AlÃ¡n Aspuru Guzik

List of Publications by Year
in descending order

377 papers	46,721 citations	2795 94 h-index	2171 202 g-index
416 all docs	416 docs citations	416 times ranked	31972 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	A variational eigenvalue solver on a photonic quantum processor. Nature Communications, 2014, 5, 4213.	5.8	2,210
3	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. ACS Central Science, 2018, 4, 268-276.	5.3	1,761
4	A metal-free organicâ€“inorganic aqueous flow battery. Nature, 2014, 505, 195-198.	13.7	1,333
5	The theory of variational hybrid quantum-classical algorithms. New Journal of Physics, 2016, 18, 023023.	1.2	1,186
6	Inverse molecular design using machine learning: Generative models for matter engineering. Science, 2018, 361, 360-365.	6.0	1,055
7	Tuning charge transport in solution-sheared organic semiconductors using lattice strain. Nature, 2011, 480, 504-508.	13.7	981
8	Environment-assisted quantum walks in photosynthetic energy transfer. Journal of Chemical Physics, 2008, 129, 174106.	1.2	939
9	High Electrical Conductivity in Ni₃(2,3,6,7,10,11-hexaiminotriphenylene)₂, a Semiconducting Metalâ€“Organic Graphene Analogue. Journal of the American Chemical Society, 2014, 136, 8859-8862.	6.6	893
10	Simulated Quantum Computation of Molecular Energies. Science, 2005, 309, 1704-1707.	6.0	852
11	Quantum Chemistry in the Age of Quantum Computing. Chemical Reviews, 2019, 119, 10856-10915.	23.0	748
12	Quantum computational chemistry. Reviews of Modern Physics, 2020, 92, .	16.4	726
13	Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. Nature Materials, 2016, 15, 1120-1127.	13.3	708
14	Environment-assisted quantum transport. New Journal of Physics, 2009, 11, 033003.	1.2	694
15	Photonic quantum simulators. Nature Physics, 2012, 8, 285-291.	6.5	681
16	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nature Biotechnology, 2019, 37, 1038-1040.	9.4	671
17	Rational design of layered oxide materials for sodium-ion batteries. Science, 2020, 370, 708-711.	6.0	616
18	Scalable Quantum Simulation of Molecular Energies. Physical Review X, 2016, 6, .	2.8	577

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19	Towards quantum chemistry on a quantum computer. Nature Chemistry, 2010, 2, 106-111.	6.6	568
20	Noisy intermediate-scale quantum algorithms. Reviews of Modern Physics, 2022, 94, .	16.4	521
21	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
22	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	23.3	489
23	Observation of topologically protected bound states in photonic quantum walks. Nature Communications, 2012, 3, 882.	5.8	488
24	Using coherence to enhance function in chemical and biophysical systems. Nature, 2017, 543, 647-656.	13.7	477
25	The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid. Journal of Physical Chemistry Letters, 2011, 2, 2241-2251.	2.1	470
26	A redox-flow battery with an alloxazine-based organic electrolyte. Nature Energy, 2016, 1, .	19.8	427
27	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
28	Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. Quantum Science and Technology, 2019, 4, 014008.	2.6	381
29	Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems. Physical Chemistry Chemical Physics, 2015, 17, 31371-31396.	1.3	376
30	Discrete Single-Photon Quantum Walks with Tunable Decoherence. Physical Review Letters, 2010, 104, 153602.	2.9	346
31	Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator. Physical Review X, 2018, 8, .	2.8	342
32	Computational design of molecules for an all-quinone redox flow battery. Chemical Science, 2015, 6, 885-893.	3.7	341
33	From computational discovery to experimental characterization of a high hole mobility organic crystal. Nature Communications, 2011, 2, 437.	5.8	321
34	Neural Networks for the Prediction of Organic Chemistry Reactions. ACS Central Science, 2016, 2, 725-732.	5.3	321
