Sabre Kais

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7455862/publications.pdf

Version: 2024-02-01

243	6,191	76196	106150
papers	citations	40 h-index	65 g-index

256	256	256	5570
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Revealing the role of organic cations in hybrid halide perovskite CH3NH3PbI3. Nature Communications, 2015, 6, 7026.	5.8	564
2	Manipulation of molecules with electromagnetic fields. Molecular Physics, 2013, 111, 1648-1682.	0.8	235
3	Theoretical limits of photovoltaics efficiency and possible improvements by intuitive approaches learned from photosynthesis and quantum coherence. Renewable and Sustainable Energy Reviews, 2015, 43, 1073-1089.	8.2	153
4	Qudits and High-Dimensional Quantum Computing. Frontiers in Physics, 2020, 8, .	1.0	149
5	Modified Scaled Hierarchical Equation of Motion Approach for the Study of Quantum Coherence in Photosynthetic Complexes. Journal of Physical Chemistry B, 2011, 115, 1531-1537.	1.2	120
6	Hydrogen Bonding and Stability of Hybrid Organicâ€“Inorganic Perovskites. ChemSusChem, 2016, 9, 2648-2655.	3.6	109
7	Quantum algorithm and circuit design solving the Poisson equation. New Journal of Physics, 2013, 15, 013021.	1.2	102
8	Entanglement as measure of electronâ€“electron correlation in quantum chemistry calculations. Chemical Physics Letters, 2005, 413, 1-5.	1.2	99
9	Quantum machine learning for electronic structure calculations. Nature Communications, 2018, 9, 4195.	5.8	99
10	Quantum Annealing for Prime Factorization. Scientific Reports, 2018, 8, 17667.	1.6	98
11	Cation Effect on Hot Carrier Cooling in Halide Perovskite Materials. Journal of Physical Chemistry Letters, 2017, 8, 4439-4445.	2.1	97
12	Quantum algorithm for obtaining the energy spectrum of molecular systems. Physical Chemistry Chemical Physics, 2008, 10, 5388.	1.3	95
13	Experimental realization of quantum algorithm for solving linear systems of equations. Physical Review A, 2014, 89, .	1.0	82
14	A quantum algorithm for evolving open quantum dynamics on quantum computing devices. Scientific Reports, 2020, 10, 3301.	1.6	73
15	Electronic Structure Calculations and the Ising Hamiltonian. Journal of Physical Chemistry B, 2018, 122, 3384-3395.	1.2	68
16	Entropic uncertainty relations for Markovian and non-Markovian processes under a structured bosonic reservoir. Scientific Reports, 2017, 7, 1066.	1.6	67
17	Prospects for quantum computing with an array of ultracold polar paramagnetic molecules. Journal of Chemical Physics, 2016, 144, 094301.	1.2	62
18	Coherent states for the Morse oscillator. Physical Review A, 1990, 41, 2301-2305.	1.0	61

#	Article	IF	Citations
19	Enhancing the carrier thermalization time in organometallic perovskites by halide mixing. Physical Chemistry Chemical Physics, 2016, 18, 5219-5231.	1.3	61
20	Implementation of quantum logic gates using polar molecules in pendular states. Journal of Chemical Physics, 2013, 138, 024104.	1.2	60
21	Tuning the entanglement for a one-dimensional magnetic system with anisotropic coupling and impurities. Physical Review A, 2003, 67, .	1.0	58
22	Entanglement of polar symmetric top molecules as candidate qubits. Journal of Chemical Physics, 2011, 135, 154102.	1.2	55
23	Entanglement of polar molecules in pendular states. Journal of Chemical Physics, 2011, 134, 124107.	1.2	53
24	Quantum coherence and entanglement in the avian compass. Physical Review E, 2013, 87, 062704.	0.8	52
25	Dimensional interpolation of hard sphere virial coefficients. Journal of Chemical Physics, 1991, 95, 4525-4544.	1.2	51
26	Finite size scaling for the atomic Shannon-information entropy. Journal of Chemical Physics, 2004, 121, 5611-5617.	1.2	49
27	Delocalized quantum states enhance photocell efficiency. Physical Chemistry Chemical Physics, 2015, 17, 5743-5750.	1.3	49
28	Electronic Structure Critical Parameters From Finite-Size Scaling. Physical Review Letters, 1997, 79, 3142-3145.	2.9	48
29	Entanglement and electron correlation in quantum chemistry calculations. Journal of Modern Optics, 2006, 53, 2543-2558.	0.6	48
30	Effects of Hawking Radiation on the Entropic Uncertainty in a Schwarzschild Spaceâ€Time. Annalen Der Physik, 2018, 530, 1800080.	0.9	48
31	Quantum criticality and stability of three-body Coulomb systems. Physical Review A, 2000, 62, .	1.0	46
32	Decomposition of unitary matrices for finding quantum circuits: Application to molecular Hamiltonians. Journal of Chemical Physics, 2011, 134, 144112.	1.2	45
33	Correlated Protein Environments Drive Quantum Coherence Lifetimes in Photosynthetic Pigment-Protein Complexes. CheM, 2018, 4, 138-149.	5.8	45
34	Qubit coupled cluster singles and doubles variational quantum eigensolver ansatz for electronic structure calculations. Quantum Science and Technology, 2021, 6, 015001.	2.6	45
35	Study of phase changes of the water octamer using parallel tempering and multihistogram methods. Journal of Chemical Physics, 2001, 115, 2621-2628.	1.2	44
36	Finite-Size Scaling for Atomic and Molecular Systems. Advances in Chemical Physics, 2003, , 1-99.	0.3	44

