AlÃ¡n Aspuru Guzik

List of Publications by Year
in descending order

377 papers	46,721 citations	2802 94 h-index	2127 203 g-index
416 all docs	416 docs citations	416 times ranked	31972 citing authors

#	Article	IF	Citations
1	A Comprehensive Discovery Platform for Organophosphorus Ligands for Catalysis. Journal of the American Chemical Society, 2022, 144, 1205-1217.	13.7	97
2	Routescore: Punching the Ticket to More Efficient Materials Development. ACS Central Science, 2022, 8, 122-131.	11.3	8
3	In silico design of microporous polymers for chemical separations and storage. Current Opinion in Chemical Engineering, 2022, 36, 100795.	7.8	6
4	A forward view for Digital Discovery: the scientific challenges of the twenty-first century require accelerated discovery approaches. , 2022, 1, 6-7.		2
5	A quantum computing view on unitary coupled cluster theory. Chemical Society Reviews, 2022, 51, 1659-1684.	38.1	83
6	Noisy intermediate-scale quantum algorithms. Reviews of Modern Physics, 2022, 94, .	45.6	521
7	Experimental High-Dimensional Greenberger-Horne-Zeilinger Entanglement with Superconducting Transmon Qutrits. Physical Review Applied, 2022, 17, .	3.8	41
8	Updated Calibrated Model for the Prediction of Molecular Frontier Orbital Energies and Its Application to Boron Subphthalocyanines. Journal of Chemical Information and Modeling, 2022, 62, 829-840.	5.4	2
9	Optimized low-depth quantum circuits for molecular electronic structure using a separable-pair approximation. Physical Review A, 2022, 105, .	2.5	19
10	Learning quantum dynamics with latent neural ordinary differential equationsÂ. Physical Review A, 2022, 105, .	2.5	10
11	Parallel tempered genetic algorithm guided by deep neural networks for inverse molecular design. , 2022, 1, 390-404.		22
12	Toward Quantum Computing with Molecular Electronics. Journal of Chemical Theory and Computation, 2022, 18, 3318-3326.	5.3	5
13	Improving the accuracy of the variational quantum eigensolver for molecular systems by the explicitly-correlated perturbative [2]_{R12}-correction. Physical Chemistry Chemical Physics, 2022, 24, 13550-13564.	2.8	12
14	Language models can learn complex molecular distributions. Nature Communications, 2022, 13, .	12.8	51
15	Learning interpretable representations of entanglement in quantum optics experiments using deep generative models. Nature Machine Intelligence, 2022, 4, 544-554.	16.0	12
16	Curiosity in exploring chemical spaces: intrinsic rewards for molecular reinforcement learning. Machine Learning: Science and Technology, 2022, 3, 035008.	5.0	7
17	The influence of sorbitol doping on aggregation and electronic properties of PEDOT:PSS: a theoretical study. Machine Learning: Science and Technology, 2021, 2, 01LT01.	5.0	4
18	Reducing Qubit Requirements while Maintaining Numerical Precision for the Variational Quantum Eigensolver: A Basis-Set-Free Approach. Journal of Physical Chemistry Letters, 2021, 12, 663-673.	4.6	33

