules and solids. Chemical Physics Letters, 2009, 478, 1-10.	1.2	60
23	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
24	A new generation of effective core potentials from correlated calculations: 3d transition metal series. Journal of Chemical Physics, 2018, 149, 134108.	1.2	54
25	Structure of Fermion Nodes and Nodal Cells. Physical Review Letters, 2006, 96, 240402.	2.9	53
26	Quantum Monte Carlo calculation of the Fe atom. Physical Review A, 1994, 49, 4411-4414.	1.0	51
27	High Accuracy Molecular Heats of Formation and Reaction Barriers: Essential Role of Electron Correlation. Physical Review Letters, 1997, 79, 4353-4356.	2.9	51
28	Quantum Monte Carlo for noncovalent interactions: an efficient protocol attaining benchmark accuracy. Physical Chemistry Chemical Physics, 2014, 16, 20915-20923.	1.3	46
29	Electronic structure by quantum Monte Carlo: atoms, molecules and solids. Computer Physics Communications, 1996, 96, 107-117.	3.0	45
30	Role of dynamic cartography in simulations of landscape processes based on multivariate fields. Computers and Geosciences, 1997, 23, 437-446.	2.0	45
31	A new generation of effective core potentials from correlated calculations: 2nd row elements. Journal of Chemical Physics, 2018, 149, 104108.	1.2	42
32	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
33	Real-time landscape model interaction using a tangible geospatial modeling environment. IEEE Computer Graphics and Applications, 2006, 26, 55-63.	1.0	30
34	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
35	Electronic structure quantum Monte Carlo. Acta Physica Slovaca, 2009, 59, .	1.4	26
36	Spin-orbit interactions in electronic structure quantum Monte Carlo methods. Physical Review A, 2016, 93, .	1.0	25

#	Article	IF	Citations
37	Core-valence partitioning and quasiparticle pseudopotentials. Physical Review B, 1991, 44, 3395-3398.	1.1	24
38	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
39	Precision benchmark calculations for four particles at unitarity. Physical Review A, 2011, 83, .	1.0	18
40	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
41	Quantum Monte Carlo with variable spins. Journal of Chemical Physics, 2016, 144, 244113.	1.2	17
42	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
43	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
44	Density dependence of fixed-node errors in diffusion quantum Monte Carlo: Triplet pair correlations. Chemical Physics Letters, 2014, 591, 170-174.	1.2	13
45	Toward Accurate Hydrogen Bonds by Scalable Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 3552-3557.	2.3	12
46	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
47	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><m by real-space quantum Monte Carlo. Physical Review B, 2020, 102, .	1.1	10
48	Study of dipole moments of LiSr and KRb molecules by quantum Monte Carlo methods. Molecular Physics, 2013, 111, 1744-1752.	0.8	8
49	Binding and excitations in SixHy molecular systems using quantum Monte Carlo. Journal of Chemical Physics, 2020, 153, 144303.	1.2	8
50	Repulsive atomic Fermi gas with Rashba spin-orbit coupling: A quantum Monte Carlo study. Physical Review A, 2015, 91, .	1.0	7
51	Quantum Monte Carlo with variable spins: Fixed-phase and fixed-node approximations. Physical Review E, 2017, 96, 043305.	0.8	7
52	Quantum Monte Carlo. Current Opinion in Solid State and Materials Science, 1997, 2, 696-700.	5.6	5
53	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
54	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

#	Article	IF	Citations
55	A global address space approach to automated data management for parallel Quantum Monte Carlo applications. , 2012, , .		4
56	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
57	Weighted nodal domain averages of eigenstates for quantum Monte Carlo and beyond. Chemical Physics, 2022, 557, 111483.	0.9	3
58	Many-Body Nodal Hypersurface and Domain Averages for Correlated Wave Functions. ACS Symposium Series, 2012, , 77-87.	0.5	2
59	A quantum Monte Carlo study of systems with effective core potentials and node nonlinearities. Chemical Physics, 2022, 554, 111402.	0.9	2
60	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
61	Assessing the accuracy of compound formation energies with quantum Monte Carlo. Physical Review B, 2022, 105, .	1.1	2
62	Quantum monte carlo methods for electronic structure of nanosystems. Israel Journal of Chemistry, 2002, 42, 261-268.	1.0	1