#	Article	IF	Citations
37	Discontinuity of Shannon information entropy for two-electron atoms. Chemical Physics, 2005, 309, 127-131.	0.9	44
38	Infrared-dressed entanglement of cold open-shell polar molecules for universal matchgate quantum computing. New Journal of Physics, 2014, 16, 075001.	1.2	44
39	Critical Phenomena for Electronic Structure at the Large-Dimension Limit. Physical Review Letters, 1996, 77, 466-469.	2.9	42
40	Comparison study of pivot methods for global optimization. Journal of Chemical Physics, 1997, 106, 7170-7177.	1.2	42
41	Multipartite quantum entanglement evolution in photosynthetic complexes. Journal of Chemical Physics, 2012, 137, 074112.	1.2	42
42	Enhancing Intrinsic Stability of Hybrid Perovskite Solar Cell by Strong, yet Balanced, Electronic Coupling. Scientific Reports, 2016, 6, 30305.	1.6	42
43	Large-Z and -N dependence of atomic energies from renormalization of the large-dimension limit. International Journal of Quantum Chemistry, 1994, 49, 657-674.	1.0	41
44	Domain Walls Conductivity in Hybrid Organometallic Perovskites and Their Essential Role in CH3NH3PbI3 Solar Cell High Performance. Scientific Reports, 2015, 5, 11467.	1.6	41
45	Degree Distribution in Quantum Walks on Complex Networks. Physical Review X, 2013, 3, .	2.8	40
46	Electronic Structure Critical Parameters For the Lithium Isoelectronic Series. Physical Review Letters, 1998, 80, 5293-5296.	2.9	39
47	Entanglement evolution of one-dimensional spin systems in external magnetic fields. Physical Review A, 2006, 73, .	1.0	39
48	An efficient descriptor model for designing materials for solar cells. Npj Computational Materials, 2015, 1, .	3.5	39
49	Quantum critical phenomena and stability of atomic and molecular ions. International Reviews in Physical Chemistry, 2000, 19, 97-121.	0.9	38
50	On the interactions between atmospheric radicals and cloud droplets: A molecular picture of the interface. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 9686-9690.	3.3	38
51	Quantum circuit design for solving linear systems of equations. Molecular Physics, 2012, 110, 1675-1680.	0.8	38
52	Interfaces Select Specific Stereochemical Conformations: The Isomerization of Glyoxal at the Liquid Water Interface. Journal of the American Chemical Society, 2017, 139, 27-30.	6.6	38
53	Large order dimensional perturbation theory for complex energy eigenvalues. Journal of Chemical Physics, 1993, 99, 7739-7747.	1.2	36
54	Pivot method for global optimization: a study of water clusters (H2O)N with 2â©½Nâ©½33. Chemical Physics Letters, 1999, 305, 433-438.	1.2	36