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19	Quantum computing at the frontiers of biological sciences. Nature Methods, 2021, 18, 701-709.	19.0	64
20	A feasible approach for automatically differentiable unitary coupled-cluster on quantum computers. Chemical Science, 2021, 12, 3497-3508.	7.4	43
21	Inverse design of nanoporous crystalline reticular materials with deep generative models. Nature Machine Intelligence, 2021, 3, 76-86.	16.0	172
22	Coronene derivatives for transparent organic photovoltaics through inverse materials design. Journal of Materials Chemistry C, 2021, 9, 1310-1317.	5.5	12
23	Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning. Trends in Chemistry, 2021, 3, 96-110.	8.5	39
24	Data-Driven Strategies for Accelerated Materials Design. Accounts of Chemical Research, 2021, 54, 849-860.	15.6	168
25	Automated design of superconducting circuits and its application to 4-local couplers. Npj Quantum Information, 2021, 7, .	6.7	17
26	TEQUILA: a platform for rapid development of quantum algorithms. Quantum Science and Technology, 2021, 6, 024009.	5.8	36
27	Analog Quantum Simulation of Non-Condon Effects in Molecular Spectroscopy. ACS Photonics, 2021, 8, 2007-2016.	6.6	8
28	Scientific intuition inspired by machine learning-generated hypotheses. Machine Learning: Science and Technology, 2021, 2, 025027.	5.0	23
29	A molecular computing approach to solving optimization problems via programmable microdroplet arrays. Matter, 2021, 4, 1107-1124.	10.0	7
30	Noise Robustness and Experimental Demonstration of a Quantum Generative Adversarial Network for Continuous Distributions. Advanced Quantum Technologies, 2021, 4, 2000069.	3.9	8
31	An artificial spiking quantum neuron. Npj Quantum Information, 2021, 7, .	6.7	12
32	Machine-learned potentials for next-generation matter simulations. Nature Materials, 2021, 20, 750-761.	27.5	214
33	Organic molecules with inverted gaps between first excited singlet and triplet states and appreciable fluorescence rates. Matter, 2021, 4, 1654-1682.	10.0	67
34	Meta-Variational Quantum Eigensolver: Learning Energy Profiles of Parameterized Hamiltonians for Quantum Simulation. PRX Quantum, 2021, 2, .	9.2	33
35	Machine learning the quantum-chemical properties of metalâ€“organic frameworks for accelerated materials discovery. Matter, 2021, 4, 1578-1597.	10.0	170
36	Assigning confidence to molecular property prediction. Expert Opinion on Drug Discovery, 2021, 16, 1009-1023.	5.0	34

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37	Deep molecular dreaming: inverse machine learning for de-novo molecular design and interpretability with surjective representations. Machine Learning: Science and Technology, 2021, 2, 03LT02.	5.0	22
38	Natural evolutionary strategies for variational quantum computation. Machine Learning: Science and Technology, 2021, 2, 045012.	5.0	16
39	Nanoparticle synthesis assisted by machine learning. Nature Reviews Materials, 2021, 6, 701-716.	48.7	179
40	Mutual information-assisted adaptive variational quantum eigensolver. Quantum Science and Technology, 2021, 6, 035001.	5.8	26
41	Quantum computer-aided design of quantum optics hardware. Quantum Science and Technology, 2021, 6, 035010.	5.8	13
42	Neural message passing on high order paths. Machine Learning: Science and Technology, 2021, 2, 045009.	5.0	16
43	Olympus: a benchmarking framework for noisy optimization and experiment planning. Machine Learning: Science and Technology, 2021, 2, 035021.	5.0	31
44	MPGVAE: improved generation of small organic molecules using message passing neural nets. Machine Learning: Science and Technology, 2021, 2, 045010.	5.0	7
45	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
46	Data-science driven autonomous process optimization. Communications Chemistry, 2021, 4, .	4.5	94
47	Machine learning directed drug formulation development. Advanced Drug Delivery Reviews, 2021, 175, 113806.	13.7	99
48	Conceptual Understanding through Efficient Automated Design of Quantum Optical Experiments. Physical Review X, 2021, 11, .	8.9	17
49	Selfâ€Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. Advanced Functional Materials, 2021, 31, 2106725.	14.9	57
50	G<scp>ryffin</scp>: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. Applied Physics Reviews, 2021, 8, .	11.3	61
51	You Wouldnâ€™t Download a Molecule! Now, ChemSCAD Makes It Possible. ACS Central Science, 2021, 7, 228-230.	11.3	1
52	Beyond generative models: superfast traversal, optimization, novelty, exploration and discovery (STONED) algorithm for molecules using SELFIES. Chemical Science, 2021, 12, 7079-7090.	7.4	64
53	Quantum computation of eigenvalues within target intervals. Quantum Science and Technology, 2021, 6, 015004.	5.8	7
54	Golem: an algorithm for robust experiment and process optimization. Chemical Science, 2021, 12, 14792-14807.	7.4	12

