Aln Aspuru Guzik

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

376 papers	29,808 citations	81 h-index	164 g-index
416 ext. papers	38,118 ext. citations	10.7 avg, IF	7.7 L-index

#	Paper	IF	Citations
376	A Comprehensive Discovery Platform for Organophosphorus Ligands for Catalysis.. *Journal of the American Chemical Society*, **2022**,	16.4	9
375	Routescore: Punching the Ticket to More Efficient Materials Development.. *ACS Central Science*, **2022**, 8, 122-131	16.8	1
374	In silico design of microporous polymers for chemical separations and storage. *Current Opinion in Chemical Engineering*, **2022**, 36, 100795	5.4	1
373	A quantum computing view on unitary coupled cluster theory.. *Chemical Society Reviews*, **2022**,	58.5	4
372	Noisy intermediate-scale quantum algorithms. *Reviews of Modern Physics*, **2022**, 94,	40.5	49
371	Experimental High-Dimensional Greenberger-Horne-Zeilinger Entanglement with Superconducting Transmon Qutrits. *Physical Review Applied*, **2022**, 17,	4.3	1
370	Quantum Computer-Aided Design: Digital Quantum Simulation of Quantum Processors. *Physical Review Applied*, **2021**, 16,	4.3	2
369	Golem: an algorithm for robust experiment and process optimization. *Chemical Science*, **2021**, 12, 14792-14807	9.4	4
368	funsies: A minimalist, distributed and dynamic workflow engine. *Journal of Open Source Software*, **2021**, 6, 3274	5.2	
367	Quantum computation of eigenvalues within target intervals. *Quantum Science and Technology*, **2021**, 6, 015004	5.5	5
366	Automated design of superconducting circuits and its application to 4-local couplers. *Npj Quantum Information*, **2021**, 7,	8.6	3
365	TEQUILA: a platform for rapid development of quantum algorithms. *Quantum Science and Technology*, **2021**, 6, 024009	5.5	10
364	Analog Quantum Simulation of Non-Condon Effects in Molecular Spectroscopy. *ACS Photonics*, **2021**, 8, 2007-2016	6.3	1
363	Scientific intuition inspired by machine learning-generated hypotheses. *Machine Learning: Science and Technology*, **2021**, 2, 025027	5.1	10
362	A molecular computing approach to solving optimization problems via programmable microdroplet arrays. *Matter*, **2021**, 4, 1107-1124	12.7	1
361	Noise Robustness and Experimental Demonstration of a Quantum Generative Adversarial Network for Continuous Distributions. *Advanced Quantum Technologies*, **2021**, 4, 2000069	4.3	1
360	An artificial spiking quantum neuron. *Npj Quantum Information*, **2021**, 7,	8.6	2

359	Machine-learned potentials for next-generation matter simulations. *Nature Materials*, **2021**, 20, 750-761	27	54
358	Organic molecules with inverted gaps between first excited singlet and triplet states and appreciable fluorescence rates. *Matter*, **2021**, 4, 1654-1682	12.7	19
357	Meta-Variational Quantum Eigensolver: Learning Energy Profiles of Parameterized Hamiltonians for Quantum Simulation. *PRX Quantum*, **2021**, 2,	6.1	9
356	Machine learning the quantum-chemical properties of metal–organic frameworks for accelerated materials discovery. *Matter*, **2021**, 4, 1578-1597	12.7	43
355	Assigning confidence to molecular property prediction. *Expert Opinion on Drug Discovery*, **2021**, 16, 1009-1023	6.1	10
354	Deep molecular dreaming: inverse machine learning for de-novo molecular design and interpretability with surjective representations. *Machine Learning: Science and Technology*, **2021**, 2, 03LT02	5.1	7
353	Natural evolutionary strategies for variational quantum computation. *Machine Learning: Science and Technology*, **2021**, 2, 045012	5.1	4
352	Nanoparticle synthesis assisted by machine learning. *Nature Reviews Materials*, **2021**, 6, 701-716	73.3	38
351	Mutual information-assisted adaptive variational quantum eigensolver. *Quantum Science and Technology*, **2021**, 6, 035001	5.5	5
350	The influence of sorbitol doping on aggregation and electronic properties of PEDOT:PSS: a theoretical study. *Machine Learning: Science and Technology*, **2021**, 2, 01LT01	5.1	4
349	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	6.4	6
348	Quantum computing at the frontiers of biological sciences. *Nature Methods*, **2021**, 18, 701-709	21.6	14
347	A feasible approach for automatically differentiable unitary coupled-cluster on quantum computers. *Chemical Science*, **2021**, 12, 3497-3508	9.4	18
346	Inverse design of nanoporous crystalline reticular materials with deep generative models. *Nature Machine Intelligence*, **2021**, 3, 76-86	22.5	58
345	Coronene derivatives for transparent organic photovoltaics through inverse materials design. *Journal of Materials Chemistry C*, **2021**, 9, 1310-1317	7.1	5
344	Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning. *Trends in Chemistry*, **2021**, 3, 96-110	14.8	16
343	Data-Driven Strategies for Accelerated Materials Design. *Accounts of Chemical Research*, **2021**, 54, 849-860	24.3	61
342	Quantum computer-aided design of quantum optics hardware. *Quantum Science and Technology*, **2021**, 6, 035010	5.5	2