35	Simulation of electronic structure Hamiltonians using quantum computers. Molecular Physics, 2011, 109, 735-750.	0.8	310
36	Self-driving laboratory for accelerated discovery of thin-film materials. Science Advances, 2020, 6, eaaz8867.	4.7	306

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37	Role of Quantum Coherence and Environmental Fluctuations in Chromophoric Energy Transport. Journal of Physical Chemistry B, 2009, 113, 9942-9947.	1.2	300
38	Expressibility and Entangling Capability of Parameterized Quantum Circuits for Hybrid Quantumâ€Classical Algorithms. Advanced Quantum Technologies, 2019, 2, 1900070.	1.8	298
39	Quantum autoencoders for efficient compression of quantum data. Quantum Science and Technology, 2017, 2, 045001.	2.6	295
40	Alkaline Quinone Flow Battery with Long Lifetime at pH 12. Joule, 2018, 2, 1894-1906.	11.7	293
41	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. Machine Learning: Science and Technology, 2020, 1, 045024.	2.4	272
42	Molecular Sets (MOSES): A Benchmarking Platform for Molecular Generation Models. Frontiers in Pharmacology, 2020, 11, 565644.	1.6	266
43	Reinforced Adversarial Neural Computer for de Novo Molecular Design. Journal of Chemical Information and Modeling, 2018, 58, 1194-1204.	2.5	256
44	Finding low-energy conformations of lattice protein models by quantum annealing. Scientific Reports, 2012, 2, 571.	1.6	247
45	Quantum Simulation of Electronic Structure with Linear Depth and Connectivity. Physical Review Letters, 2018, 120, 110501.	2.9	243
46	Polynomial-time quantum algorithm for the simulation of chemical dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 18681-18686.	3.3	241
47	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
48	Boson sampling for molecular vibronic spectra. Nature Photonics, 2015, 9, 615-620.	15.6	230
49	Interface chemistry of an amide electrolyte for highly reversible lithium metal batteries. Nature Communications, 2020, 11, 4188.	5.8	226
50	Simulating Chemistry Using Quantum Computers. Annual Review of Physical Chemistry, 2011, 62, 185-207.	4.8	224
51	Phoenics: A Bayesian Optimizer for Chemistry. ACS Central Science, 2018, 4, 1134-1145.	5.3	215
52	Machine-learned potentials for next-generation matter simulations. Nature Materials, 2021, 20, 750-761.	13.3	214
53	Revealing High Na-Content P2-Type Layered Oxides as Advanced Sodium-Ion Cathodes. Journal of the American Chemical Society, 2020, 142, 5742-5750.	6.6	206
54	What Is High-Throughput Virtual Screening? A Perspective from Organic Materials Discovery. Annual Review of Materials Research, 2015, 45, 195-216.	4.3	203

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55	Inverse Design of Solid-State Materials via a Continuous Representation. Matter, 2019, 1, 1370-1384.	5.0	198
56	Photonics meets excitonics: natural and artificial molecular aggregates. Nanophotonics, 2013, 2, 21-38.	2.9	195
57	Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry â€“ the Harvard Clean Energy Project. Energy and Environmental Science, 2014, 7, 698-704.	15.6	189
58	Anthraquinone Derivatives in Aqueous Flow Batteries. Advanced Energy Materials, 2017, 7, 1601488.	10.2	189
59	Atomistic Study of the Long-Lived Quantum Coherences in the Fenna-Matthews-Olson Complex. Biophysical Journal, 2012, 102, 649-660.	0.2	188
60	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	0.7	181
61	Understanding Polymorphism in Organic Semiconductor Thin Films through Nanoconfinement. Journal of the American Chemical Society, 2014, 136, 17046-17057.	6.6	179
62	Nanoparticle synthesis assisted by machine learning. Nature Reviews Materials, 2021, 6, 701-716.	23.3	179
63	Next-Generation Experimentation with Self-Driving Laboratories. Trends in Chemistry, 2019, 1, 282-291.	4.4	175
64	From transistor to trapped-ion computers for quantum chemistry. Scientific Reports, 2014, 4, 3589.	1.6	172
