

AlĀ;n Aspuru Guzik

List of Publications by Year in descending order

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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	A Comprehensive Discovery Platform for Organophosphorus Ligands for Catalysis. <i>Journal of the American Chemical Society</i> , 2022, 144, 1205-1217.	6.6	97
2	Routescor: Punching the Ticket to More Efficient Materials Development. <i>ACS Central Science</i> , 2022, 8, 122-131.	5.3	8
3	In silico design of microporous polymers for chemical separations and storage. <i>Current Opinion in Chemical Engineering</i> , 2022, 36, 100795.	3.8	6
4	A forward view for <i>Digital Discovery</i> : 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. <i>Chemical Society Reviews</i> , 2022, 51, 1659-1684.	18.7	83
6	Noisy intermediate-scale quantum algorithms. <i>Reviews of Modern Physics</i> , 2022, 94, .	16.4	521
7	Experimental High-Dimensional Greenberger-Horne-Zeilinger Entanglement with Superconducting Transmon Qubits. <i>Physical Review Applied</i> , 2022, 17, .	1.5	41
8	Updated Calibrated Model for the Prediction of Molecular Frontier Orbital Energies and Its Application to Boron Subphthalocyanines. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 829-840.	2.5	2
9	Optimized low-depth quantum circuits for molecular electronic structure using a separable-pair approximation. <i>Physical Review A</i> , 2022, 105, .	1.0	19
10	Learning quantum dynamics with latent neural ordinary differential equations. <i>Physical Review A</i> , 2022, 105, .	1.0	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. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3318-3326.	2.3	5
13	Improving the accuracy of the variational quantum eigensolver for molecular systems by the explicitly-correlated perturbative [2] _{R12} correction. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13550-13564.	1.3	12
14	Language models can learn complex molecular distributions. <i>Nature Communications</i> , 2022, 13, .	5.8	51
15	Learning interpretable representations of entanglement in quantum optics experiments using deep generative models. <i>Nature Machine Intelligence</i> , 2022, 4, 544-554.	8.3	12
16	Curiosity in exploring chemical spaces: intrinsic rewards for molecular reinforcement learning. <i>Machine Learning: Science and Technology</i> , 2022, 3, 035008.	2.4	7
17	The influence of sorbitol doping on aggregation and electronic properties of PEDOT:PSS: a theoretical study. <i>Machine Learning: Science and Technology</i> , 2021, 2, 01LT01.	2.4	4
18	Reducing Qubit Requirements while Maintaining Numerical Precision for the Variational Quantum Eigensolver: A Basis-Set-Free Approach. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 663-673.	2.1	33

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19	Quantum computing at the frontiers of biological sciences. <i>Nature Methods</i> , 2021, 18, 701-709.	9.0	64
20	A feasible approach for automatically differentiable unitary coupled-cluster on quantum computers. <i>Chemical Science</i> , 2021, 12, 3497-3508.	3.7	43
21	Inverse design of nanoporous crystalline reticular materials with deep generative models. <i>Nature Machine Intelligence</i> , 2021, 3, 76-86.	8.3	172
22	Coronene derivatives for transparent organic photovoltaics through inverse materials design. <i>Journal of Materials Chemistry C</i> , 2021, 9, 1310-1317.	2.7	12
23	Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning. <i>Trends in Chemistry</i> , 2021, 3, 96-110.	4.4	39
24	Data-Driven Strategies for Accelerated Materials Design. <i>Accounts of Chemical Research</i> , 2021, 54, 849-860.	7.6	168
25	Automated design of superconducting circuits and its application to 4-local couplers. <i>Npj Quantum Information</i> , 2021, 7, .	2.8	17
26	TEQUILA: a platform for rapid development of quantum algorithms. <i>Quantum Science and Technology</i> , 2021, 6, 024009.	2.6	36
27	Analog Quantum Simulation of Non-Condon Effects in Molecular Spectroscopy. <i>ACS Photonics</i> , 2021, 8, 2007-2016.	3.2	8
28	Scientific intuition inspired by machine learning-generated hypotheses. <i>Machine Learning: Science and Technology</i> , 2021, 2, 025027.	2.4	23
29	A molecular computing approach to solving optimization problems via programmable microdroplet arrays. <i>Matter</i> , 2021, 4, 1107-1124.	5.0	7
30	Noise Robustness and Experimental Demonstration of a Quantum Generative Adversarial Network for Continuous Distributions. <i>Advanced Quantum Technologies</i> , 2021, 4, 2000069.	1.8	8
31	An artificial spiking quantum neuron. <i>Npj Quantum Information</i> , 2021, 7, .	2.8	12
32	Machine-learned potentials for next-generation matter simulations. <i>Nature Materials</i> , 2021, 20, 750-761.	13.3	214
33	Organic molecules with inverted gaps between first excited singlet and triplet states and appreciable fluorescence rates. <i>Matter</i> , 2021, 4, 1654-1682.	5.0	67
34	Meta-Variational Quantum Eigensolver: Learning Energy Profiles of Parameterized Hamiltonians for Quantum Simulation. <i>PRX Quantum</i> , 2021, 2, .	3.5	33
35	Machine learning the quantum-chemical properties of metal-organic frameworks for accelerated materials discovery. <i>Matter</i> , 2021, 4, 1578-1597.	5.0	170
36	Assigning confidence to molecular property prediction. <i>Expert Opinion on Drug Discovery</i> , 2021, 16, 1009-1023.	2.5	34