341	Neural message passing on high order paths. *Machine Learning: Science and Technology*, **2021**, 2, 045009	5.1	3
340	Olympus: a benchmarking framework for noisy optimization and experiment planning. *Machine Learning: Science and Technology*, **2021**, 2, 035021	5.1	14
339	MPGVAE: improved generation of small organic molecules using message passing neural nets. *Machine Learning: Science and Technology*, **2021**, 2, 045010	5.1	0
338	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
337	Data-science driven autonomous process optimization. *Communications Chemistry*, **2021**, 4,	6.3	19
336	Machine learning directed drug formulation development. *Advanced Drug Delivery Reviews*, **2021**, 175, 113806	18.5	17
335	Conceptual Understanding through Efficient Automated Design of Quantum Optical Experiments. *Physical Review X*, **2021**, 11,	9.1	4
334	Gryffin: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. *Applied Physics Reviews*, **2021**, 8, 031406	17.3	14
333	Beyond generative models: superfast traversal, optimization, novelty, exploration and discovery (STONED) algorithm for molecules using SELFIES. *Chemical Science*, **2021**, 12, 7079-7090	9.4	16
332	Rational design of layered oxide materials for sodium-ion batteries. *Science*, **2020**, 370, 708-711	33.3	209
331	Optically Induced Molecular Logic Operations. *ACS Nano*, **2020**, 14, 15248-15255	16.7	1
330	A machine learning workflow for molecular analysis: application to melting points. *Machine Learning: Science and Technology*, **2020**, 1, 025015	5.1	6
329	Self-driving laboratory for accelerated discovery of thin-film materials. *Science Advances*, **2020**, 6, eaaz8867	14.3	138
328	Materials Acceleration Platforms: On the way to autonomous experimentation. *Current Opinion in Green and Sustainable Chemistry*, **2020**, 25, 100370	7.9	28
327	Quantum computational chemistry. *Reviews of Modern Physics*, **2020**, 92,	40.5	256
326	Boramidine: A Versatile Structural Motif for the Design of Fluorescent Heterocycles. *Journal of the American Chemical Society*, **2020**, 142, 13544-13549	16.4	3
325	The Cyclopropane Ring as a Reporter of Radical Leaving-Group Reactivity for Ni-Catalyzed C(sp)-O Arylation. *Journal of the American Chemical Society*, **2020**, 142, 13246-13254	16.4	17
324	Machine learning for analysing ab initio molecular dynamics simulations. *Journal of Physics: Conference Series*, **2020**, 1412, 042003	0.3	1