65	Inverse design of nanoporous crystalline reticular materials with deep generative models. Nature Machine Intelligence, 2021, 3, 76-86.	8.3	172
66	Machine learning the quantum-chemical properties of metalâ€“organic frameworks for accelerated materials discovery. Matter, 2021, 4, 1578-1597.	5.0	170
67	Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics. Energy and Environmental Science, 2011, 4, 4849.	15.6	169
68	Data-Driven Strategies for Accelerated Materials Design. Accounts of Chemical Research, 2021, 54, 849-860.	7.6	168
69	Alkaline Benzoquinone Aqueous Flow Battery for Largeâ€Scale Storage of Electrical Energy. Advanced Energy Materials, 2018, 8, 1702056.	10.2	161
70	Learning from the Harvard Clean Energy Project: The Use of Neural Networks to Accelerate Materials Discovery. Advanced Functional Materials, 2015, 25, 6495-6502.	7.8	160
71	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. Joule, 2017, 1, 857-870.	11.7	157
72	Extending the Lifetime of Organic Flow Batteries via Redox State Management. Journal of the American Chemical Society, 2019, 141, 8014-8019.	6.6	151

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73	Beyond Ternary OPV: Highâ€Throughput Experimentation and Selfâ€Driving Laboratories Optimize Multicomponent Systems. Advanced Materials, 2020, 32, e1907801.	11.1	138
74	Bioinspiration in light harvesting and catalysis. Nature Reviews Materials, 2020, 5, 828-846.	23.3	136
75	Accelerating Resolution-of-the-Identity Second-Order MÃ¸llerâ^'Plesset Quantum Chemistry Calculations with Graphical Processing Units. Journal of Physical Chemistry A, 2008, 112, 2049-2057.	1.1	133
76	Chemical basis of Trotter-Suzuki errors in quantum chemistry simulation. Physical Review A, 2015, 91, .	1.0	133
77	Potential of quantum computing for drug discovery. IBM Journal of Research and Development, 2018, 62, 6:1-6:20.	3.2	130
78	Mapping the frontiers of quinone stability in aqueous media: implications for organic aqueous redox flow batteries. Journal of Materials Chemistry A, 2019, 7, 12833-12841.	5.2	128
79	Identification Schemes for Metalâ€“Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. Crystal Growth and Design, 2019, 19, 6682-6697.	1.4	123
80	On the alternatives for bath correlators and spectral densities from mixed quantum-classical simulations. Journal of Chemical Physics, 2012, 137, 224103.	1.2	121
81	Non-Markovian quantum jumps in excitonic energy transfer. Journal of Chemical Physics, 2009, 131, 184102.	1.2	120
82	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
83	Adiabatic Quantum Simulation of Quantum Chemistry. Scientific Reports, 2014, 4, 6603.	1.6	120
84	Quantum Simulation of Helium Hydride Cation in a Solid-State Spin Register. ACS Nano, 2015, 9, 7769-7774.	7.3	113
85	ChemOS: Orchestrating autonomous experimentation. Science Robotics, 2018, 3, .	9.9	113
86	Conformation of self-assembled porphyrin dimers in liposome vesicles by phase-modulation 2D fluorescence spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16521-16526.	3.3	112
87	Machine learning exciton dynamics. Chemical Science, 2016, 7, 5139-5147.	3.7	112
88	Separation of Electromagnetic and Chemical Contributions to Surface-Enhanced Raman Spectra on Nanoengineered Plasmonic Substrates. Journal of Physical Chemistry Letters, 2010, 1, 2740-2746.	2.1	106
89	Programmed coherent coupling in a synthetic DNA-based excitonic circuit. Nature Materials, 2018, 17, 159-166.	13.3	106
90	Scalable High-Performance Algorithm for the Simulation of Exciton Dynamics. Application to the Light-Harvesting Complex II in the Presence of Resonant Vibrational Modes. Journal of Chemical Theory and Computation, 2014, 10, 4045-4054.	2.3	103

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91	An Alternative Host Material for Longâ€Lifespan Blue Organic Lightâ€Emitting Diodes Using Thermally Activated Delayed Fluorescence. Advanced Science, 2017, 4, 1600502.	5.6	103
