Aln Aspuru Guzik

List of Publications by Citations

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	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
375	A variational eigenvalue solver on a photonic quantum processor. *Nature Communications*, **2014**, 5, 4213	17.4	1030
374	A metal-free organic-inorganic aqueous flow battery. *Nature*, **2014**, 505, 195-8	50.4	1025
373	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. *ACS Central Science*, **2018**, 4, 268-276	16.8	950
372	Tuning charge transport in solution-sheared organic semiconductors using lattice strain. *Nature*, **2011**, 480, 504-8	50.4	855
371	Environment-assisted quantum walks in photosynthetic energy transfer. *Journal of Chemical Physics* , **2008**, 129, 174106	3.9	820
370	High electrical conductivity in Ni(2,3,6,7,10,11-hexaiminotriphenylene)a semiconducting metal-organic graphene analogue. *Journal of the American Chemical Society*, **2014**, 136, 8859-62	16.4	691
369	Inverse molecular design using machine learning: Generative models for matter engineering. *Science*, **2018**, 361, 360-365	33.3	624
368	The theory of variational hybrid quantum-classical algorithms. *New Journal of Physics*, **2016**, 18, 023023	2.9	615
367	Environment-assisted quantum transport. *New Journal of Physics*, **2009**, 11, 033003	2.9	606
366	Simulated quantum computation of molecular energies. *Science*, **2005**, 309, 1704-7	33.3	555
365	Photonic quantum simulators. *Nature Physics*, **2012**, 8, 285-291	16.2	522
364	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
363	Towards quantum chemistry on a quantum computer. *Nature Chemistry*, **2010**, 2, 106-11	17.6	416
362	Observation of topologically protected bound states in photonic quantum walks. *Nature Communications*, **2012**, 3, 882	17.4	376
361	Using coherence to enhance function in chemical and biophysical systems. *Nature*, **2017**, 543, 647-656	50.4	367
360	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	6.4	367

359	Scalable Quantum Simulation of Molecular Energies. *Physical Review X*, **2016**, 6,	9.1	355
358	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. *Nature Biotechnology*, **2019**, 37, 1038-1040	44.5	338
357	Accelerating the discovery of materials for clean energy in the era of smart automation. *Nature Reviews Materials*, **2018**, 3, 5-20	73.3	308
356	A redox-flow battery with an alloxazine-based organic electrolyte. *Nature Energy*, **2016**, 1,	62.3	307
355	Quantum Chemistry in the Age of Quantum Computing. *Chemical Reviews*, **2019**, 119, 10856-10915	68.1	288
354	Discrete single-photon quantum walks with tunable decoherence. *Physical Review Letters*, **2010**, 104, 153602	7.4	288
353	From computational discovery to experimental characterization of a high hole mobility organic crystal. *Nature Communications*, **2011**, 2, 437	17.4	281
352	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, 31371-96	3.6	276
351	Role of quantum coherence and environmental fluctuations in chromophoric energy transport. *Journal of Physical Chemistry B*, **2009**, 113, 9942-7	3.4	268
350	Quantum computational chemistry. *Reviews of Modern Physics*, **2020**, 92,	40.5	256
349	Computational design of molecules for an all-quinone redox flow battery. *Chemical Science*, **2015**, 6, 885-893	9.4	245
348	Neural Networks for the Prediction of Organic Chemistry Reactions. *ACS Central Science*, **2016**, 2, 725-732	16.8	234
347	Simulation of electronic structure Hamiltonians using quantum computers. *Molecular Physics*, **2011**, 109, 735-750	1.7	213
346	Rational design of layered oxide materials for sodium-ion batteries. *Science*, **2020**, 370, 708-711	33.3	209
345	Quantum Chemistry Calculations on a Trapped-Ion Quantum Simulator. *Physical Review X*, **2018**, 8,	9.1	197
344	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
343	Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. *Quantum Science and Technology*, **2019**, 4, 014008	5.5	189
342	Simulating chemistry using quantum computers. *Annual Review of Physical Chemistry*, **2011**, 62, 185-207	15.7	179