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55	funsies: A minimalist, distributed and dynamic workflow engine. Journal of Open Source Software, 2021, 6, 3274.	4.6	0
56	Quantum Computer-Aided Design: Digital Quantum Simulation of Quantum Processors. Physical Review Applied, 2021, 16, .	3.8	12
57	When robotics met fluidics. Lab on A Chip, 2020, 20, 709-716.	6.0	27
58	Effect of Molecular Structure of Quinones and Carbon Electrode Surfaces on the Interfacial Electron Transfer Process. ACS Applied Energy Materials, 2020, 3, 1933-1943.	5.1	38
59	Generative Adversarial Networks for Crystal Structure Prediction. ACS Central Science, 2020, 6, 1412-1420.	11.3	102
60	Resource-efficient digital quantum simulation of d-level systems for photonic, vibrational, and spin-s Hamiltonians. Npj Quantum Information, 2020, 6, .	6.7	74
61	Molecular Sets (MOSES): A Benchmarking Platform for Molecular Generation Models. Frontiers in Pharmacology, 2020, 11, 565644.	3.5	266
62	Bioinspiration in light harvesting and catalysis. Nature Reviews Materials, 2020, 5, 828-846.	48.7	136
63	Computer Vision for Recognition of Materials and Vessels in Chemistry Lab Settings and the Vector-LabPics Data Set. ACS Central Science, 2020, 6, 1743-1752.	11.3	25
64	Designing and understanding light-harvesting devices with machine learning. Nature Communications, 2020, 11, 4587.	12.8	57
65	Interface chemistry of an amide electrolyte for highly reversible lithium metal batteries. Nature Communications, 2020, 11, 4188.	12.8	226
66	Rational design of layered oxide materials for sodium-ion batteries. Science, 2020, 370, 708-711.	12.6	616
67	Optically Induced Molecular Logic Operations. ACS Nano, 2020, 14, 15248-15255.	14.6	6
68	A machine learning workflow for molecular analysis: application to melting points. Machine Learning: Science and Technology, 2020, 1, 025015.	5.0	23
69	Self-driving laboratory for accelerated discovery of thin-film materials. Science Advances, 2020, 6, eaaz8867.	10.3	306
70	Materials Acceleration Platforms: On the way to autonomous experimentation. Current Opinion in Green and Sustainable Chemistry, 2020, 25, 100370.	5.9	67
71	Quantum computational chemistry. Reviews of Modern Physics, 2020, 92, .	45.6	726
72	Boramidine: A Versatile Structural Motif for the Design of Fluorescent Heterocycles. Journal of the American Chemical Society, 2020, 142, 13544-13549.	13.7	7