323	Team-Based Learning for Scientific Computing and Automated Experimentation: Visualization of Colored Reactions. *Journal of Chemical Education*, **2020**, 97, 689-694	2.4	4
322	Constructing Na-Ion Cathodes via Alkali-Site Substitution. *Advanced Functional Materials*, **2020**, 30, 1910840	18.5	11
321	Revealing High Na-Content P2-Type Layered Oxides as Advanced Sodium-Ion Cathodes. *Journal of the American Chemical Society*, **2020**, 142, 5742-5750	16.4	84
320	Optical monitoring of polymerizations in droplets with high temporal dynamic range. *Chemical Science*, **2020**, 11, 2647-2656	9.4	6
319	Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems. *Advanced Materials*, **2020**, 32, e1907801	24	66
318	Reply to 'Assessing the impact of generative AI on medicinal chemistry'. *Nature Biotechnology*, **2020**, 38, 146	44.5	8
317	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
316	Film Fabrication Techniques: Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems (Adv. Mater. 14/2020). *Advanced Materials*, **2020**, 32, 2070110	24	2
315	Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. *Chemical Science*, **2020**, 11, 4584-4601	9.4	47
314	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. *ACS Nano*, **2020**, 14, 6589-6598	16.7	8
313	Machine Learning and Big-Data in Computational Chemistry **2020**, 1939-1962		2
312	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	11.5	4
311	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. *Machine Learning: Science and Technology*, **2020**, 1, 045024	5.1	85
310	When robotics met fluidics. *Lab on A Chip*, **2020**, 20, 709-716	7.2	16
309	Effect of Molecular Structure of Quinones and Carbon Electrode Surfaces on the Interfacial Electron Transfer Process. *ACS Applied Energy Materials*, **2020**, 3, 1933-1943	6.1	17
308	Generative Adversarial Networks for Crystal Structure Prediction. *ACS Central Science*, **2020**, 6, 1412-1420	16.8	35
307	Resource-efficient digital quantum simulation of d-level systems for photonic, vibrational, and spin-s Hamiltonians. *Npj Quantum Information*, **2020**, 6,	8.6	27
306	Molecular Sets (MOSES): A Benchmarking Platform for Molecular Generation Models. *Frontiers in Pharmacology*, **2020**, 11, 565644	5.6	82

305	Bioinspiration in light harvesting and catalysis. *Nature Reviews Materials*, **2020**, 5, 828-846	73.3	54
304	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	16.8	9
303	Designing and understanding light-harvesting devices with machine learning. *Nature Communications*, **2020**, 11, 4587	17.4	21
302	Interface chemistry of an amide electrolyte for highly reversible lithium metal batteries. *Nature Communications*, **2020**, 11, 4188	17.4	90
301	ChemOS: An orchestration software to democratize autonomous discovery. *PLoS ONE*, **2020**, 15, e0229862	3.7	35
300	Oscillatory Active-site Motions Correlate with Kinetic Isotope Effects in Formate Dehydrogenase. *ACS Catalysis*, **2019**, 9, 11199-11206	13.1	13
299	Quantum Chemistry in the Age of Quantum Computing. *Chemical Reviews*, **2019**, 119, 10856-10915	68.1	288
298	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. *Nature Biotechnology*, **2019**, 37, 1038-1040	44.5	338
297	Identification Schemes for Metal–Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. *Crystal Growth and Design*, **2019**, 19, 6682-6697	3.5	59
296	Discovery of blue singlet exciton fission molecules via a high-throughput virtual screening and experimental approach. *Journal of Chemical Physics*, **2019**, 151, 121102	3.9	16
295	Inverse Design of Solid-State Materials via a Continuous Representation. *Matter*, **2019**, 1, 1370-1384	12.7	99
294	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. *ACS Central Science*, **2019**, 5, 1199-1210	16.8	35
293	Predicting Feasible Organic Reaction Pathways Using Heuristically Aided Quantum Chemistry. *Journal of Chemical Theory and Computation*, **2019**, 15, 4099-4112	6.4	17
292	Next-Generation Experimentation with Self-Driving Laboratories. *Trends in Chemistry*, **2019**, 1, 282-291	14.8	91
291	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	13	78
290	Autonomous Molecular Design: Then and Now. *ACS Applied Materials & Interfaces*, **2019**, 11, 24825-24836	9.5	48
289	Variational Quantum Factoring. *Lecture Notes in Computer Science*, **2019**, 74-85	0.9	26
288	Extending the Lifetime of Organic Flow Batteries via Redox State Management. *Journal of the American Chemical Society*, **2019**, 141, 8014-8019	16.4	93