341	Atomistic study of the long-lived quantum coherences in the Fenna-Matthews-Olson complex. *Biophysical Journal*, **2012**, 102, 649-60	2.9	178
340	Alkaline Quinone Flow Battery with Long Lifetime at pH 12. *Joule*, **2018**, 2, 1894-1906	27.8	175
339	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, 18681-6	11.5	168
338	Finding low-energy conformations of lattice protein models by quantum annealing. *Scientific Reports*, **2012**, 2, 571	4.9	166
337	Photonics meets excitonics: natural and artificial molecular aggregates. *Nanophotonics*, **2013**, 2, 21-38	6.3	165
336	Predicting synthesizability. *Journal Physics D: Applied Physics*, **2019**, 52,	3	161
335	Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry the Harvard Clean Energy Project. *Energy and Environmental Science*, **2014**, 7, 698-704	35.4	158
334	Understanding polymorphism in organic semiconductor thin films through nanoconfinement. *Journal of the American Chemical Society*, **2014**, 136, 17046-57	16.4	155
333	Quantum autoencoders for efficient compression of quantum data. *Quantum Science and Technology*, **2017**, 2, 045001	5.5	154
332	Reinforced Adversarial Neural Computer for de Novo Molecular Design. *Journal of Chemical Information and Modeling*, **2018**, 58, 1194-1204	6.1	151
331	Boson sampling for molecular vibronic spectra. *Nature Photonics*, **2015**, 9, 615-620	33.9	148
330	Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics. *Energy and Environmental Science*, **2011**, 4, 4849	35.4	147
329	Anthraquinone Derivatives in Aqueous Flow Batteries. *Advanced Energy Materials*, **2017**, 7, 1601488	21.8	141
328	What Is High-Throughput Virtual Screening? A Perspective from Organic Materials Discovery. *Annual Review of Materials Research*, **2015**, 45, 195-216	12.8	141
327	Self-driving laboratory for accelerated discovery of thin-film materials. *Science Advances*, **2020**, 6, eaaz8867	14.3	138
326	Quantum Simulation of Electronic Structure with Linear Depth and Connectivity. *Physical Review Letters*, **2018**, 120, 110501	7.4	136
325	Time-dependent density-functional theory in massively parallel computer architectures: the OCTOPUS project. *Journal of Physics Condensed Matter*, **2012**, 24, 233202	1.8	135
324	Phoenics: A Bayesian Optimizer for Chemistry. *ACS Central Science*, **2018**, 4, 1134-1145	16.8	126

323	Learning from the Harvard Clean Energy Project: The Use of Neural Networks to Accelerate Materials Discovery. *Advanced Functional Materials*, **2015**, 25, 6495-6502	15.6	121
322	Accelerating resolution-of-the-identity second-order Møller-Plesset quantum chemistry calculations with graphical processing units. *Journal of Physical Chemistry A*, **2008**, 112, 2049-57	2.8	121
321	From transistor to trapped-ion computers for quantum chemistry. *Scientific Reports*, **2014**, 4, 3589	4.9	120
320	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. *Joule*, **2017**, 1, 857-870	27.8	120
319	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
318	Alkaline Benzoquinone Aqueous Flow Battery for Large-Scale Storage of Electrical Energy. *Advanced Energy Materials*, **2018**, 8, 1702056	21.8	113
317	Non-Markovian quantum jumps in excitonic energy transfer. *Journal of Chemical Physics*, **2009**, 131, 184102	3.9	111
316	Modified scaled hierarchical equation of motion approach for the study of quantum coherence in photosynthetic complexes. *Journal of Physical Chemistry B*, **2011**, 115, 1531-7	3.4	110
315	On the alternatives for bath correlators and spectral densities from mixed quantum-classical simulations. *Journal of Chemical Physics*, **2012**, 137, 224103	3.9	107
314	Inverse Design of Solid-State Materials via a Continuous Representation. *Matter*, **2019**, 1, 1370-1384	12.7	99
313	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, 16521-6	11.5	96
312	Extending the Lifetime of Organic Flow Batteries via Redox State Management. *Journal of the American Chemical Society*, **2019**, 141, 8014-8019	16.4	93
311	Next-Generation Experimentation with Self-Driving Laboratories. *Trends in Chemistry*, **2019**, 1, 282-291	14.8	91
310	Separation of Electromagnetic and Chemical Contributions to Surface-Enhanced Raman Spectra on Nanoengineered Plasmonic Substrates. *Journal of Physical Chemistry Letters*, **2010**, 1, 2740-2746	6.4	90
309	Interface chemistry of an amide electrolyte for highly reversible lithium metal batteries. *Nature Communications*, **2020**, 11, 4188	17.4	90
308	Machine learning exciton dynamics. *Chemical Science*, **2016**, 7, 5139-5147	9.4	90
307	Quantum Simulation of Helium Hydride Cation in a Solid-State Spin Register. *ACS Nano*, **2015**, 9, 7769-74	16.7	89
306	Communication: Exciton-phonon information flow in the energy transfer process of photosynthetic complexes. *Journal of Chemical Physics*, **2011**, 134, 101103	3.9	89