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73	The Cyclopropane Ring as a Reporter of Radical Leaving-Group Reactivity for Ni-Catalyzed C(sp³)â€“O Arylation. Journal of the American Chemical Society, 2020, 142, 13246-13254.	13.7	34
74	Machine learning for analysing ab initio molecular dynamics simulations. Journal of Physics: Conference Series, 2020, 1412, 042003.	0.4	6
75	Team-Based Learning for Scientific Computing and Automated Experimentation: Visualization of Colored Reactions. Journal of Chemical Education, 2020, 97, 689-694.	2.3	15
76	Constructing Naâ€Ion Cathodes via Alkaliâ€Site Substitution. Advanced Functional Materials, 2020, 30, 1910840.	14.9	28
77	Revealing High Na-Content P2-Type Layered Oxides as Advanced Sodium-Ion Cathodes. Journal of the American Chemical Society, 2020, 142, 5742-5750.	13.7	206
78	Optical monitoring of polymerizations in droplets with high temporal dynamic range. Chemical Science, 2020, 11, 2647-2656.	7.4	18
79	Beyond Ternary OPV: Highâ€Throughput Experimentation and Selfâ€Driving Laboratories Optimize Multicomponent Systems. Advanced Materials, 2020, 32, e1907801.	21.0	138
80	Reply to â€˜Assessing the impact of generative AI on medicinal chemistryâ€™. Nature Biotechnology, 2020, 38, 146-146.	17.5	11
81	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
82	Film Fabrication Techniques: Beyond Ternary OPV: Highâ€Throughput Experimentation and Selfâ€Driving Laboratories Optimize Multicomponent Systems (Adv. Mater. 14/2020). Advanced Materials, 2020, 32, 2070110.	21.0	2
83	Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. Chemical Science, 2020, 11, 4584-4601.	7.4	93
84	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. ACS Nano, 2020, 14, 6589-6598.	14.6	12
85	ChemOS: An orchestration software to democratize autonomous discovery. PLoS ONE, 2020, 15, e0229862.	2.5	77
86	Machine Learning and Big-Data in Computational Chemistry. , 2020, , 1939-1962.		5
87	A thermodynamic atlas of carbon redox chemical space. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 32910-32918.	7.1	11
88	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. Machine Learning: Science and Technology, 2020, 1, 045024.	5.0	272
89	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	2.8	236
90	Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. Quantum Science and Technology, 2019, 4, 014008.	5.8	381

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91	In Situ Electron Microscopy Investigation of Sodiation of Titanium Disulfide Nanoflakes. ACS Nano, 2019, 13, 9421-9430.	14.6	30
92	Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer. Quantum Science and Technology, 2019, 4, 045005.	5.8	69
93	Interface Molecular Engineering for Laminated Monolithic Perovskite/Silicon Tandem Solar Cells with 80.4% Fill Factor. Advanced Functional Materials, 2019, 29, 1901476.	14.9	43
94	Molecular Engineering of an Alkaline Naphthoquinone Flow Battery. ACS Energy Letters, 2019, 4, 1880-1887.	17.4	90
95	Design rules for high mobility xanthene-based hole transport materials. Chemical Science, 2019, 10, 8360-8366.	7.4	20
96	Generalized Kashaâ€™s Model: T-Dependent Spectroscopy Reveals Short-Range Structures of 2D Excitonic Systems. CheM, 2019, 5, 3135-3150.	11.7	20
97	Oscillatory Active-Site Motions Correlate with Kinetic Isotope Effects in Formate Dehydrogenase. ACS Catalysis, 2019, 9, 11199-11206.	11.2	29
98	Quantum Chemistry in the Age of Quantum Computing. Chemical Reviews, 2019, 119, 10856-10915.	47.7	748
99	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nature Biotechnology, 2019, 37, 1038-1040.	17.5	671
100	Identification Schemes for Metalâ€“Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. Crystal Growth and Design, 2019, 19, 6682-6697.	3.0	123
101	Discovery of blue singlet exciton fission molecules via a high-throughput virtual screening and experimental approach. Journal of Chemical Physics, 2019, 151, 121102.	3.0	24
102	Inverse Design of Solid-State Materials via a Continuous Representation. Matter, 2019, 1, 1370-1384.	10.0	198
103	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.	11.3	61
104	Predicting Feasible Organic Reaction Pathways Using Heuristically Aided Quantum Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 4099-4112.	5.3	27
105	Next-Generation Experimentation with Self-Driving Laboratories. Trends in Chemistry, 2019, 1, 282-291.	8.5	175
106	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.	10.3	128
107	Autonomous Molecular Design: Then and Now. ACS Applied Materials & Interfaces, 2019, 11, 24825-24836.	8.0	69
108	Variational Quantum Factoring. Lecture Notes in Computer Science, 2019, , 74-85.	1.3	52