#	Article	IF	Citations
55	Reduced work function of graphene by metal adatoms. Applied Surface Science, 2017, 394, 98-107.	3.1	36
56	Entanglement, Electron Correlation, and Density Matrices. Advances in Chemical Physics, 2007, , 493-535.	0.3	35
57	Finite-size scaling approach for the SchrÃ¶dinger equation. Physical Review A, 1998, 57, R1481-R1484.	1.0	34
58	Group leaders optimization algorithm. Molecular Physics, 2011, 109, 761-772.	0.8	34
59	Hydrogen bonding and orientation effects on the accommodation of methylamine at the air-water interface. Journal of Chemical Physics, 2016, 144, 214701.	1.2	34
60	Elucidation of near-resonance vibronic coherence lifetimes by nonadiabatic electronic-vibrational state character mixing. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18263-18268.	3.3	34
61	Pivot method for global optimization. Physical Review E, 1997, 55, 1162-1165.	0.8	33
62	Critical nuclear charges forN-electron atoms. International Journal of Quantum Chemistry, 1999, 75, 533-542.	1.0	33
63	Quantum computing methods for electronic states of the water molecule. Molecular Physics, 2019, 117, 2069-2082.	0.8	33
64	Hydrogen bonding: a mechanism for tuning electronic and optical properties of hybrid organicâ€“inorganic frameworks. Npj Computational Materials, 2016, 2, .	3.5	32
65	Entanglement of formation for one-dimensional magnetic systems with defects. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 322, 137-145.	0.9	29
66	The radical pair mechanism and the avian chemical compass: Quantum coherence and entanglement. International Journal of Quantum Chemistry, 2015, 115, 1327-1341.	1.0	29
67	The 1/Z expansion and renormalization of the largeâ€dimension limit for manyâ€electron atoms. Journal of Chemical Physics, 1994, 100, 4367-4376.	1.2	28
68	Ground-state stability and criticality of two-electron atoms with screened Coulomb potentials using the B-splines basis set. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 235003.	0.6	28
69	Probing entropic uncertainty relations under a two-atom system coupled with structured bosonic reservoirs. Quantum Information Processing, 2018, 17, 1.	1.0	28
70	Quantum Phase Estimation with Timeâ€Frequency Qudits in a Single Photon. Advanced Quantum Technologies, 2020, 3, 1900074.	1.8	28
71	A general quantum algorithm for open quantum dynamics demonstrated with the Fenna-Matthews-Olson complex. Quantum - the Open Journal for Quantum Science, 0, 6, 726.	0.0	28
72	Sensitivity and entanglement in the avian chemical compass. Physical Review E, 2014, 90, 042707.	0.8	26

#	Article	IF	Citations
73	Entanglement, Berry phases, and level crossings for the atomic Breit-Rabi Hamiltonian. Physical Review A, 2008, 78, .	1.0	25
74	Quantum cusp. Physical Review A, 1986, 34, 2442-2452.	1.0	24
75	Finite-size scaling for critical conditions for stable quadrupole-bound anions. Journal of Chemical Physics, 2004, 120, 8412-8419.	1.2	24
76	Universal programmable quantum circuit schemes to emulate an operator. Journal of Chemical Physics, 2012, 137, 234112.	1.2	24
77	Multicritical phenomena for the hydrogen molecule at the large-dimension limit. Chemical Physics Letters, 1996, 260, 302-308.	1.2	23
78	Critical parameters for the heliumlike atoms: A phenomenological renormalization study. Journal of Chemical Physics, 1998, 108, 2765-2770.	1.2	23
79	Finite size scaling for critical conditions for stable dipole-bound anions. Chemical Physics Letters, 2003, 372, 205-209.	1.2	23
80	Generalized Remote Preparation of Arbitrary m-qubit Entangled States via Genuine Entanglements. Entropy, 2015, 17, 1755-1774.	1.1	23
81	Tuning the Stereoselectivity and Solvation Selectivity at Interfacial and Bulk Environments by Changing Solvent Polarity: Isomerization of Glyoxal in Different Solvent Environments. Journal of the American Chemical Society, 2018, 140, 5535-5543.	6.6	23
82	Crossover phenomena and resonances in quantum systems. Physical Review A, 2001, 64, .	1.0	22
83	Quantum Computation using Arrays of N Polar Molecules in Pendular States. ChemPhysChem, 2016, 17, 3714-3722.	1.0	22
84	Quantum Machine-Learning for Eigenstate Filtration in Two-Dimensional Materials. Journal of the American Chemical Society, 2021, 143, 18426-18445.	6.6	22
85	Phase transitions for N-electron atoms at the large-dimension limit. Physical Review A, 1997, 55, 238-247.	1.0	21
86	Communications: Entanglement switch for dipole arrays. Journal of Chemical Physics, 2010, 132, 121104.	1.2	21
87	Pursuit of the Kramers-Henneberger atom. Chemical Physics Letters, 2017, 683, 240-246.	1.2	21
88	New stable multiply charged negative atomic ions in linearly polarized superintense laser fields. Journal of Chemical Physics, 2006, 124, 201108.	1.2	20
89	Dynamics of entanglement in a two-dimensional spin system. Physical Review A, 2011, 83, .	1.0	20
90	Population and coherence dynamics in light harvesting complex II (LH2). Journal of Chemical Physics, 2012, 137, 084110.	1.2	20