305	Chemical basis of Trotter-Suzuki errors in quantum chemistry simulation. *Physical Review A*, **2015**, 91,	2.6	87
304	Expressibility and Entangling Capability of Parameterized Quantum Circuits for Hybrid Quantum-Classical Algorithms. *Advanced Quantum Technologies*, **2019**, 2, 1900070	4.3	87
303	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, 4045-54	6.4	86
302	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. *Machine Learning: Science and Technology*, **2020**, 1, 045024	5.1	85
301	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
300	Hydrogen-bonded diketopyrrolopyrrole (DPP) pigments as organic semiconductors. *Organic Electronics*, **2014**, 15, 3521-3528	3.5	83
299	Quantum algorithm for obtaining the energy spectrum of molecular systems. *Physical Chemistry Chemical Physics*, **2008**, 10, 5388-93	3.6	83
298	Adiabatic quantum simulation of quantum chemistry. *Scientific Reports*, **2014**, 4, 6603	4.9	82
297	Molecular Sets (MOSES): A Benchmarking Platform for Molecular Generation Models. *Frontiers in Pharmacology*, **2020**, 11, 565644	5.6	82
296	On the chemical bonding effects in the Raman response: benzenethiol adsorbed on silver clusters. *Physical Chemistry Chemical Physics*, **2009**, 11, 9401-11	3.6	81
295	Strong coupling between chlorosomes of photosynthetic bacteria and a confined optical cavity mode. *Nature Communications*, **2014**, 5, 5561	17.4	80
294	Absence of Quantum Oscillations and Dependence on Site Energies in Electronic Excitation Transfer in the Fenna□Matthews□Olson Trimer. *Journal of Physical Chemistry Letters*, **2011**, 2, 2912-2917	6.4	79
293	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
292	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
291	ChemOS: Orchestrating autonomous experimentation. *Science Robotics*, **2018**, 3,	18.6	73
290	Complex Chemical Reaction Networks from Heuristics-Aided Quantum Chemistry. *Journal of Chemical Theory and Computation*, **2014**, 10, 897-907	6.4	73
289	Programmed coherent coupling in a synthetic DNA-based excitonic circuit. *Nature Materials*, **2018**, 17, 159-166	27	73
288	Multiple coherent states for first-principles semiclassical initial value representation molecular dynamics. *Journal of Chemical Physics*, **2009**, 130, 234113	3.9	72

287	Effects of odd-even side chain length of alkyl-substituted diphenylbithiophenes on first monolayer thin film packing structure. *Journal of the American Chemical Society*, **2013**, 135, 11006-14	16.4	71
286	Accelerating Correlated Quantum Chemistry Calculations Using Graphical Processing Units and a Mixed Precision Matrix Multiplication Library. *Journal of Chemical Theory and Computation*, **2010**, 6, 135-44	6.4	71
285	Exponentially more precise quantum simulation of fermions in second quantization. *New Journal of Physics*, **2016**, 18, 033032	2.9	71
284	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
283	Atomistic study of energy funneling in the light-harvesting complex of green sulfur bacteria. *Journal of the American Chemical Society*, **2014**, 136, 2048-57	16.4	69
282	Quantum stochastic walks: A generalization of classical random walks and quantum walks. *Physical Review A*, **2010**, 81,	2.6	69
281	Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems. *Advanced Materials*, **2020**, 32, e1907801	24	66
280	The Matter Simulation (R)evolution. *ACS Central Science*, **2018**, 4, 144-152	16.8	66
279	Theoretical Characterization of the Air-Stable, High-Mobility Dinaphtho[2,3-b:2?3?-f]thieno[3,2-b]-thiophene Organic Semiconductor. *Journal of Physical Chemistry C*, **2010**, 114, 2334-2340	3.8	66
278	Strongly Coupled Quantum Heat Machines. *Journal of Physical Chemistry Letters*, **2015**, 6, 3477-82	6.4	65
277	Quantum simulator of an open quantum system using superconducting qubits: exciton transport in photosynthetic complexes. *New Journal of Physics*, **2012**, 14, 105013	2.9	65
276	Exploiting Locality in Quantum Computation for Quantum Chemistry. *Journal of Physical Chemistry Letters*, **2014**, 5, 4368-80	6.4	64
275	Faster quantum chemistry simulation on fault-tolerant quantum computers. *New Journal of Physics*, **2012**, 14, 115023	2.9	64
274	Use machine learning to find energy materials. *Nature*, **2017**, 552, 23-27	50.4	63
273	Time-dependent density functional theory for open quantum systems with unitary propagation. *Physical Review Letters*, **2010**, 104, 043001	7.4	61
272	First-principles semiclassical initial value representation molecular dynamics. *Physical Chemistry Chemical Physics*, **2009**, 11, 3861-7	3.6	61
271	Data-Driven Strategies for Accelerated Materials Design. *Accounts of Chemical Research*, **2021**, 54, 849-860	24.3	61
270	Exciton transport in thin-film cyanine dye J-aggregates. *Journal of Chemical Physics*, **2012**, 137, 034109	3.9	60