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37	Deep molecular dreaming: inverse machine learning for de-novo molecular design and interpretability with surjective representations. <i>Machine Learning: Science and Technology</i> , 2021, 2, 03LT02.	2.4	22
38	Natural evolutionary strategies for variational quantum computation. <i>Machine Learning: Science and Technology</i> , 2021, 2, 045012.	2.4	16
39	Nanoparticle synthesis assisted by machine learning. <i>Nature Reviews Materials</i> , 2021, 6, 701-716.	23.3	179
40	Mutual information-assisted adaptive variational quantum eigensolver. <i>Quantum Science and Technology</i> , 2021, 6, 035001.	2.6	26
41	Quantum computer-aided design of quantum optics hardware. <i>Quantum Science and Technology</i> , 2021, 6, 035010.	2.6	13
42	Neural message passing on high order paths. <i>Machine Learning: Science and Technology</i> , 2021, 2, 045009.	2.4	16
43	Olympus: a benchmarking framework for noisy optimization and experiment planning. <i>Machine Learning: Science and Technology</i> , 2021, 2, 035021.	2.4	31
44	MPGVAE: improved generation of small organic molecules using message passing neural nets. <i>Machine Learning: Science and Technology</i> , 2021, 2, 045010.	2.4	7
45	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
46	Data-science driven autonomous process optimization. <i>Communications Chemistry</i> , 2021, 4, .	2.0	94
47	Machine learning directed drug formulation development. <i>Advanced Drug Delivery Reviews</i> , 2021, 175, 113806.	6.6	99
48	Conceptual Understanding through Efficient Automated Design of Quantum Optical Experiments. <i>Physical Review X</i> , 2021, 11, .	2.8	17
49	Self-Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. <i>Advanced Functional Materials</i> , 2021, 31, 2106725.	7.8	57
50	G _{ryffin} : An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. <i>Applied Physics Reviews</i> , 2021, 8, .	5.5	61
51	You Wouldn't Download a Molecule! Now, ChemSCAD Makes It Possible. <i>ACS Central Science</i> , 2021, 7, 228-230.	5.3	1
52	Beyond generative models: superfast traversal, optimization, novelty, exploration and discovery (STONED) algorithm for molecules using SELFIES. <i>Chemical Science</i> , 2021, 12, 7079-7090.	3.7	64
53	Quantum computation of eigenvalues within target intervals. <i>Quantum Science and Technology</i> , 2021, 6, 015004.	2.6	7
54	Golem: an algorithm for robust experiment and process optimization. <i>Chemical Science</i> , 2021, 12, 14792-14807.	3.7	12