#	Article	IF	Citations
91	Atomic energies from renormalization of the largeâ€dimension limit. Journal of Chemical Physics, 1993, 99, 5184-5196.	1.2	19
92	Study of electronic structure and dynamics of interacting free radicals influenced by water. Journal of Chemical Physics, 2009, 130, 124312.	1.2	19
93	Hamiltonian gadgets with reduced resource requirements. Physical Review A, 2015, 91, .	1.0	19
94	Enhancement of Photovoltaic Current through Dark States in Donorâ€Acceptor Pairs of Tungstenâ€Based Transition Metal Diâ€Chalcogenides. Advanced Functional Materials, 2021, 31, 2100387.	7.8	19
95	Training Restricted Boltzmann Machines With a D-Wave Quantum Annealer. Frontiers in Physics, 2021, 9, .	1.0	19
96	Square-well potential by an algebraic approach. Physical Review A, 1986, 34, 4615-4620.	1.0	18
97	Resonance states of atomic anions. International Journal of Quantum Chemistry, 2001, 82, 255-261.	1.0	18
98	Quantum Entanglement and Electron Correlation in Molecular Systems. Israel Journal of Chemistry, 2007, 47, 59-65.	1.0	18
99	A universal quantum circuit scheme for finding complex eigenvalues. Quantum Information Processing, 2014, 13, 333-353.	1.0	18
100	Dark states and delocalization: Competing effects of quantum coherence on the efficiency of light harvesting systems. Journal of Chemical Physics, 2018, 148, 064304.	1.2	18
101	Training a Quantum Annealing Based Restricted Boltzmann Machine on Cybersecurity Data. IEEE Transactions on Emerging Topics in Computational Intelligence, 2022, 6, 417-428.	3.4	18
102	The Repulsive Coulomb Barrier along a Dissociation Path of the Be Dianion. Journal of the American Chemical Society, 2002, 124, 11723-11729.	6.6	17
103	Quantum teleportation in one-dimensional quantum dots system. Chemical Physics Letters, 2006, 421, 338-342.	1.2	17
104	Efficient Remote Preparation of Four-Qubit Cluster-Type Entangled States with Multi-Party Over Partially Entangled Channels. International Journal of Theoretical Physics, 2016, 55, 3454-3466.	0.5	17
105	Maximal Entropy Approach for Quantum State Tomography. PRX Quantum, 2021, 2, .	3.5	17
106	Implementation of Quantum Machine Learning for Electronic Structure Calculations of Periodic Systems on Quantum Computing Devices. Journal of Chemical Information and Modeling, 2021, 61, 2667-2674.	2.5	17
107	Gas-Phase Reactions of Fe(CH2O)+ and Fe(CH2S)+ with Small Alkanes:â€‰ An Experimental and Theoretical Study. Journal of the American Chemical Society, 1997, 119, 12879-12888.	6.6	16
108	Scaling of entanglement at a quantum phase transition for a two-dimensional array of quantum dots. Physical Review A, 2004, 70, .	1.0	16

#	Article	IF	Citations
109	DYNAMICS OF ENTANGLEMENT FOR ONE-DIMENSIONAL SPIN SYSTEMS IN AN EXTERNAL TIME-DEPENDENT MAGNETIC FIELD. International Journal of Quantum Information, 2005, 03, 483-500.	0.6	16
110	Dimensional scaling treatment of stability of simple diatomic molecules induced by superintense, high-frequency laser fields. Journal of Chemical Physics, 2008, 129, 214110.	1.2	16
111	Exact calculation of entanglement in a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>19</mml:mn></mml:mrow></mml:math>-site two-dimensional spin system. Physical Review A, 2010, 81, .	1.0	16
112	Entanglement dynamics of one-dimensional driven spin systems in time-varying magnetic fields. Physical Review A, 2011, 84, .	1.0	16
113	Neuroreceptor Activation by Vibration-Assisted Tunneling. Scientific Reports, 2015, 5, 9990.	1.6	16
114	Experimental evaluation of the generalized vibrational theory of G protein-coupled receptor activation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 5595-5600.	3.3	16
115	Time evolution of a single spin inhomogeneously coupled to an interacting spin environment. Journal of Chemical Physics, 2006, 124, 144513.	1.2	15
116	Dimensional scaling treatment of stability of atomic anions induced by superintense, high-frequency laser fields. Journal of Chemical Physics, 2007, 127, 094301.	1.2	15
117	Frequency-dependent stabilization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mtext>He</mml:mtext></mml:mrow><mml:mo>â^’</mml:mo> a superintense laser field. Physical Review A, 2007, 76, .	1.0	15
118	Role of Water on the Rotational Dynamics of the Organic Methylammonium Cation: A First Principles Analysis. Scientific Reports, 2019, 9, 668.	1.6	15
119	Hybrid Quantum-Classical Neural Network for Calculating Ground State Energies of Molecules. Entropy, 2020, 22, 828.	1.1	15
120	A new approach to global minimization. Journal of Computational Chemistry, 1997, 18, 594-599.	1.5	14
121	Graph Theory for Fused Cubic Clusters of Water Dodecamer. Journal of Physical Chemistry A, 2005, 109, 12036-12045.	1.1	14
122	Supersymmetry identifies molecular Stark states whose eigenproperties can be obtained analytically. New Journal of Physics, 2011, 13, 063036.	1.2	14
123	Tuning entanglement and ergodicity in two-dimensional spin systems using impurities and anisotropy. Physical Review A, 2012, 85, .	1.0	14
124	The interference effect of laser-assisted bremsstrahlung emission in Coulomb fields of two nuclei. Journal of Applied Physics, 2013, 114, 124904.	1.1	14
125	Machine learning framework for quantum sampling of highly constrained, continuous optimization problems. Applied Physics Reviews, 2021, 8, .	5.5	14
126	Electronic tunneling in H+2 evaluated from the large-dimension limit. Chemical Physics, 1992, 161, 393-402.	0.9	13