287	Predicting synthesizability. *Journal Physics D: Applied Physics*, **2019**, 52,	3	161
286	Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. *Quantum Science and Technology*, **2019**, 4, 014008	5.5	189
285	Electron Microscopy Investigation of Sodiation of Titanium Disulfide Nanoflakes. *ACS Nano*, **2019**, 13, 9421-9430	16.7	23
284	Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer. *Quantum Science and Technology*, **2019**, 4, 045005	5.5	36
283	Interface Molecular Engineering for Laminated Monolithic Perovskite/Silicon Tandem Solar Cells with 80.4% Fill Factor. *Advanced Functional Materials*, **2019**, 29, 1901476	15.6	27
282	Molecular Engineering of an Alkaline Naphthoquinone Flow Battery. *ACS Energy Letters*, **2019**, 4, 1880-1887	19.1	52
281	Design rules for high mobility xanthene-based hole transport materials. *Chemical Science*, **2019**, 10, 8360-8366	9.4	14
280	Generalized Kasha Model: T-Dependent Spectroscopy Reveals Short-Range Structures of 2D Excitonic Systems. *CheM*, **2019**, 5, 3135-3150	16.2	11
279	Quantum Coherences as a Thermodynamic Potential. *Open Systems and Information Dynamics*, **2019**, 26, 1950022	0.4	2
278	Expressibility and Entangling Capability of Parameterized Quantum Circuits for Hybrid Quantum-Classical Algorithms. *Advanced Quantum Technologies*, **2019**, 2, 1900070	4.3	87
277	A Bayesian Approach to Predict Solubility Parameters. *Advanced Theory and Simulations*, **2019**, 2, 1800069	3.5	36
276	How machine learning can assist the interpretation of molecular dynamics simulations and conceptual understanding of chemistry. *Chemical Science*, **2019**, 10, 2298-2307	9.4	58
275	Molecular realization of a quantum NAND tree. *Quantum Science and Technology*, **2019**, 4, 015013	5.5	3
274	Discovery of Calcium-Metal Alloy Anodes for Reversible Ca-Ion Batteries. *Advanced Energy Materials*, **2019**, 9, 1802994	21.8	38
273	Temperature-dependent conformations of exciton-coupled Cy3 dimers in double-stranded DNA. *Journal of Chemical Physics*, **2018**, 148, 085101	3.9	35
272	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	6.4	27
271	Single-Atom Heat Machines Enabled by Energy Quantization. *Physical Review Letters*, **2018**, 120, 170601	7.4	32
270	The Matter Simulation (R)evolution. *ACS Central Science*, **2018**, 4, 144-152	16.8	66

269	Exploring Electronic Structure and Order in Polymers via Single-Particle Microresonator Spectroscopy. *Nano Letters*, **2018**, 18, 1600-1607	11.5	18
268	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. *ACS Central Science*, **2018**, 4, 268-276	16.8	950
267	Oxidation of rubrene, and implications for device stability. *Journal of Materials Chemistry C*, **2018**, 6, 3757-3761	7.1	11
266	Accelerating the discovery of materials for clean energy in the era of smart automation. *Nature Reviews Materials*, **2018**, 3, 5-20	73.3	308
265	Photochemical Control of Exciton Superradiance in Light-Harvesting Nanotubes. *ACS Nano*, **2018**, 12, 4556-4564	16.7	23
264	Flow Batteries: Alkaline Benzoquinone Aqueous Flow Battery for Large-Scale Storage of Electrical Energy (Adv. Energy Mater. 8/2018). *Advanced Energy Materials*, **2018**, 8, 1870034	21.8	15
263	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	9.4	12
262	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	11.5	47
261	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	6.4	1
260	Quantum Simulation of Electronic Structure with Linear Depth and Connectivity. *Physical Review Letters*, **2018**, 120, 110501	7.4	136
259	Exponentially more precise quantum simulation of fermions in the configuration interaction representation. *Quantum Science and Technology*, **2018**, 3, 015006	5.5	37
258	Alkaline Quinone Flow Battery with Long Lifetime at pH 12. *Joule*, **2018**, 2, 1894-1906	27.8	175
257	Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator. *Physical Review X*, **2018**, 8,	9.1	197
256	Inverse molecular design using machine learning: Generative models for matter engineering. *Science*, **2018**, 361, 360-365	33.3	624
255	High-Voltage-Assisted Mechanical Stabilization of Single-Molecule Junctions. *Nano Letters*, **2018**, 18, 4727-4733	11.5	14
254	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartree-Fock. *ACS Central Science*, **2018**, 4, 559-566	16.8	35
253	Phoenics: A Bayesian Optimizer for Chemistry. *ACS Central Science*, **2018**, 4, 1134-1145	16.8	126
252	ChemOS: Orchestrating autonomous experimentation. *Science Robotics*, **2018**, 3,	18.6	73