269	Identification Schemes for Metal-Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. *Crystal Growth and Design*, **2019**, 19, 6682-6697	3.5	59
268	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
267	Memory-Assisted Exciton Diffusion in the Chlorosome Light-Harvesting Antenna of Green Sulfur Bacteria. *Journal of Physical Chemistry Letters*, **2012**, 3, 2357-61	6.4	58
266	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	6.4	58
265	A quantum-quantum Metropolis algorithm. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 754-9	11.5	58
264	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,	2.6	58
263	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
262	Inverse design of nanoporous crystalline reticular materials with deep generative models. *Nature Machine Intelligence*, **2021**, 3, 76-86	22.5	58
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260	Soft pseudopotentials for efficient quantum Monte Carlo calculations: From Be to Ne and Al to Ar. *Journal of Chemical Physics*, **2001**, 114, 7790-7794	3.9	56
259	Machine learning for quantum dynamics: deep learning of excitation energy transfer properties. *Chemical Science*, **2017**, 8, 8419-8426	9.4	55
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257	Disentangling electronic and vibronic coherences in two-dimensional echo spectra. *Journal of Physical Chemistry B*, **2013**, 117, 9380-5	3.4	54
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255	Machine-learned potentials for next-generation matter simulations. *Nature Materials*, **2021**, 20, 750-761	27	54
254	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, 17615-20	11.5	53
253	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. *Chemical Science*, **2018**, 9, 7642-7655	9.4	53
252	Molecular Engineering of an Alkaline Naphthoquinone Flow Battery. *ACS Energy Letters*, **2019**, 4, 1880-1887	23.1	52

251	Optimizing distributions over molecular space. An Objective-Reinforced Generative Adversarial Network for Inverse-design Chemistry (ORGANIC)		51
250	Bayesian network structure learning using quantum annealing. *European Physical Journal: Special Topics*, **2015**, 224, 163-188	2.3	50
249	A two-qubit photonic quantum processor and its application to solving systems of linear equations. *Scientific Reports*, **2014**, 4, 6115	4.9	49
248	Linear assignment maps for correlated system-environment states. *Physical Review A*, **2010**, 81,	2.6	49
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246	Quantum Monte Carlo for electronic excitations of free-base porphyrin. *Journal of Chemical Physics*, **2004**, 120, 3049-50	3.9	49
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244	Autonomous Molecular Design: Then and Now. *ACS Applied Materials & Interfaces*, **2019**, 11, 24825-24836	9.5	48
243	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	7.4	48
242	Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. *Chemical Science*, **2020**, 11, 4584-4601	9.4	47
241	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
240	Topologically protected excitons in porphyrin thin films. *Nature Materials*, **2014**, 13, 1026-32	27	47
239	Potential of quantum computing for drug discovery. *IBM Journal of Research and Development*, **2018**, 62, 6:1-6:20	2.5	47
238	Adiabatic quantum simulators. *AIP Advances*, **2011**, 1, 022126	1.5	45
237	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	3.9	44
236	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	3.9	43
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234	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, 4360-73	6.4	42