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109	Extending the Lifetime of Organic Flow Batteries via Redox State Management. Journal of the American Chemical Society, 2019, 141, 8014-8019.	13.7	151
110	Quantum Coherences as a Thermodynamic Potential. Open Systems and Information Dynamics, 2019, 26, 1950022.	1.2	2
111	Expressibility and Entangling Capability of Parameterized Quantum Circuits for Hybrid Quantumâ€Classical Algorithms. Advanced Quantum Technologies, 2019, 2, 1900070.	3.9	298
112	A Bayesian Approach to Predict Solubility Parameters. Advanced Theory and Simulations, 2019, 2, 1800069.	2.8	62
113	How machine learning can assist the interpretation of ab initio molecular dynamics simulations and conceptual understanding of chemistry. Chemical Science, 2019, 10, 2298-2307.	7.4	80
114	Molecular realization of a quantum <tt>NAND</tt> tree. Quantum Science and Technology, 2019, 4, 015013.	5.8	6
115	Discovery of Calciumâ€Metal Alloy Anodes for Reversible Caâ€Ion Batteries. Advanced Energy Materials, 2019, 9, 1802994.	19.5	61
116	Closed-loop discovery platform integration is needed for artificial intelligence to make an impact in drug discovery. Expert Opinion on Drug Discovery, 2019, 14, 1-4.	5.0	37
117	Temperature-dependent conformations of exciton-coupled Cy3 dimers in double-stranded DNA. Journal of Chemical Physics, 2018, 148, 085101.	3.0	58
118	Mechanistic Regimes of Vibronic Transport in a Heterodimer and the Design Principle of Incoherent Vibronic Transport in Phycobiliproteins. Journal of Physical Chemistry Letters, 2018, 9, 2665-2670.	4.6	32
119	Single-Atom Heat Machines Enabled by Energy Quantization. Physical Review Letters, 2018, 120, 170601.	7.8	41
120	The Matter Simulation (R)evolution. ACS Central Science, 2018, 4, 144-152.	11.3	88
121	Exploring Electronic Structure and Order in Polymers via Single-Particle Microresonator Spectroscopy. Nano Letters, 2018, 18, 1600-1607.	9.1	23
122	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. ACS Central Science, 2018, 4, 268-276.	11.3	1,761
123	Oxidation of rubrene, and implications for device stability. Journal of Materials Chemistry C, 2018, 6, 3757-3761.	5.5	17
124	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
125	Photochemical Control of Exciton Superradiance in Light-Harvesting Nanotubes. ACS Nano, 2018, 12, 4556-4564.	14.6	34
126	Flow Batteries: Alkaline Benzoquinone Aqueous Flow Battery for Largeâ€Scale Storage of Electrical Energy (Adv. Energy Mater. 8/2018). Advanced Energy Materials, 2018, 8, 1870034.	19.5	30

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127	Disentanglement of excited-state dynamics with implications for FRET measurements: two-dimensional electronic spectroscopy of a BODIPY-functionalized cavitand. Chemical Science, 2018, 9, 3694-3703.	7.4	13
128	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.	7.1	61
129	Reproducing Quantum Probability Distributions at the Speed of Classical Dynamics: A New Approach for Developing Force-Field Functors. Journal of Physical Chemistry Letters, 2018, 9, 1721-1727.	4.6	1
130	Quantum Simulation of Electronic Structure with Linear Depth and Connectivity. Physical Review Letters, 2018, 120, 110501.	7.8	243
131	Exponentially more precise quantum simulation of fermions in the configuration interaction representation. Quantum Science and Technology, 2018, 3, 015006.	5.8	53
132	Alkaline Benzoquinone Aqueous Flow Battery for Largeâ€Scale Storage of Electrical Energy. Advanced Energy Materials, 2018, 8, 1702056.	19.5	161
133	Programmed coherent coupling in a synthetic DNA-based excitonic circuit. Nature Materials, 2018, 17, 159-166.	27.5	106
134	Quantum Computer Simulates Excited States of Molecule. Physics Magazine, 2018, 11, .	0.1	4
135	qTorch: The quantum tensor contraction handler. PLoS ONE, 2018, 13, e0208510.	2.5	31
136	Potential of quantum computing for drug discovery. IBM Journal of Research and Development, 2018, 62, 6:1-6:20.	3.1	130
137	Precise Control of Thermal and Redox Properties of Organic Holeâ€Transport Materials. Angewandte Chemie - International Edition, 2018, 57, 15529-15533.	13.8	41
138	Alkaline Quinone Flow Battery with Long Lifetime at pH 12. Joule, 2018, 2, 1907-1908.	24.0	37
139	Precise Control of Thermal and Redox Properties of Organic Holeâ€Transport Materials. Angewandte Chemie, 2018, 130, 15755-15759.	2.0	15
140	Machine Learning and Big-Data in Computational Chemistry. , 2018, , 1-24.		4
141	Quantum chemistry reveals thermodynamic principles of redox biochemistry. PLoS Computational Biology, 2018, 14, e1006471.	3.2	22
142	Mapping Forbidden Emission to Structure in Self-Assembled Organic Nanoparticles. Journal of the American Chemical Society, 2018, 140, 15827-15841.	13.7	21
143	Origin of the 1/fÎ± spectral noise in chaotic and regular quantum systems. Physical Review E, 2018, 98, .	2.1	8
144	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. Chemical Science, 2018, 9, 7642-7655.	7.4	86