92	Strong coupling between chlorosomes of photosynthetic bacteria and a confined optical cavity mode. Nature Communications, 2014, 5, 5561.	5.8	102
93	Generative Adversarial Networks for Crystal Structure Prediction. ACS Central Science, 2020, 6, 1412-1420.	5.3	102
94	Complex Chemical Reaction Networks from Heuristics-Aided Quantum Chemistry. Journal of Chemical Theory and Computation, 2014, 10, 897-907.	2.3	100
95	Exponentially more precise quantum simulation of fermions in second quantization. New Journal of Physics, 2016, 18, 033032.	1.2	100
96	Hydrogen-bonded diketopyrrolopyrrole (DPP) pigments as organic semiconductors. Organic Electronics, 2014, 15, 3521-3528.	1.4	99
97	Machine learning directed drug formulation development. Advanced Drug Delivery Reviews, 2021, 175, 113806.	6.6	99
98	A Comprehensive Discovery Platform for Organophosphorus Ligands for Catalysis. Journal of the American Chemical Society, 2022, 144, 1205-1217.	6.6	97
99	Quantum algorithm for obtaining the energy spectrum of molecular systems. Physical Chemistry Chemical Physics, 2008, 10, 5388.	1.3	95
100	Data-science driven autonomous process optimization. Communications Chemistry, 2021, 4, .	2.0	94
101	Exploiting Locality in Quantum Computation for Quantum Chemistry. Journal of Physical Chemistry Letters, 2014, 5, 4368-4380.	2.1	93
102	Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. Chemical Science, 2020, 11, 4584-4601.	3.7	93
103	Communication: Excitonâ€“phonon information flow in the energy transfer process of photosynthetic complexes. Journal of Chemical Physics, 2011, 134, 101103.	1.2	92
104	A quantumâ€“quantum Metropolis algorithm. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 754-759.	3.3	92
105	On the chemical bonding effects in the Raman response: Benzenethiol adsorbed on silver clusters. Physical Chemistry Chemical Physics, 2009, 11, 9401.	1.3	91
106	Faster quantum chemistry simulation on fault-tolerant quantum computers. New Journal of Physics, 2012, 14, 115023.	1.2	91
107	Molecular Engineering of an Alkaline Naphthoquinone Flow Battery. ACS Energy Letters, 2019, 4, 1880-1887.	8.8	90
108	The Matter Simulation (R)evolution. ACS Central Science, 2018, 4, 144-152.	5.3	88

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109	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. Chemical Science, 2018, 9, 7642-7655.	3.7	86
110	The Harvard organic photovoltaic dataset. Scientific Data, 2016, 3, 160086.	2.4	85
111	Use machine learning to find energy materials. Nature, 2017, 552, 23-27.	13.7	85
112	Improved Fault-Tolerant Quantum Simulation of Condensed-Phase Correlated Electrons via Trotterization. Quantum - the Open Journal for Quantum Science, 0, 4, 296.	0.0	85
113	Construction of model Hamiltonians for adiabatic quantum computation and its application to finding low-energy conformations of lattice protein models. Physical Review A, 2008, 78, .	1.0	84
114	Quantum stochastic walks: A generalization of classical random walks and quantum walks. Physical Review A, 2010, 81, .	1.0	83
115	Absence of Quantum Oscillations and Dependence on Site Energies in Electronic Excitation Transfer in the Fennaâ€“Matthewsâ€“Olson Trimer. Journal of Physical Chemistry Letters, 2011, 2, 2912-2917.	2.1	83
116	A quantum computing view on unitary coupled cluster theory. Chemical Society Reviews, 2022, 51, 1659-1684.	18.7	83
117	Multiple coherent states for first-principles semiclassical initial value representation molecular dynamics. Journal of Chemical Physics, 2009, 130, 234113.	1.2	82
118	Influence of Force Fields and Quantum Chemistry Approach on Spectral Densities of BChl a in Solution and in FMO Proteins. Journal of Physical Chemistry B, 2015, 119, 9995-10004.	1.2	82