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232	A study of heuristic guesses for adiabatic quantum computation. *Quantum Information Processing*, **2011**, 10, 33-52	1.6	42
231	Coherent exciton dynamics in supramolecular light-harvesting nanotubes revealed by ultrafast quantum process tomography. *ACS Nano*, **2014**, 8, 5527-34	16.7	41
230	Digital quantum simulation of the statistical mechanics of a frustrated magnet. *Nature Communications*, **2012**, 3, 880	17.4	41
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228	A witness for coherent electronic vs vibronic-only oscillations in ultrafast spectroscopy. *Journal of Chemical Physics*, **2012**, 136, 234501	3.9	40
227	Accelerating Correlated Quantum Chemistry Calculations Using Graphical Processing Units. *Computing in Science and Engineering*, **2010**, 12, 40-51	1.5	40
226	Preparation of many-body states for quantum simulation. *Journal of Chemical Physics*, **2009**, 130, 194105	3.9	39
225	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
224	Nonradiative lifetimes in intermediate band photovoltaics□Absence of lifetime recovery. *Journal of Applied Physics*, **2012**, 112, 013707	2.5	38
223	Solving quantum ground-state problems with nuclear magnetic resonance. *Scientific Reports*, **2011**, 1, 88	4.9	38
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221	Nanoparticle synthesis assisted by machine learning. *Nature Reviews Materials*, **2021**, 6, 701-716	73.3	38
220	Discovery of Calcium-Metal Alloy Anodes for Reversible Ca-Ion Batteries. *Advanced Energy Materials* , **2019**, 9, 1802994	21.8	38
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217	Low-depth circuit ansatz for preparing correlated fermionic states on a quantum computer. *Quantum Science and Technology*, **2019**, 4, 045005	5.5	36
216	A Nanophotonic Structure Containing Living Photosynthetic Bacteria. *Small*, **2017**, 13, 1701777	11	36

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213	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
212	Temperature-dependent conformations of exciton-coupled Cy3 dimers in double-stranded DNA. *Journal of Chemical Physics*, **2018**, 148, 085101	3.9	35
211	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartree-Fock. *ACS Central Science*, **2018**, 4, 559-566	16.8	35
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207	Generative Adversarial Networks for Crystal Structure Prediction. *ACS Central Science*, **2020**, 6, 1412-1420	16.8	35
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205	ChemOS: An orchestration software to democratize autonomous discovery. *PLoS ONE*, **2020**, 15, e0229862	3.7	35
204	Theoretical characterization of excitation energy transfer in chlorosome light-harvesting antennae from green sulfur bacteria. *Photosynthesis Research*, **2014**, 120, 273-89	3.7	34
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202	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
201	Demon-like algorithmic quantum cooling and its realization with quantum optics. *Nature Photonics*, **2014**, 8, 113-118	33.9	33
200	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
199	Improved Fault-Tolerant Quantum Simulation of Condensed-Phase Correlated Electrons via Trotterization. *Quantum - the Open Journal for Quantum Science*,4, 296		33
198	Single-Atom Heat Machines Enabled by Energy Quantization. *Physical Review Letters*, **2018**, 120, 170601	7.4	32

197	Unification of witnessing initial system-environment correlations and witnessing non-Markovianity. *Europhysics Letters*, **2012**, 99, 20010	1.6	32
196	Proposal for Microwave Boson Sampling. *Physical Review Letters*, **2016**, 117, 140505	7.4	32
195	Quantum Nonlinear Optics with Polar J-Aggregates in Microcavities. *Journal of Physical Chemistry Letters*, **2014**, 5, 3708-15	6.4	31
194	Optimizing distributions over molecular space. An Objective-Reinforced Generative Adversarial Network for Inverse-design Chemistry (ORGANIC)		31
193	Chiral Sugars Drive Enantioenrichment in Prebiotic Amino Acid Synthesis. *ACS Central Science*, **2017**, 3, 322-328	16.8	30
192	Computational complexity in electronic structure. *Physical Chemistry Chemical Physics*, **2013**, 15, 397-411	3.6	30
191	Charge Tunneling along Short Oligoglycine Chains. *Angewandte Chemie - International Edition*, **2015**, 54, 14743-7	16.4	30
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189	Multipartite quantum entanglement evolution in photosynthetic complexes. *Journal of Chemical Physics*, **2012**, 137, 074112	3.9	30
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185	Ultrafast Spectroscopy		28
184	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
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