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145	Reinforced Adversarial Neural Computer for de Novo Molecular Design. Journal of Chemical Information and Modeling, 2018, 58, 1194-1204.	5.4	256
146	Excitonics: A Set of Gates for Molecular Exciton Processing and Signaling. ACS Nano, 2018, 12, 6410-6420.	14.6	26
147	Alkaline Quinone Flow Battery with Long Lifetime at pH 12. Joule, 2018, 2, 1894-1906.	24.0	293
148	Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator. Physical Review X, 2018, 8, .	8.9	342
149	Inverse molecular design using machine learning: Generative models for matter engineering. Science, 2018, 361, 360-365.	12.6	1,055
150	High-Voltage-Assisted Mechanical Stabilization of Single-Molecule Junctions. Nano Letters, 2018, 18, 4727-4733.	9.1	20
151	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartreeâ€“Fock. ACS Central Science, 2018, 4, 559-566.	11.3	57
152	Phoenics: A Bayesian Optimizer for Chemistry. ACS Central Science, 2018, 4, 1134-1145.	11.3	215
153	ChemOS: Orchestrating autonomous experimentation. Science Robotics, 2018, 3, .	17.6	113
154	Learning More, with Less. ACS Central Science, 2017, 3, 275-277.	11.3	6
155	Anomalously Rapid Tunneling: Charge Transport across Self-Assembled Monolayers of Oligo(ethylene) Tj ETQq1 1 0.784314 rgBT /Overl	13.7	41
156	Equivalence between spin Hamiltonians and boson sampling. Physical Review A, 2017, 95, .	2.5	13
157	An Alternative Host Material for Longâ€Lifespan Blue Organic Lightâ€Emitting Diodes Using Thermally Activated Delayed Fluorescence. Advanced Science, 2017, 4, 1600502.	11.2	103
158	Chiral Sugars Drive Enantioenrichment in Prebiotic Amino Acid Synthesis. ACS Central Science, 2017, 3, 322-328.	11.3	42
159	Using coherence to enhance function in chemical and biophysical systems. Nature, 2017, 543, 647-656.	27.8	477
160	MultiDK: A Multiple Descriptor Multiple Kernel Approach for Molecular Discovery and Its Application to Organic Flow Battery Electrolytes. Journal of Chemical Information and Modeling, 2017, 57, 657-668.	5.4	24
161	A Study of the Degree of Fluorination in Regioregular Poly(3-hexylthiophene). Macromolecules, 2017, 50, 162-174.	4.8	30
162	Emulation of complex open quantum systems using superconducting qubits. Quantum Information Processing, 2017, 16, 1.	2.2	23