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55	funsies: A minimalist, distributed and dynamic workflow engine. <i>Journal of Open Source Software</i> , 2021, 6, 3274.	2.0	0
56	Quantum Computer-Aided Design: Digital Quantum Simulation of Quantum Processors. <i>Physical Review Applied</i> , 2021, 16, .	1.5	12
57	When robotics met fluidics. <i>Lab on A Chip</i> , 2020, 20, 709-716.	3.1	27
58	Effect of Molecular Structure of Quinones and Carbon Electrode Surfaces on the Interfacial Electron Transfer Process. <i>ACS Applied Energy Materials</i> , 2020, 3, 1933-1943.	2.5	38
59	Generative Adversarial Networks for Crystal Structure Prediction. <i>ACS Central Science</i> , 2020, 6, 1412-1420.	5.3	102
60	Resource-efficient digital quantum simulation of d-level systems for photonic, vibrational, and spin-S Hamiltonians. <i>Npj Quantum Information</i> , 2020, 6, .	2.8	74
61	Molecular Sets (MOSES): A Benchmarking Platform for Molecular Generation Models. <i>Frontiers in Pharmacology</i> , 2020, 11, 565644.	1.6	266
62	Bioinspiration in light harvesting and catalysis. <i>Nature Reviews Materials</i> , 2020, 5, 828-846.	23.3	136
63	Computer Vision for Recognition of Materials and Vessels in Chemistry Lab Settings and the Vector-LabPics Data Set. <i>ACS Central Science</i> , 2020, 6, 1743-1752.	5.3	25
64	Designing and understanding light-harvesting devices with machine learning. <i>Nature Communications</i> , 2020, 11, 4587.	5.8	57
65	Interface chemistry of an amide electrolyte for highly reversible lithium metal batteries. <i>Nature Communications</i> , 2020, 11, 4188.	5.8	226
66	Rational design of layered oxide materials for sodium-ion batteries. <i>Science</i> , 2020, 370, 708-711.	6.0	616
67	Optically Induced Molecular Logic Operations. <i>ACS Nano</i> , 2020, 14, 15248-15255.	7.3	6
68	A machine learning workflow for molecular analysis: application to melting points. <i>Machine Learning: Science and Technology</i> , 2020, 1, 025015.	2.4	23
69	Self-driving laboratory for accelerated discovery of thin-film materials. <i>Science Advances</i> , 2020, 6, eaaz8867.	4.7	306
70	Materials Acceleration Platforms: On the way to autonomous experimentation. <i>Current Opinion in Green and Sustainable Chemistry</i> , 2020, 25, 100370.	3.2	67
71	Quantum computational chemistry. <i>Reviews of Modern Physics</i> , 2020, 92, .	16.4	726
72	Boramidine: A Versatile Structural Motif for the Design of Fluorescent Heterocycles. <i>Journal of the American Chemical Society</i> , 2020, 142, 13544-13549.	6.6	7

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73	The Cyclopropane Ring as a Reporter of Radical Leaving-Group Reactivity for Ni-Catalyzed C(sp ³) ³ Arylation. <i>Journal of the American Chemical Society</i> , 2020, 142, 13246-13254.	6.6	34
74	Machine learning for analysing ab initio molecular dynamics simulations. <i>Journal of Physics: Conference Series</i> , 2020, 1412, 042003.	0.3	6
75	Team-Based Learning for Scientific Computing and Automated Experimentation: Visualization of Colored Reactions. <i>Journal of Chemical Education</i> , 2020, 97, 689-694.	1.1	15
76	Constructing Na-Ion Cathodes via Alkali-Site Substitution. <i>Advanced Functional Materials</i> , 2020, 30, 1910840.	7.8	28
77	Revealing High Na-Content P2-Type Layered Oxides as Advanced Sodium-Ion Cathodes. <i>Journal of the American Chemical Society</i> , 2020, 142, 5742-5750.	6.6	206
78	Optical monitoring of polymerizations in droplets with high temporal dynamic range. <i>Chemical Science</i> , 2020, 11, 2647-2656.	3.7	18
79	Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems. <i>Advanced Materials</i> , 2020, 32, e1907801.	11.1	138
80	Reply to "Assessing the impact of generative AI on medicinal chemistry". <i>Nature Biotechnology</i> , 2020, 38, 146-146.	9.4	11
81	QSAR without borders. <i>Chemical Society Reviews</i> , 2020, 49, 3525-3564.	18.7	427
82	Film Fabrication Techniques: Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems (Adv. Mater. 14/2020). <i>Advanced Materials</i> , 2020, 32, 2070110.	11.1	2
83	Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. <i>Chemical Science</i> , 2020, 11, 4584-4601.	3.7	93
84	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. <i>ACS Nano</i> , 2020, 14, 6589-6598.	7.3	12
85	ChemOS: An orchestration software to democratize autonomous discovery. <i>PLoS ONE</i> , 2020, 15, e0229862.	1.1	77
86	Machine Learning and Big-Data in Computational Chemistry. , 2020, , 1939-1962.		5
87	A thermodynamic atlas of carbon redox chemical space. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 32910-32918.	3.3	11
88	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. <i>Machine Learning: Science and Technology</i> , 2020, 1, 045024.	2.4	272
89	The 2019 materials by design roadmap. <i>Journal Physics D: Applied Physics</i> , 2019, 52, 013001.	1.3	236
90	Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. <i>Quantum Science and Technology</i> , 2019, 4, 014008.	2.6	381