251	Alkaline Benzoquinone Aqueous Flow Battery for Large-Scale Storage of Electrical Energy. *Advanced Energy Materials*, **2018**, 8, 1702056	21.8	113
250	Programmed coherent coupling in a synthetic DNA-based excitonic circuit. *Nature Materials*, **2018**, 17, 159-166	27	73
249	qTorch: The quantum tensor contraction handler. *PLoS ONE*, **2018**, 13, e0208510	3.7	21
248	Potential of quantum computing for drug discovery. *IBM Journal of Research and Development*, **2018**, 62, 6:1-6:20	2.5	47
247	Precise Control of Thermal and Redox Properties of Organic Hole-Transport Materials. *Angewandte Chemie - International Edition*, **2018**, 57, 15529-15533	16.4	26
246	Alkaline Quinone Flow Battery with Long Lifetime at pH 12. *Joule*, **2018**, 2, 1907-1908	27.8	26
245	Precise Control of Thermal and Redox Properties of Organic Hole-Transport Materials. *Angewandte Chemie*, **2018**, 130, 15755-15759	3.6	7
244	Machine Learning and Big-Data in Computational Chemistry **2018**, 1-24		3
243	Quantum chemistry reveals thermodynamic principles of redox biochemistry. *PLoS Computational Biology*, **2018**, 14, e1006471	5	15
242	Mapping Forbidden Emission to Structure in Self-Assembled Organic Nanoparticles. *Journal of the American Chemical Society*, **2018**, 140, 15827-15841	16.4	19
241	Origin of the 1/f□spectral noise in chaotic and regular quantum systems. *Physical Review E*, **2018**, 98,	2.4	6
240	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. *Chemical Science*, **2018**, 9, 7642-7655	9.4	53
239	Reinforced Adversarial Neural Computer for de Novo Molecular Design. *Journal of Chemical Information and Modeling*, **2018**, 58, 1194-1204	6.1	151
238	Excitonics: A Set of Gates for Molecular Exciton Processing and Signaling. *ACS Nano*, **2018**, 12, 6410-6420	16.7	15
237	Anomalously Rapid Tunneling: Charge Transport across Self-Assembled Monolayers of Oligo(ethylene glycol). *Journal of the American Chemical Society*, **2017**, 139, 7624-7631	16.4	33
236	Equivalence between spin Hamiltonians and boson sampling. *Physical Review A*, **2017**, 95,	2.6	8
235	An Alternative Host Material for Long-Lifespan Blue Organic Light-Emitting Diodes Using Thermally Activated Delayed Fluorescence. *Advanced Science*, **2017**, 4, 1600502	13.6	69
234	Chiral Sugars Drive Enantioenrichment in Prebiotic Amino Acid Synthesis. *ACS Central Science*, **2017**, 3, 322-328	16.8	30

233	Using coherence to enhance function in chemical and biophysical systems. *Nature*, **2017**, 543, 647-656	50.4	367
232	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	6.1	14
231	A Study of the Degree of Fluorination in Regioregular Poly(3-hexylthiophene). *Macromolecules*, **2017**, 50, 162-174	5.5	26
230	Emulation of complex open quantum systems using superconducting qubits. *Quantum Information Processing*, **2017**, 16, 1	1.6	15
229	Anthraquinone Derivatives in Aqueous Flow Batteries. *Advanced Energy Materials*, **2017**, 7, 1601488	21.8	141
228	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	3.8	15
227	Machine learning for quantum dynamics: deep learning of excitation energy transfer properties. *Chemical Science*, **2017**, 8, 8419-8426	9.4	55
226	Absence of Selection for Quantum Coherence in the Fenna-Matthews-Olson Complex: A Combined Evolutionary and Excitonic Study. *ACS Central Science*, **2017**, 3, 1086-1095	16.8	7
225	Bounding the costs of quantum simulation of many-body physics in real space. *Journal of Physics A: Mathematical and Theoretical*, **2017**, 50, 305301	2	33
224	A Nanophotonic Structure Containing Living Photosynthetic Bacteria. *Small*, **2017**, 13, 1701777	11	36
223	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	3.6	35
222	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. *Joule*, **2017**, 1, 857-870	27.8	120
221	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	3.8	38
220	Taking six-dimensional spectra in finite time. *Science*, **2017**, 356, 1333	33.3	2
219	On thermodynamic inconsistencies in several photosynthetic and solar cell models and how to fix them. *Chemical Science*, **2017**, 8, 1008-1014	9.4	16
218	Quantum autoencoders for efficient compression of quantum data. *Quantum Science and Technology*, **2017**, 2, 045001	5.5	154
217	Use machine learning to find energy materials. *Nature*, **2017**, 552, 23-27	50.4	63
216	Response to: Comment on benchmarking compressed sensing, super-resolution, and filter diagonalization *International Journal of Quantum Chemistry*, **2016**, 116, 1818-1821	2.1	

