Artur F Izmaylov

List of Publications by Year
in descending order

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65 papers	7,621 citations	172207 29 h-index	114278 63 g-index
65 all docs	65 docs citations	65 times ranked	8814 citing authors

#	Article	IF	Citations
1	Influence of the exchange screening parameter on the performance of screened hybrid functionals. Journal of Chemical Physics, 2006, 125, 224106.	1.2	4,894
2	Efficient evaluation of short-range Hartree-Fock exchange in large molecules and periodic systems. Journal of Chemical Physics, 2006, 125, 104103.	1.2	200
3	Qubit Coupled Cluster Method: A Systematic Approach to Quantum Chemistry on a Quantum Computer. Journal of Chemical Theory and Computation, 2018, 14, 6317-6326.	2.3	182
4	Assessment of a Middle-Range Hybrid Functional. Journal of Chemical Theory and Computation, 2008, 4, 1254-1262.	2.3	155
5	The importance of middle-range Hartree-Fock-type exchange for hybrid density functionals. Journal of Chemical Physics, 2007, 127, 221103.	1.2	152
6	Measurement optimization in the variational quantum eigensolver using a minimum clique cover. Journal of Chemical Physics, 2020, 152, 124114.	1.2	138
7	Iterative Qubit Coupled Cluster Approach with Efficient Screening of Generators. Journal of Chemical Theory and Computation, 2020, 16, 1055-1063.	2.3	109
8	Unitary Partitioning Approach to the Measurement Problem in the Variational Quantum Eigensolver Method. Journal of Chemical Theory and Computation, 2020, 16, 190-195.	2.3	107
9	Measuring All Compatible Operators in One Series of Single-Qubit Measurements Using Unitary Transformations. Journal of Chemical Theory and Computation, 2020, 16, 2400-2409.	2.3	95
10	A quantum computing view on unitary coupled cluster theory. Chemical Society Reviews, 2022, 51, 1659-1684.	18.7	83
11	Geometric Phase Effects in Nonadiabatic Dynamics near Conical Intersections. Accounts of Chemical Research, 2017, 50, 1785-1793.	7.6	80
12	Fast Numerical Evaluation of Time-Derivative Nonadiabatic Couplings for Mixed Quantumâ€“Classical Methods. Journal of Physical Chemistry Letters, 2015, 6, 4200-4203.	2.1	75
13	Constrained Variational Quantum Eigensolver: Quantum Computer Search Engine in the Fock Space. Journal of Chemical Theory and Computation, 2019, 15, 249-255.	2.3	74
14	Nonequilibrium Fermi golden rule for electronic transitions through conical intersections. Journal of Chemical Physics, 2011, 135, 234106.	1.2	73
15	Terahertz spectroscopy of enantiopure and racemic polycrystalline valine. Physical Chemistry Chemical Physics, 2011, 13, 11719.	1.3	70
16	Geometric Phase Effects in Dynamics Near Conical Intersections: Symmetry Breaking and Spatial Localization. Physical Review Letters, 2013, 111, 220406.	2.9	68
17	When do we need to account for the geometric phase in excited state dynamics?. Journal of Chemical Physics, 2014, 140, 214116.	1.2	62
18	Resolution of the identity atomic orbital Laplace transformed second order MÃ¸llerâ€“Plesset theory for nonconducting periodic systems. Physical Chemistry Chemical Physics, 2008, 10, 3421.	1.3	60

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19	Revising the measurement process in the variational quantum eigensolver: is it possible to reduce the number of separately measured operators?. Chemical Science, 2019, 10, 3746-3755.	3.7	53
20	Linear-scaling calculation of static and dynamic polarizabilities in Hartree-Fock and density functional theory for periodic systems. Journal of Chemical Physics, 2006, 125, 224105.	1.2	52
21	Active-Space<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>-Representability Constraints for Variational Two-Particle Reduced Density Matrix Calculations. Physical Review Letters, 2010, 105, 213003.	2.9	45
22	Geometric phase effects in low-energy dynamics near conical intersections: A study of the multidimensional linear vibronic coupling model. Journal of Chemical Physics, 2013, 139, 234103.	1.2	41
23	Why Do Mixed Quantum-Classical Methods Describe Short-Time Dynamics through Conical Intersections So Well? Analysis of Geometric Phase Effects. Journal of Chemical Theory and Computation, 2015, 11, 1375-1382.	2.3	36
24	On the order problem in construction of unitary operators for the variational quantum eigensolver. Physical Chemistry Chemical Physics, 2020, 22, 12980-12986.	1.3	36
25	Unitary Transformation of the Electronic Hamiltonian with an Exact Quadratic Truncation of the Baker-Campbell-Hausdorff Expansion. Journal of Chemical Theory and Computation, 2021, 17, 66-78.	2.3	36
26	TEQUILA: a platform for rapid development of quantum algorithms. Quantum Science and Technology, 2021, 6, 024009.	2.6	36
27	Shape-Dependent Interactions of Palladium Nanocrystals with Hydrogen. Small, 2016, 12, 2450-2458.	5.2	34
28	New Insights into the State Trapping of UV-Excited Thymine. Molecules, 2016, 21, 1603.	1.7	31
29	Entanglement in the Bornâ€“Oppenheimer Approximation. Journal of Chemical Theory and Computation, 2017, 13, 20-28.	2.3	30
30	Exact and approximate symmetry projectors for the electronic structure problem on a quantum computer. Journal of Chemical Physics, 2019, 151, 164111.	1.2	30
31	Topologically Correct Quantum Nonadiabatic Formalism for On-the-Fly Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 452-456.	2.1	29
32	Efficient evaluation of analytic vibrational frequencies in Hartree-Fock and density functional theory for periodic nonconducting systems. Journal of Chemical Physics, 2007, 127, 144106.	1.2	28
33	On the inclusion of the diagonal Born-Oppenheimer correction in surface hopping methods. Journal of Chemical Physics, 2016, 144, 154103.	1.2	28
34	Multipartitioning many-body perturbation theory calculations on temporary anions: applications to NÂ2and COÂ. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, 2321-2329.	0.6	27
35	Analytically Calculated Polarizability of Carbon Nanotubes:â€‰ Single Wall, Coaxial, and Bundled Systems. Journal of Physical Chemistry C, 2008, 112, 1396-1400.	1.5	26
36	A perturbative formalism for electronic transitions through conical intersections in a fully quadratic vibronic model. Journal of Chemical Physics, 2014, 141, 034104.	1.2	26