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91	<i>In Situ</i> Electron Microscopy Investigation of Sodiation of Titanium Disulfide Nanoflakes. <i>ACS Nano</i> , 2019, 13, 9421-9430.	7.3	30
92	Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer. <i>Quantum Science and Technology</i> , 2019, 4, 045005.	2.6	69
93	Interface Molecular Engineering for Laminated Monolithic Perovskite/Silicon Tandem Solar Cells with 80.4% Fill Factor. <i>Advanced Functional Materials</i> , 2019, 29, 1901476.	7.8	43
94	Molecular Engineering of an Alkaline Naphthoquinone Flow Battery. <i>ACS Energy Letters</i> , 2019, 4, 1880-1887.	8.8	90
95	Design rules for high mobility xanthene-based hole transport materials. <i>Chemical Science</i> , 2019, 10, 8360-8366.	3.7	20
96	Generalized Kasha's Model: T-Dependent Spectroscopy Reveals Short-Range Structures of 2D Excitonic Systems. <i>Chem</i> , 2019, 5, 3135-3150.	5.8	20
97	Oscillatory Active-Site Motions Correlate with Kinetic Isotope Effects in Formate Dehydrogenase. <i>ACS Catalysis</i> , 2019, 9, 11199-11206.	5.5	29
98	Quantum Chemistry in the Age of Quantum Computing. <i>Chemical Reviews</i> , 2019, 119, 10856-10915.	23.0	748
99	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. <i>Nature Biotechnology</i> , 2019, 37, 1038-1040.	9.4	671
100	Identification Schemes for Metal-Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. <i>Crystal Growth and Design</i> , 2019, 19, 6682-6697.	1.4	123
101	Discovery of blue singlet exciton fission molecules via a high-throughput virtual screening and experimental approach. <i>Journal of Chemical Physics</i> , 2019, 151, 121102.	1.2	24
102	Inverse Design of Solid-State Materials via a Continuous Representation. <i>Matter</i> , 2019, 1, 1370-1384.	5.0	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 315,000 Redox Reactions. <i>ACS Central Science</i> , 2019, 5, 1199-1210.	5.3	61
104	Predicting Feasible Organic Reaction Pathways Using Heuristically Aided Quantum Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4099-4112.	2.3	27
105	Next-Generation Experimentation with Self-Driving Laboratories. <i>Trends in Chemistry</i> , 2019, 1, 282-291.	4.4	175
106	Mapping the frontiers of quinone stability in aqueous media: implications for organic aqueous redox flow batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 12833-12841.	5.2	128
107	Autonomous Molecular Design: Then and Now. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 24825-24836.	4.0	69
108	Variational Quantum Factoring. <i>Lecture Notes in Computer Science</i> , 2019, , 74-85.	1.0	52