#	Article	IF	Citations
127	Finite Size Scaling in Quantum Mechanics. Journal of Physical Chemistry A, 1998, 102, 9518-9522.	1.1	13
128	Size Effects in the Electronic Properties of Finite Arrays of Exchange-Coupled Quantum Dots. Journal of Physical Chemistry B, 2002, 106, 12847-12850.	1.2	13
129	Time-dependent density functional theory of coupled electronic lattice motion in quasi-two-dimensional crystals. Physical Review B, 2014, 89, .	1.1	13
130	Dark states enhance the photocell power via phononic dissipation. Physical Chemistry Chemical Physics, 2016, 18, 31845-31849.	1.3	13
131	Double-excitation manifold's effect on exciton transfer dynamics and the efficiency of coherent light harvesting. Physical Chemistry Chemical Physics, 2018, 20, 30032-30040.	1.3	13
132	Finite size scaling for critical parameters of simple diatomic molecules. Molecular Physics, 2000, 98, 1485-1493.	0.8	12
133	Supersymmetric factorization yields exact solutions to the molecular Stark-effect problem for stretched states. Physical Review A, 2011, 83, .	1.0	12
134	Persistence of entanglement in thermal states of spin systems. Journal of Physics B: Atomic, Molecular and Optical Physics, 2013, 46, 245501.	0.6	12
135	Canonical Schottky barrier heights of transition metal dichalcogenide monolayers in contact with a metal. Physical Review B, 2018, 97, .	1.1	12
136	Entanglement classifier in chemical reactions. Science Advances, 2019, 5, eaax5283.	4.7	12
137	Electronic Isomerism: Symmetry Breaking and Electronic Phase Diagrams for Diatomic Molecules at the Large-Dimension Limit. ChemPhysChem, 2001, 2, 434-442.	1.0	11
138	Real-space renormalization group study of the Hubbard model on a non-bipartite lattice. International Journal of Molecular Sciences, 2002, 3, 4-16.	1.8	11
139	Potential energy surface for the hydroperoxy and water (HO2Â·H2O) radical complex. Molecular Physics, 2002, 100, 247-253.	0.8	11
140	Simulated two-dimensional electronic spectroscopy of the eight-bacteriochlorophyll FMO complex. Journal of Chemical Physics, 2014, 141, 234105.	1.2	11
141	Direct application of the phase estimation algorithm to find the eigenvalues of the Hamiltonians. Chemical Physics, 2018, 514, 87-94.	0.9	11
142	Orientational Dynamics of Transition Dipoles and Exciton Relaxation in LH2 from Ultrafast Two-Dimensional Anisotropy. Journal of Physical Chemistry Letters, 2019, 10, 270-277.	2.1	11
143	Mean field phase diagrams for one-electron molecules. Journal of Physics A, 1997, 30, 1483-1493.	1.6	10
144	Dimensional perturbation theory for Regge poles. Journal of Chemical Physics, 1997, 106, 599-604.	1.2	10