215	Accelerating the computation of bath spectral densities with super-resolution. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	2
214	Layer-by-Layer Assembled Films of Perylene Diimide- and Squaraine-Containing Metal-Organic Framework-like Materials: Solar Energy Capture and Directional Energy Transfer. *ACS Applied Materials & Interfaces*, **2016**, 8, 24983-8	9.5	37
213	Scalable Quantum Simulation of Molecular Energies. *Physical Review X*, **2016**, 6,	9.1	355
212	Neural Networks for the Prediction of Organic Chemistry Reactions. *ACS Central Science*, **2016**, 2, 725-732	6.8	234
211	Optical Spectra of p-Doped PEDOT Nanoaggregates Provide Insight into the Material Disorder. *ACS Energy Letters*, **2016**, 1, 1100-1105	20.1	5
210	A redox-flow battery with an alloxazine-based organic electrolyte. *Nature Energy*, **2016**, 1,	62.3	307
209	The Harvard organic photovoltaic dataset. *Scientific Data*, **2016**, 3, 160086	8.2	57
208	Application of Graphics Processing Units to Accelerate Real-Space Density Functional Theory and Time-Dependent Density Functional Theory Calculations **2016**, 211-238		
207	GPU Acceleration of Second-Order Møller-Plesset Perturbation Theory with Resolution of Identity **2016**, 259-278		1
206	The theory of variational hybrid quantum-classical algorithms. *New Journal of Physics*, **2016**, 18, 023023	2.9	615
205	Coherent Dynamics of Mixed Frenkel and Charge-Transfer Excitons in Dinaphtho[2,3-b:2′3′-f]thieno[3,2-b]-thiophene Thin Films: The Importance of Hole Delocalization. *Journal of Physical Chemistry Letters*, **2016**, 7, 1374-80	6.4	23
204	A Bayesian approach to calibrating high-throughput virtual screening results and application to organic photovoltaic materials. *Materials Horizons*, **2016**, 3, 226-233	14.4	58
203	The role of interparticle interaction and environmental coupling in a two-particle open quantum system. *Physical Chemistry Chemical Physics*, **2016**, 18, 436-47	3.6	1
202	Analytical nuclear gradients for the range-separated many-body dispersion model of noncovalent interactions. *Chemical Science*, **2016**, 7, 1712-1728	9.4	29
201	Renewables need a grand-challenge strategy. *Nature*, **2016**, 538, 27-29	50.4	22
200	Benchmarking compressed sensing, super-resolution, and filter diagonalization. *International Journal of Quantum Chemistry*, **2016**, 116, 1097-1106	2.1	3
199	Exponentially more precise quantum simulation of fermions in second quantization. *New Journal of Physics*, **2016**, 18, 033032	2.9	71
198	Error Sensitivity to Environmental Noise in Quantum Circuits for Chemical State Preparation. *Journal of Chemical Theory and Computation*, **2016**, 12, 3097-108	6.4	21

197	Faster than classical quantum algorithm for dense formulas of exact satisfiability and occupation problems. *New Journal of Physics*, **2016**, 18, 073003	2.9	11
196	Machine learning exciton dynamics. *Chemical Science*, **2016**, 7, 5139-5147	9.4	90
195	Tunneling across SAMs Containing Oligophenyl Groups. *Journal of Physical Chemistry C*, **2016**, 120, 11331-11337	4.8	35
194	Efficiency of energy funneling in the photosystem II supercomplex of higher plants. *Chemical Science*, **2016**, 7, 4174-4183	9.4	21
193	Turbocharged molecular discovery of OLED emitters: from high-throughput quantum simulation to highly efficient TADF devices **2016**,		3
192	Quantum simulation with a boson sampling circuit. *Physical Review A*, **2016**, 94,	2.6	6
191	Proposal for Microwave Boson Sampling. *Physical Review Letters*, **2016**, 117, 140505	7.4	32
190	Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. *Nature Materials*, **2016**, 15, 1120-7	27	492
189	Bayesian network structure learning using quantum annealing. *European Physical Journal: Special Topics*, **2015**, 224, 163-188	2.3	50
188	Fast delocalization leads to robust long-range excitonic transfer in a large quantum chlorosome model. *Nano Letters*, **2015**, 15, 1722-9	11.5	24
187	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	3.4	74
186	Chemical basis of Trotter-Suzuki errors in quantum chemistry simulation. *Physical Review A*, **2015**, 91,	2.6	87
185	Compressed Sensing for the Fast Computation of Matrices: Application to Molecular Vibrations. *ACS Central Science*, **2015**, 1, 24-32	16.8	6
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