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109	Extending the Lifetime of Organic Flow Batteries via Redox State Management. <i>Journal of the American Chemical Society</i> , 2019, 141, 8014-8019.	6.6	151
110	Quantum Coherences as a Thermodynamic Potential. <i>Open Systems and Information Dynamics</i> , 2019, 26, 1950022.	0.5	2
111	Expressibility and Entangling Capability of Parameterized Quantum Circuits for Hybrid Quantum-Classical Algorithms. <i>Advanced Quantum Technologies</i> , 2019, 2, 1900070.	1.8	298
112	A Bayesian Approach to Predict Solubility Parameters. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800069.	1.3	62
113	How machine learning can assist the interpretation of <i>ab initio</i> molecular dynamics simulations and conceptual understanding of chemistry. <i>Chemical Science</i> , 2019, 10, 2298-2307.	3.7	80
114	Molecular realization of a quantum NAND tree. <i>Quantum Science and Technology</i> , 2019, 4, 015013.	2.6	6
115	Discovery of Calcium-Metal Alloy Anodes for Reversible Ca-Ion Batteries. <i>Advanced Energy Materials</i> , 2019, 9, 1802994.	10.2	61
116	Closed-loop discovery platform integration is needed for artificial intelligence to make an impact in drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2019, 14, 1-4.	2.5	37
117	Temperature-dependent conformations of exciton-coupled Cy3 dimers in double-stranded DNA. <i>Journal of Chemical Physics</i> , 2018, 148, 085101.	1.2	58
118	Mechanistic Regimes of Vibronic Transport in a Heterodimer and the Design Principle of Incoherent Vibronic Transport in Phycobiliproteins. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2665-2670.	2.1	32
119	Single-Atom Heat Machines Enabled by Energy Quantization. <i>Physical Review Letters</i> , 2018, 120, 170601.	2.9	41
120	The Matter Simulation (R)evolution. <i>ACS Central Science</i> , 2018, 4, 144-152.	5.3	88
121	Exploring Electronic Structure and Order in Polymers via Single-Particle Microresonator Spectroscopy. <i>Nano Letters</i> , 2018, 18, 1600-1607.	4.5	23
122	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. <i>ACS Central Science</i> , 2018, 4, 268-276.	5.3	1,761
123	Oxidation of rubrene, and implications for device stability. <i>Journal of Materials Chemistry C</i> , 2018, 6, 3757-3761.	2.7	17
124	Accelerating the discovery of materials for clean energy in the era of smart automation. <i>Nature Reviews Materials</i> , 2018, 3, 5-20.	23.3	489
125	Photochemical Control of Exciton Superradiance in Light-Harvesting Nanotubes. <i>ACS Nano</i> , 2018, 12, 4556-4564.	7.3	34
126	Flow Batteries: Alkaline Benzoquinone Aqueous Flow Battery for Large-Scale Storage of Electrical Energy (<i>Adv. Energy Mater.</i> 8/2018). <i>Advanced Energy Materials</i> , 2018, 8, 1870034.	10.2	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. <i>Chemical Science</i> , 2018, 9, 3694-3703.	3.7	13
128	Local protein solvation drives direct down-conversion in phycobiliprotein PC645 via incoherent vibronic transport. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E3342-E3350.	3.3	61
129	Reproducing Quantum Probability Distributions at the Speed of Classical Dynamics: A New Approach for Developing Force-Field Functors. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1721-1727.	2.1	1
130	Quantum Simulation of Electronic Structure with Linear Depth and Connectivity. <i>Physical Review Letters</i> , 2018, 120, 110501.	2.9	243
131	Exponentially more precise quantum simulation of fermions in the configuration interaction representation. <i>Quantum Science and Technology</i> , 2018, 3, 015006.	2.6	53
132	Alkaline Benzoquinone Aqueous Flow Battery for Large-Scale Storage of Electrical Energy. <i>Advanced Energy Materials</i> , 2018, 8, 1702056.	10.2	161
133	Programmed coherent coupling in a synthetic DNA-based excitonic circuit. <i>Nature Materials</i> , 2018, 17, 159-166.	13.3	106
134	Quantum Computer Simulates Excited States of Molecule. <i>Physics Magazine</i> , 2018, 11, .	0.1	4
135	qTorch: The quantum tensor contraction handler. <i>PLoS ONE</i> , 2018, 13, e0208510.	1.1	31
136	Potential of quantum computing for drug discovery. <i>IBM Journal of Research and Development</i> , 2018, 62, 6:1-6:20.	3.2	130
137	Precise Control of Thermal and Redox Properties of Organic Hole-Transport Materials. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 15529-15533.	7.2	41
138	Alkaline Quinone Flow Battery with Long Lifetime at pH 12. <i>Joule</i> , 2018, 2, 1907-1908.	11.7	37
139	Precise Control of Thermal and Redox Properties of Organic Hole-Transport Materials. <i>Angewandte Chemie</i> , 2018, 130, 15755-15759.	1.6	15
140	Machine Learning and Big-Data in Computational Chemistry. , 2018, , 1-24.		4
141	Quantum chemistry reveals thermodynamic principles of redox biochemistry. <i>PLoS Computational Biology</i> , 2018, 14, e1006471.	1.5	22
142	Mapping Forbidden Emission to Structure in Self-Assembled Organic Nanoparticles. <i>Journal of the American Chemical Society</i> , 2018, 140, 15827-15841.	6.6	21
143	Origin of the $1/f$ spectral noise in chaotic and regular quantum systems. <i>Physical Review E</i> , 2018, 98, .	0.8	8
144	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. <i>Chemical Science</i> , 2018, 9, 7642-7655.	3.7	86