119	Effects of Oddâ€“Even Side Chain Length of Alkyl-Substituted Diphenylbithiophenes on First Monolayer Thin Film Packing Structure. Journal of the American Chemical Society, 2013, 135, 11006-11014.	6.6	81
120	How machine learning can assist the interpretation of ab initio molecular dynamics simulations and conceptual understanding of chemistry. Chemical Science, 2019, 10, 2298-2307.	3.7	80
121	Quantum simulator of an open quantum system using superconducting qubits: exciton transport in photosynthetic complexes. New Journal of Physics, 2012, 14, 105013.	1.2	79
122	Atomistic Study of Energy Funneling in the Light-Harvesting Complex of Green Sulfur Bacteria. Journal of the American Chemical Society, 2014, 136, 2048-2057.	6.6	78
123	ChemOS: An orchestration software to democratize autonomous discovery. PLoS ONE, 2020, 15, e0229862.	1.1	77
124	Accelerating Correlated Quantum Chemistry Calculations Using Graphical Processing Units and a Mixed Precision Matrix Multiplication Library. Journal of Chemical Theory and Computation, 2010, 6, 135-144.	2.3	75
125	Strongly Coupled Quantum Heat Machines. Journal of Physical Chemistry Letters, 2015, 6, 3477-3482.	2.1	75
126	Resource-efficient digital quantum simulation of d-level systems for photonic, vibrational, and spin-s Hamiltonians. Npj Quantum Information, 2020, 6, .	2.8	74

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127	Theoretical Characterization of the Air-Stable, High-Mobility Dinaphtho[2,3-‹i›b‹/i›:2â€²3â€²-‹i›f‹/i›]thieno[3,2-‹i›b‹/i›]-thiophene Organic Semiconductor. Journal of Physical Chemistry C, 2010, 114, 2334-2340.	1.5	73
128	First-principles semiclassical initial value representation molecular dynamics. Physical Chemistry Chemical Physics, 2009, 11, 3861.	1.3	70
129	A two-qubit photonic quantum processor and its application to solving systems of linear equations. Scientific Reports, 2014, 4, 6115.	1.6	70
130	A Bayesian approach to calibrating high-throughput virtual screening results and application to organic photovoltaic materials. Materials Horizons, 2016, 3, 226-233.	6.4	70
131	Machine learning for quantum dynamics: deep learning of excitation energy transfer properties. Chemical Science, 2017, 8, 8419-8426.	3.7	70
132	Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer. Quantum Science and Technology, 2019, 4, 045005.	2.6	69
133	Autonomous Molecular Design: Then and Now. ACS Applied Materials & Interfaces, 2019, 11, 24825-24836.	4.0	69
134	A study of heuristic guesses for adiabatic quantum computation. Quantum Information Processing, 2011, 10, 33-52.	1.0	67
135	Conformation and Electronic Population Transfer in Membrane-Supported Self-Assembled Porphyrin Dimers by 2D Fluorescence Spectroscopy. Journal of Physical Chemistry B, 2012, 116, 10757-10770.	1.2	67
136	Bayesian network structure learning using quantum annealing. European Physical Journal: Special Topics, 2015, 224, 163-188.	1.2	67
137	Materials Acceleration Platforms: On the way to autonomous experimentation. Current Opinion in Green and Sustainable Chemistry, 2020, 25, 100370.	3.2	67
138	Organic molecules with inverted gaps between first excited singlet and triplet states and appreciable fluorescence rates. Matter, 2021, 4, 1654-1682.	5.0	67
139	Time-Dependent Density Functional Theory for Open Quantum Systems with Unitary Propagation. Physical Review Letters, 2010, 104, 043001.	2.9	65
140	Exciton transport in thin-film cyanine dye J-aggregates. Journal of Chemical Physics, 2012, 137, 034109.	1.2	65
141	Quantum computing at the frontiers of biological sciences. Nature Methods, 2021, 18, 701-709.	9.0	64
142	Beyond generative models: superfast traversal, optimization, novelty, exploration and discovery (STONED) algorithm for molecules using SELFIES. Chemical Science, 2021, 12, 7079-7090.	3.7	64
143	Soft pseudopotentials for efficient quantum Monte Carlo calculations: From Be to Ne and Al to Ar. Journal of Chemical Physics, 2001, 114, 7790-7794.	1.2	63