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37	Deuterium isotope effect in fluorescence of gaseous oxazine dyes. Physical Chemistry Chemical Physics, 2019, 21, 5759-5770.	1.3	24
38	A posteriori corrections to the iterative qubit coupled cluster method to minimize the use of quantum resources in large-scale calculations. Quantum Science and Technology, 2021, 6, 024012.	2.6	24
39	Cartan Subalgebra Approach to Efficient Measurements of Quantum Observables. PRX Quantum, 2021, 2, .	3.5	24
40	Analysis of geometric phase effects in the quantum-classical Liouville formalism. Journal of Chemical Physics, 2014, 140, 084104.	1.2	22
41	Analytic gradients in variational quantum algorithms: Algebraic extensions of the parameter-shift rule to general unitary transformations. Physical Review A, 2021, 104, .	1.0	20
42	Perturbative wave-packet spawning procedure for non-adiabatic dynamics in diabatic representation. Journal of Chemical Physics, 2013, 138, 104115.	1.2	18
43	Diabatic Definition of Geometric Phase Effects. Journal of Chemical Theory and Computation, 2016, 12, 5278-5283.	2.3	18
44	Mixed Quantum-Classical Dynamics Using Collective Electronic Variables: A Better Alternative to Electronic Friction Theories. Journal of Physical Chemistry Letters, 2017, 8, 440-444.	2.1	15
45	Nonadiabatic Quantum Dynamics with Frozen-Width Gaussians. Journal of Physical Chemistry A, 2018, 122, 6031-6042.	1.1	15
46	Ab initio study of temporary anions of benzene and fluorobenzenes using the multipartitioning many-body perturbation theory. Physical Chemistry Chemical Physics, 2005, 7, 3933.	1.3	13
47	Variational nonadiabatic dynamics in the moving crude adiabatic representation: Further merging of nuclear dynamics and electronic structure. Journal of Chemical Physics, 2018, 148, 114102.	1.2	13
48	Relation between fermionic and qubit mean fields in the electronic structure problem. Journal of Chemical Physics, 2018, 149, 214105.	1.2	12
49	Problem-free time-dependent variational principle for open quantum systems. Journal of Chemical Physics, 2015, 142, 134107.	1.2	11
50	Topological Origins of Bound States in the Continuum for Systems with Conical Intersections. Journal of Physical Chemistry Letters, 2018, 9, 146-149.	2.1	11
51	Relativistic Interactions in the Radical Pair Model of Magnetic Field Sense in CRY-1 Protein of Arabidopsis thaliana. Journal of Physical Chemistry A, 2009, 113, 12276-12284.	1.1	10
52	Molecular â€œtopological insulatorsâ€• a case study of electron transfer in the bis(methylene) adamantyl carbocation. Chemical Communications, 2017, 53, 7365-7368.	2.2	10
53	Quantum Nonadiabatic Cloning of Entangled Coherent States. Journal of Physical Chemistry Letters, 2017, 8, 1793-1797.	2.1	10
54	Geometric phase effects in excited state dynamics through a conical intersection in large molecules: N-dimensional linear vibronic coupling model study. Journal of Chemical Physics, 2017, 147, 064106.	1.2	9

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55	On Calculating a Polymer's Enthalpy of Formation with Quantum Chemical Methods. Journal of Physical Chemistry B, 2007, 111, 13869-13872.	1.2	8
56	On Construction of Projection Operators. Journal of Physical Chemistry A, 2019, 123, 3429-3433.	1.1	8
57	Exploring vibrational ladder climbing in vibronic coupling models: Toward experimental observation of a geometric phase signature of a conical intersection. Chemical Physics, 2018, 515, 28-35.	0.9	7
58	Non-stochastic matrix SchrÃ¶dinger equation for open systems. Journal of Chemical Physics, 2014, 141, 234112.	1.2	5
59	On the breakdown of the Ehrenfest method for molecular dynamics on surfaces. Journal of Chemical Physics, 2018, 149, 214101.	1.2	5
60	An efficient implementation of the localized operator partitioning method for electronic energy transfer. Journal of Chemical Physics, 2015, 142, 084114.	1.2	2
61	Localized operator partitioning method for electronic excitation energies in the time-dependent density functional formalism. Journal of Chemical Physics, 2016, 145, 244111.	1.2	2
62	How to define quantum mean-field solvable Hamiltonians using Lie algebras. Quantum Science and Technology, 2021, 6, 044006.	2.6	2
63	Computational approaches to efficient generation of the stationary state for incoherent light excitation. Journal of Chemical Physics, 2021, 154, 124126.	1.2	1
64	Controlling energy conservation in quantum dynamics with independently moving basis functions: Application to Multi-Configuration Ehrenfest. Journal of Chemical Physics, 0, , .	1.2	1
65	Explaining electric conductivity using the particle-in-a-box model: quantum superposition is the key. Canadian Journal of Physics, 2017, 95, 1181-1188.	0.4	0