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145	Reinforced Adversarial Neural Computer for <i>de Novo</i> Molecular Design. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1194-1204.	2.5	256
146	Excitronics: A Set of Gates for Molecular Exciton Processing and Signaling. <i>ACS Nano</i> , 2018, 12, 6410-6420.	7.3	26
147	Alkaline Quinone Flow Battery with Long Lifetime at pH 12. <i>Joule</i> , 2018, 2, 1894-1906.	11.7	293
148	Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator. <i>Physical Review X</i> , 2018, 8, .	2.8	342
149	Inverse molecular design using machine learning: Generative models for matter engineering. <i>Science</i> , 2018, 361, 360-365.	6.0	1,055
150	High-Voltage-Assisted Mechanical Stabilization of Single-Molecule Junctions. <i>Nano Letters</i> , 2018, 18, 4727-4733.	4.5	20
151	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartree-Fock. <i>ACS Central Science</i> , 2018, 4, 559-566.	5.3	57
152	Phoenics: A Bayesian Optimizer for Chemistry. <i>ACS Central Science</i> , 2018, 4, 1134-1145.	5.3	215
153	ChemOS: Orchestrating autonomous experimentation. <i>Science Robotics</i> , 2018, 3, .	9.9	113
154	Learning More, with Less. <i>ACS Central Science</i> , 2017, 3, 275-277.	5.3	6
155	Anomalous Rapid Tunneling: Charge Transport across Self-Assembled Monolayers of Oligo(ethylene) Tj ETQq1 1 0,784314 rgBT /Overl 6,6 41	0.6	41
156	Equivalence between spin Hamiltonians and boson sampling. <i>Physical Review A</i> , 2017, 95, .	1.0	13
157	An Alternative Host Material for Long-Lifespan Blue Organic Light-Emitting Diodes Using Thermally Activated Delayed Fluorescence. <i>Advanced Science</i> , 2017, 4, 1600502.	5.6	103
158	Chiral Sugars Drive Enantioenrichment in Prebiotic Amino Acid Synthesis. <i>ACS Central Science</i> , 2017, 3, 322-328.	5.3	42
159	Using coherence to enhance function in chemical and biophysical systems. <i>Nature</i> , 2017, 543, 647-656.	13.7	477
160	MultiDK: A Multiple Descriptor Multiple Kernel Approach for Molecular Discovery and Its Application to Organic Flow Battery Electrolytes. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 657-668.	2.5	24
161	A Study of the Degree of Fluorination in Regioregular Poly(3-hexylthiophene). <i>Macromolecules</i> , 2017, 50, 162-174.	2.2	30
162	Emulation of complex open quantum systems using superconducting qubits. <i>Quantum Information Processing</i> , 2017, 16, 1.	1.0	23

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163	Anthraquinone Derivatives in Aqueous Flow Batteries. <i>Advanced Energy Materials</i> , 2017, 7, 1601488.	10.2	189
164	On the Long-Range Exciton Transport in Molecular Systems: The Application to H-Aggregated Heterotriangulene Chains. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24994-25002.	1.5	21
165	Machine learning for quantum dynamics: deep learning of excitation energy transfer properties. <i>Chemical Science</i> , 2017, 8, 8419-8426.	3.7	70
166	Absence of Selection for Quantum Coherence in the Fennaâ€œMatthewsâ€œOlson Complex: A Combined Evolutionary and Excitonic Study. <i>ACS Central Science</i> , 2017, 3, 1086-1095.	5.3	11
167	Bounding the costs of quantum simulation of many-body physics in real space. <i>Journal of Physics A: Mathematical and Theoretical</i> , 2017, 50, 305301.	0.7	47
168	A Nanophotonic Structure Containing Living Photosynthetic Bacteria. <i>Small</i> , 2017, 13, 1701777.	5.2	46
169	UV-Vis spectrophotometry of quinone flow battery electrolyte for <i>in situ</i> monitoring and improved electrochemical modeling of potential and quinhydrone formation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31684-31691.	1.3	57
170	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. <i>Joule</i> , 2017, 1, 857-870.	11.7	157
171	Introducing a New Potential Figure of Merit for Evaluating Microstructure Stability in Photovoltaic Polymer-Fullerene Blends. <i>Journal of Physical Chemistry C</i> , 2017, 121, 18153-18161.	1.5	52
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