144	Memory-Assisted Exciton Diffusion in the Chlorosome Light-Harvesting Antenna of Green Sulfur Bacteria. Journal of Physical Chemistry Letters, 2012, 3, 2357-2361.	2.1	63

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145	Quantum state and process tomography of energy transfer systems via ultrafast spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 17615-17620.	3.3	62
146	A Bayesian Approach to Predict Solubility Parameters. Advanced Theory and Simulations, 2019, 2, 1800069.	1.3	62
147	Failure of Conventional Density Functionals for the Prediction of Molecular Crystal Polymorphism: A Quantum Monte Carlo Study. Journal of Physical Chemistry Letters, 2010, 1, 1789-1794.	2.1	61
148	Local protein solvation drives direct down-conversion in phycobiliprotein PC645 via incoherent vibronic transport. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E3342-E3350.	3.3	61
149	A Mixed Quantum Chemistry/Machine Learning Approach for the Fast and Accurate Prediction of Biochemical Redox Potentials and Its Large-Scale Application to 315â€¯000 Redox Reactions. ACS Central Science, 2019, 5, 1199-1210.	5.3	61
150	Discovery of Calciumâ€Metal Alloy Anodes for Reversible Caâ€Ion Batteries. Advanced Energy Materials, 2019, 9, 1802994.	10.2	61
151	G<scp>ryffin</scp>: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. Applied Physics Reviews, 2021, 8, .	5.5	61
152	Environment-assisted quantum transport in ordered systems. New Journal of Physics, 2012, 14, 053041.	1.2	58
153	Efficient quantum circuits for diagonal unitaries without ancillas. New Journal of Physics, 2014, 16, 033040.	1.2	58
154	Temperature-dependent conformations of exciton-coupled Cy3 dimers in double-stranded DNA. Journal of Chemical Physics, 2018, 148, 085101.	1.2	58
155	Adiabatic quantum simulators. AIP Advances, 2011, 1, .	0.6	57
156	UV-Vis spectrophotometry of quinone flow battery electrolyte for in situ monitoring and improved electrochemical modeling of potential and quinhydrone formation. Physical Chemistry Chemical Physics, 2017, 19, 31684-31691.	1.3	57
157	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartreeâ€“Fock. ACS Central Science, 2018, 4, 559-566.	5.3	57
158	Designing and understanding light-harvesting devices with machine learning. Nature Communications, 2020, 11, 4587.	5.8	57
159	Selfâ€Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. Advanced Functional Materials, 2021, 31, 2106725.	7.8	57
160	Nonradiative lifetimes in intermediate band photovoltaicsâ€”Absence of lifetime recovery. Journal of Applied Physics, 2012, 112, .	1.1	56
161	Disentangling Electronic and Vibronic Coherences in Two-Dimensional Echo Spectra. Journal of Physical Chemistry B, 2013, 117, 9380-9385.	1.2	55
162	Topologically protected excitons in porphyrin thinÂfilms. Nature Materials, 2014, 13, 1026-1032.	13.3	55

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163	Quantum Monte Carlo for electronic excitations of free-base porphyrin. Journal of Chemical Physics, 2004, 120, 3049-3050.	1.2	54
164	Linear assignment maps for correlated system-environment states. Physical Review A, 2010, 81, .	1.0	54
165	Real-Space Density Functional Theory on Graphical Processing Units: Computational Approach and Comparison to Gaussian Basis Set Methods. Journal of Chemical Theory and Computation, 2013, 9, 4360-4373.	2.3	53
166	Exponentially more precise quantum simulation of fermions in the configuration interaction representation. Quantum Science and Technology, 2018, 3, 015006.	2.6	53
167	Quantum algorithm for molecular properties and geometry optimization. Journal of Chemical Physics, 2009, 131, 224102.	1.2	52
168	Prediction of the Derivative Discontinuity in Density Functional Theory from an Electrostatic Description of the Exchange and Correlation Potential. Physical Review Letters, 2011, 107, 183002.	2.9	52