#	Article	IF	Citations
145	Phase transitions and the stability of atomic and molecular ions. International Journal of Mass Spectrometry, 1999, 182-183, 23-29.	0.7	10
146	Solving Set Cover with Pairs Problem using Quantum Annealing. Scientific Reports, 2016, 6, 33957.	1.6	10
147	Solar Cell Materials by Design: Hybrid Pyroxene Cornerâ€Sharing VO₄ Tetrahedral Chains. ChemSusChem, 2017, 10, 1931-1942.	3.6	10
148	Mechanism of Meâ€“Re Bond Addition to Platinum(II) and Dioxygen Activation by the Resulting Ptâ€“Re Bimetallic Center. Inorganic Chemistry, 2017, 56, 2145-2152.	1.9	10
149	Convergence of a Reconstructed Density Matrix to a Pure State Using the Maximal Entropy Approach. Journal of Physical Chemistry A, 2021, 125, 7588-7595.	1.1	10
150	Quantum criticality at the large-dimensional limit: Three-body Coulomb systems. International Journal of Quantum Chemistry, 2001, 85, 307-314.	1.0	9
151	Lifetimes of metastable spherical carbon cluster dianions. Molecular Physics, 2002, 100, 475-481.	0.8	9
152	Dimensional scaling for stability of two particles in a dipole field. Chemical Physics Letters, 2008, 461, 127-130.	1.2	9
153	Quantum confinement and negative heat capacity. Europhysics Letters, 2013, 104, 16004.	0.7	9
154	Quantum criticality analysis by finite-size scaling and exponential basis sets. Physical Review E, 2013, 87, 043308.	0.8	9
155	Kinetic energy density for orbitalâ€free density functional calculations by axiomatic approach. International Journal of Quantum Chemistry, 2017, 117, e25373.	1.0	9
156	An ancilla-based quantum simulation framework for non-unitary matrices. Quantum Information Processing, 2017, 16, 1.	1.0	9
157	Kinetic energy functional derivative for the Thomas-Fermi atom inD dimensions. International Journal of Quantum Chemistry, 1997, 65, 411-413.	1.0	8
158	Finite-size scaling for Mott metal-insulator transition on a half filled nonpartite lattice. Physical Review B, 2002, 66, .	1.1	8
159	Transitionless driving on adiabatic search algorithm. Journal of Chemical Physics, 2014, 141, 224108.	1.2	8
160	Spectral Method for Solving the Nonlinear Thomas-Fermi Equation Based on Exponential Functions. Journal of Applied Mathematics, 2014, 2014, 1-8.	0.4	8
161	Quantum computing for atomic and molecular resonances. Journal of Chemical Physics, 2021, 154, 194107.	1.2	8
162	Renormalization group approach for electronic excitations in atoms. Chemical Physics Letters, 1998, 290, 199-204.	1.2	7

#	Article	IF	Citations
163	Comparison study of finite element and basis set methods for finite size scaling. Journal of Chemical Physics, 2009, 131, .	1.2	7
164	Pendular alignment and strong chemical binding are induced in helium dimer molecules by intense laser fields. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E9058-E9066.	3.3	7
165	Gap states and valley-spin filtering in transition metal dichalcogenide monolayers. Physical Review B, 2020, 101, .	1.1	7
166	Dimensional interpolation for metallic hydrogen. Physical Chemistry Chemical Physics, 2021, 23, 7841-7848.	1.3	7
167	Relaxation of stationary states on a quantum computer yields a unique spectroscopic fingerprint of the computerâ€™s noise. Communications Physics, 2022, 5, .	2.0	7
168	Symmetry breaking and stability of binary clusters. Chemical Physics Letters, 1997, 275, 211-214.	1.2	6
169	Data collapse for the SchrÃ¶dinger equation. Chemical Physics Letters, 2000, 319, 273-277.	1.2	6
170	SCALING OF ENTANGLEMENT IN FINITE ARRAYS OF EXCHANGE-COUPLED QUANTUM DOTS. International Journal of Quantum Information, 2003, 01, 375-386.	0.6	6
171	ENTANGLEMENT AND QUANTUM PHASE TRANSITION IN A ONE-DIMENSIONAL SYSTEM OF QUANTUM DOTS WITH DISORDER. International Journal of Quantum Information, 2006, 04, 827-835.	0.6	6
172	Nuclear-induced time evolution of entanglement of two-electron spins in anisotropically coupled quantum dot. Molecular Physics, 2008, 106, 1777-1786.	0.8	6
173	Critical conditions for stable dipole-bound dianions. Journal of Chemical Physics, 2008, 128, 044307.	1.2	6
174	DYNAMICS OF ENTANGLEMENT FOR TWO-ELECTRON ATOMS. International Journal of Quantum Information, 2008, 06, 303-316.	0.6	6
175	Scaling Mount Impossible: A Festschrift for Dudley Herschbach. Molecular Physics, 2012, 110, 1537-1537.	0.8	6
176	Using Quantum Games To Teach Quantum Mechanics, Part 2. Journal of Chemical Education, 2014, 91, 423-427.	1.1	6
177	Singularity of the time-energy uncertainty in adiabatic perturbation and cycloids on a Bloch sphere. Scientific Reports, 2016, 6, 20824.	1.6	6
178	Connecting bright and dark states through accidental degeneracy caused by lack of symmetry. Journal of Chemical Physics, 2018, 148, 204307.	1.2	6
179	Unorthodox Dimensional Interpolations for He, Li, Be Atoms and Hydrogen Molecule. Frontiers in Physics, 2020, 8, .	1.0	6
180	Prime factorization using quantum variational imaginary time evolution. Scientific Reports, 2021, 11, 20835.	1.6	6