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163	Anthraquinone Derivatives in Aqueous Flow Batteries. Advanced Energy Materials, 2017, 7, 1601488.	19.5	189
164	On the Long-Range Exciton Transport in Molecular Systems: The Application to H-Aggregated Heterotriangulene Chains. Journal of Physical Chemistry C, 2017, 121, 24994-25002.	3.1	21
165	Machine learning for quantum dynamics: deep learning of excitation energy transfer properties. Chemical Science, 2017, 8, 8419-8426.	7.4	70
166	Absence of Selection for Quantum Coherence in the Fennaâ€“Matthewsâ€“Olson Complex: A Combined Evolutionary and Excitonic Study. ACS Central Science, 2017, 3, 1086-1095.	11.3	11
167	Bounding the costs of quantum simulation of many-body physics in real space. Journal of Physics A: Mathematical and Theoretical, 2017, 50, 305301.	2.1	47
168	A Nanophotonic Structure Containing Living Photosynthetic Bacteria. Small, 2017, 13, 1701777.	10.0	46
169	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.	2.8	57
170	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. Joule, 2017, 1, 857-870.	24.0	157
171	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.	3.1	52
172	Taking six-dimensional spectra in finite time. Science, 2017, 356, 1333-1333.	12.6	2
173	On thermodynamic inconsistencies in several photosynthetic and solar cell models and how to fix them. Chemical Science, 2017, 8, 1008-1014.	7.4	25
174	Quantum autoencoders for efficient compression of quantum data. Quantum Science and Technology, 2017, 2, 045001.	5.8	295
175	Use machine learning to find energy materials. Nature, 2017, 552, 23-27.	27.8	85
176	Renewables need a grand-challenge strategy. Nature, 2016, 538, 30-30.	27.8	27
177	Benchmarking compressed sensing, super-resolution, and filter diagonalization. International Journal of Quantum Chemistry, 2016, 116, 1097-1106.	2.0	3
178	Exponentially more precise quantum simulation of fermions in second quantization. New Journal of Physics, 2016, 18, 033032.	2.9	100
179	Error Sensitivity to Environmental Noise in Quantum Circuits for Chemical State Preparation. Journal of Chemical Theory and Computation, 2016, 12, 3097-3108.	5.3	27
180	Faster than classical quantum algorithm for dense formulas of exact satisfiability and occupation problems. New Journal of Physics, 2016, 18, 073003.	2.9	21

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181	Machine learning exciton dynamics. Chemical Science, 2016, 7, 5139-5147.	7.4	112
182	Tunneling across SAMs Containing Oligophenyl Groups. Journal of Physical Chemistry C, 2016, 120, 11331-11337.	3.1	43
183	Efficiency of energy funneling in the photosystem II supercomplex of higher plants. Chemical Science, 2016, 7, 4174-4183.	7.4	30
184	Turbocharged molecular discovery of OLED emitters: from high-throughput quantum simulation to highly efficient TADF devices. Proceedings of SPIE, 2016, , .	0.8	3
185	Quantum simulation with a boson sampling circuit. Physical Review A, 2016, 94, .	2.5	7
186	Proposal for Microwave Boson Sampling. Physical Review Letters, 2016, 117, 140505.	7.8	40
187	Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. Nature Materials, 2016, 15, 1120-1127.	27.5	708
188	Response to: â€œComment on benchmarking compressed sensing, superâ€resolution, and filter diagonalizationâ€. International Journal of Quantum Chemistry, 2016, 116, 1818-1821.	2.0	0
189	Accelerating the computation of bath spectral densities with super-resolution. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
190	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.	8.0	44
191	Scalable Quantum Simulation of Molecular Energies. Physical Review X, 2016, 6, .	8.9	577
192	Neural Networks for the Prediction of Organic Chemistry Reactions. ACS Central Science, 2016, 2, 725-732.	11.3	321
193	Optical Spectra of p-Doped PEDOT Nanoaggregates Provide Insight into the Material Disorder. ACS Energy Letters, 2016, 1, 1100-1105.	17.4	5
194	A redox-flow battery with an alloxazine-based organic electrolyte. Nature Energy, 2016, 1, .	39.5	427
195	The Harvard organic photovoltaic dataset. Scientific Data, 2016, 3, 160086.	5.3	85
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