169	Demon-like algorithmic quantum cooling and its realization with quantum optics. Nature Photonics, 2014, 8, 113-118.	15.6	52
170	Introducing a New Potential Figure of Merit for Evaluating Microstructure Stability in Photovoltaic Polymer-Fullerene Blends. Journal of Physical Chemistry C, 2017, 121, 18153-18161.	1.5	52
171	Variational Quantum Factoring. Lecture Notes in Computer Science, 2019, , 74-85.	1.0	52
172	Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance. Scientific Reports, 2011, 1, 88.	1.6	51
173	Quantum process tomography of excitonic dimers from two-dimensional electronic spectroscopy. I. General theory and application to homodimers. Journal of Chemical Physics, 2011, 134, 134505.	1.2	51
174	Language models can learn complex molecular distributions. Nature Communications, 2022, 13, .	5.8	51
175	Digital quantum simulation of the statistical mechanics of a frustrated magnet. Nature Communications, 2012, 3, 880.	5.8	50
176	Compressed Sensing for Multidimensional Spectroscopy Experiments. Journal of Physical Chemistry Letters, 2012, 3, 2697-2702.	2.1	50
177	Bounding the costs of quantum simulation of many-body physics in real space. Journal of Physics A: Mathematical and Theoretical, 2017, 50, 305301.	0.7	47
178	Preparation of many-body states for quantum simulation. Journal of Chemical Physics, 2009, 130, 194105.	1.2	46
179	Coherent Exciton Dynamics in Supramolecular Light-Harvesting Nanotubes Revealed by Ultrafast Quantum Process Tomography. ACS Nano, 2014, 8, 5527-5534.	7.3	46
180	Uncertainty of Prebiotic Scenarios: The Case of the Non-Enzymatic Reverse Tricarboxylic Acid Cycle. Scientific Reports, 2015, 5, 8009.	1.6	46

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181	A Nanophotonic Structure Containing Living Photosynthetic Bacteria. Small, 2017, 13, 1701777.	5.2	46
182	Fighting the curse of dimensionality in first-principles semiclassical calculations: Non-local reference states for large number of dimensions. Journal of Chemical Physics, 2011, 135, 214108.	1.2	45
183	Reproducing Deep Tunneling Splittings, Resonances, and Quantum Frequencies in Vibrational Spectra From a Handful of Direct Ab Initio Semiclassical Trajectories. Journal of Physical Chemistry Letters, 2013, 4, 3407-3412.	2.1	45
184	Accelerating Correlated Quantum Chemistry Calculations Using Graphical Processing Units. Computing in Science and Engineering, 2010, 12, 40-51.	1.2	44
185	Layer-by-Layer Assembled Films of Perylene Diimide- and Squaraine-Containing Metalâ€“Organic Framework-like Materials: Solar Energy Capture and Directional Energy Transfer. ACS Applied Materials & Interfaces, 2016, 8, 24983-24988.	4.0	44
186	Tunneling across SAMs Containing Oligophenyl Groups. Journal of Physical Chemistry C, 2016, 120, 11331-11337.	1.5	43
187	Interface Molecular Engineering for Laminated Monolithic Perovskite/Silicon Tandem Solar Cells with 80.4% Fill Factor. Advanced Functional Materials, 2019, 29, 1901476.	7.8	43
188	A feasible approach for automatically differentiable unitary coupled-cluster on quantum computers. Chemical Science, 2021, 12, 3497-3508.	3.7	43
189	Multipartite quantum entanglement evolution in photosynthetic complexes. Journal of Chemical Physics, 2012, 137, 074112.	1.2	42
190	Computational complexity in electronic structure. Physical Chemistry Chemical Physics, 2013, 15, 397-411.	1.3	42
191	Chiral Sugars Drive Enantioenrichment in Prebiotic Amino Acid Synthesis. ACS Central Science, 2017, 3, 322-328.	5.3	42
192	A witness for coherent electronic vs vibronic-only oscillations in ultrafast spectroscopy. Journal of Chemical Physics, 2012, 136, 234501.	1.2	41
193	Theoretical characterization of excitation energy transfer in chlorosome light-harvesting antennae from green sulfur bacteria. Photosynthesis Research, 2014, 120, 273-289.	1.6	41
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