#	Article	IF	Citations
181	A quantum encryption design featuring confusion, diffusion, and mode of operation. Scientific Reports, 2021, 11, 23774.	1.6	6
182	On the crossing of electronic energy levels of diatomic molecules at the large-Dlimit. Journal of Chemical Physics, 2001, 114, 9697-9705.	1.2	5
183	Internal entanglement amplification by external interactions. Physical Review A, 2007, 76, .	1.0	5
184	Finite Element Method for Finite-Size Scaling in Quantum Mechanics. Journal of Physical Chemistry A, 2008, 112, 5448-5452.	1.1	5
185	Finite size scaling with gaussian basis sets. Molecular Physics, 2008, 106, 203-212.	0.8	5
186	Temperature Dependent Electron Binding in (H₂O)₈. Journal of Physical Chemistry A, 2009, 113, 10886-10890.	1.1	5
187	Using Quantum Games To Teach Quantum Mechanics, Part 1. Journal of Chemical Education, 2014, 91, 417-422.	1.1	5
188	On the divergence of gradient expansions for kinetic energy functionals in the potential functional theory. Journal of Physics A: Mathematical and Theoretical, 2016, 49, 285202.	0.7	5
189	Mechanism of Isomerization and Methyl Migration in Heterobimetallic Rheniumâ€“Iridium Complexes: Experimental and DFT Study. Organometallics, 2016, 35, 605-611.	1.1	5
190	The quantum chemical search for novel materials and the issue of data processing: The InfoMol project. Journal of Computational Science, 2016, 15, 65-73.	1.5	5
191	Time-Domain Line-Shape Analysis from 2D Spectroscopy to Precisely Determine Hamiltonian Parameters for a Photosynthetic Complex. Journal of Physical Chemistry B, 2021, 125, 2812-2820.	1.2	5
192	Finite size scaling for critical parameters of simple diatomic molecules. Molecular Physics, 2000, 98, 1485-1493.	0.8	5
193	Statistical approach to quantum phase estimation. New Journal of Physics, 2021, 23, 113027.	1.2	5
194	Quantum cluster algorithm for data classification. Materials Theory, 2021, 5, .	2.2	5
195	Variational Quantum Circuits to Prepare Low Energy Symmetry States. Symmetry, 2022, 14, 457.	1.1	5
196	Quantum criticality at the infinite complete basis set limit: A thermodynamic analog of the Yang and Lee theorem. Chemical Physics Letters, 2006, 423, 45-49.	1.2	4
197	Simulated quantum computation of global minima. Molecular Physics, 2009, 107, 2015-2023.	0.8	4
198	Dimensional scaling treatment with relativistic corrections for stable multiply charged atomic ions in high-frequency super-intense laser fields. Journal of Chemical Physics, 2012, 136, 034114.	1.2	4

#	Article	IF	Citations
199	Multiple network alignment on quantum computers. Quantum Information Processing, 2014, 13, 2653-2666.	1.0	4
200	Analytic ab initio-based molecular interaction potential for the BrOâ‹…H2O complex. Journal of Chemical Physics, 2016, 144, 204121.	1.2	4
201	Enhancing the electronic dimensionality of hybrid organicâ€“inorganic frameworks by hydrogen bonded molecular cations. Materials Horizons, 2019, 6, 1187-1196.	6.4	4
202	Introducing Open Boundary Conditions in Modeling Nonperiodic Materials and Interfaces: The Impact of the Periodicity Assumption. , 2020, 2, 247-253.		4
203	Charge renormalization at the large-D limit for atoms and molecules. International Journal of Quantum Chemistry, 1995, 56, 349-359.	1.0	3
204	Relativistic structure description and relaxation effect on krypton excitation at small squared momentum transfer. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 4123-4135.	0.6	3
205	Critical behavior of electron impact ionization of atoms. International Journal of Quantum Chemistry, 2000, 80, 575-581.	1.0	3
206	Quantum criticality for few-body systems: Path-integral approach. Physical Review E, 2001, 64, 056120.	0.8	3
207	Electron localizationâ€“delocalization transitions in dissociation of the C4â^’ anion: A large-Danalysis. Journal of Chemical Physics, 2004, 120, 2199-2207.	1.2	3
208	Finite-size scaling for quantum criticality using the finite-element method. Physical Review E, 2012, 85, 036706.	0.8	3
209	Efficient method for localised functions using domain transformation and Fourier sine series. Molecular Physics, 2014, 112, 762-769.	0.8	3
210	Correction to kinetic energy density functional using exactly solvable model. Physica Scripta, 2015, 90, 125401.	1.2	3
211	Characterization of Quantum States Based on Creation Complexity. Advanced Quantum Technologies, 2020, 3, 2000043.	1.8	3
212	Bifacial Schottkyâ€Junction Plasmonicâ€Based Solar Cell. Energy Technology, 2020, 8, 1901280.	1.8	3
213	Practical quantum encryption protocol with varying encryption configurations. Physical Review Research, 2021, 3, .	1.3	3
214	Statistical Correlation Between Quantum Entanglement and Spinâ€“Orbit Coupling in Crossed Beam Molecular Dynamics. Advanced Quantum Technologies, 2021, 4, 2100098.	1.8	3
215	Combined effects of disorders and electronâ€“electron interactions upon metalâ€–insulator transition in 2D nonbipartite lattice. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 316, 265-270.	0.9	2
216	Metal-insulator transition in the Hubbard model on a triangular lattice with disorders: Renormalization group approach. International Journal of Quantum Chemistry, 2003, 93, 360-374.	1.0	2

#	Article	IF	Citations
217	Stability conditions for hydrogen-antihydrogenâ€“like quasimolecules. Physical Review A, 2008, 77, .	1.0	2
218	Quantum random state generation with predefined entanglement constraint. International Journal of Quantum Information, 2014, 12, 1450030.	0.6	2
219	A Density-Matrix Renormalization Group Study of a One-Dimensional Incommensurate Quantum Frenkelâ€“Kontorova Model. Journal of the Physical Society of Japan, 2014, 83, 094605.	0.7	2
220	Quantum Phase Transition in One-Dimensional Commensurate Frenkelâ€“Kontorova Model. Journal of the Physical Society of Japan, 2014, 83, 124603.	0.7	2
221	Reducing the number of ancilla qubits and the gate count required for creating large controlled operations. Quantum Information Processing, 2015, 14, 891-899.	1.0	2
222	Improved Photoactivity of Pyroxene Silicates by Cation Substitutions. ChemPhysChem, 2018, 19, 943-953.	1.0	2
223	A generalized circuit for the Hamiltonian dynamics through the truncated series. Quantum Information Processing, 2018, 17, 1.	1.0	2
224	Context-aware quantum simulation of a matrix stored in quantum memory. Quantum Information Processing, 2019, 18, 1.	1.0	2
225	Spin-momentum entanglement in a Boseâ€“Einstein condensate. Physical Chemistry Chemical Physics, 2020, 22, 25669-25674.	1.3	2
226	Magnetic flux noise in superconducting qubits and the gap states continuum. Scientific Reports, 2021, 11, 1813.	1.6	2
227	Dimensional Interpolation for Random Walk. Journal of Physical Chemistry A, 2021, 125, 7581-7587.	1.1	2
228	A universal quantum circuit design for periodical functions. New Journal of Physics, 2021, 23, 103022.	1.2	2
229	Constructive Quantum Interference in Photochemical Reactions. Journal of Chemical Theory and Computation, 2021, 17, 7822-7826.	2.3	2
230	The Quantum Condition Space. Advanced Quantum Technologies, 2022, 5, 2100158.	1.8	2
231	Finite-Size Scaling on a Digital Quantum Simulator Using Quantum Restricted Boltzmann Machine. Frontiers in Physics, 0, 10, .	1.0	2
232	Statistical model for delocalized Ï€ bonding in the C60 molecule. Chemical Physics Letters, 1994, 218, 229-233.	1.2	1
233	Finite-size scaling method for the stability of atomic and molecular ions. Physica A: Statistical Mechanics and Its Applications, 2000, 283, 65-73.	1.2	1
234	Quantum critical phenomena in the SchrÃ¶dinger formulation: mapping to classical lattices. Chemical Physics Letters, 2001, 333, 451-458.	1.2	1

#	Article	IF	Citations
235	Quadratic constrained mixed discrete optimization with an adiabatic quantum optimizer. Physical Review A, 2014, 90, .	1.0	1
236	Ring flipping in heterobimetallic Re-Ir complexes and its effect on structural isomerism: Dynamic NMR and DFT study. Journal of Organometallic Chemistry, 2017, 843, 62-65.	0.8	1
237	Geometrical picture of the electronâ€“electron correlation at the large-D limit. Physical Chemistry Chemical Physics, 2022, 24, 9298-9307.	1.3	1
238	Finite Size Scaling for Criticality of the SchrÃ¶dinger Equation. , 2011, , 91-110.		0
239	Avalanches in the raise and peel model in the presence of a wall. Journal of Physics A: Mathematical and Theoretical, 2013, 46, 265001.	0.7	0
240	An agent-based model approach to multi-phase life-cycle for contact inhibited, anchorage dependent cells. Interdisciplinary Sciences, Computational Life Sciences, 2014, 6, 312-322.	2.2	0
241	Influence of the intensity gradient upon HHG from free electrons scattered by an intense laser beam. Applied Physics B: Lasers and Optics, 2014, 117, 95-101.	1.1	0
242	Plasmonically Enhanced Schottky Solar Cell. , 2018, , .		0
243	Tribute to Dor Ben-Amotz. Journal of Physical Chemistry B, 2022, 126, 2943-2945.	1.2	0