Florian Hse

List of Publications by Year in Descending Order

93 papers	15,093 citations	49 h-index	104 g-index
104 ext. papers	19,894 ext. citations	15.7 avg, IF	7.12 L-index

#	Paper	IF	Citations
93	Routescore: Punching the Ticket to More Efficient Materials Development.. *ACS Central Science*, **2022**, 8, 122-131	16.8	1
92	A quantum computing view on unitary coupled cluster theory.. *Chemical Society Reviews*, **2022**,	58.5	4
91	Noisy intermediate-scale quantum algorithms. *Reviews of Modern Physics*, **2022**, 94,	40.5	49
90	Golem: an algorithm for robust experiment and process optimization. *Chemical Science*, **2021**, 12, 14792-14807	9.4	4
89	Quantum computation of eigenvalues within target intervals. *Quantum Science and Technology*, **2021**, 6, 015004	5.5	5
88	Automated design of superconducting circuits and its application to 4-local couplers. *Npj Quantum Information*, **2021**, 7,	8.6	3
87	TEQUILA: a platform for rapid development of quantum algorithms. *Quantum Science and Technology*, **2021**, 6, 024009	5.5	10
86	Machine-learned potentials for next-generation matter simulations. *Nature Materials*, **2021**, 20, 750-761	27	54
85	Meta-Variational Quantum Eigensolver: Learning Energy Profiles of Parameterized Hamiltonians for Quantum Simulation. *PRX Quantum*, **2021**, 2,	6.1	9
84	Nanoparticle synthesis assisted by machine learning. *Nature Reviews Materials*, **2021**, 6, 701-716	73.3	38
83	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
82	A feasible approach for automatically differentiable unitary coupled-cluster on quantum computers. *Chemical Science*, **2021**, 12, 3497-3508	9.4	18
81	Inverse design of nanoporous crystalline reticular materials with deep generative models. *Nature Machine Intelligence*, **2021**, 3, 76-86	22.5	58
80	Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning. *Trends in Chemistry*, **2021**, 3, 96-110	14.8	16
79	Data-Driven Strategies for Accelerated Materials Design. *Accounts of Chemical Research*, **2021**, 54, 849-860	24.3	61
78	Quantum computer-aided design of quantum optics hardware. *Quantum Science and Technology*, **2021**, 6, 035010	5.5	2
77	Olympus: a benchmarking framework for noisy optimization and experiment planning. *Machine Learning: Science and Technology*, **2021**, 2, 035021	5.1	14

76	Data-science driven autonomous process optimization. *Communications Chemistry*, **2021**, 4,	6.3	19
75	Machine learning directed drug formulation development. *Advanced Drug Delivery Reviews*, **2021**, 175, 113806	18.5	17
74	Gryffin: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. *Applied Physics Reviews*, **2021**, 8, 031406	17.3	14
73	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
72	Self-driving laboratory for accelerated discovery of thin-film materials. *Science Advances*, **2020**, 6, eaaz8867	14.3	138
71	Materials Acceleration Platforms: On the way to autonomous experimentation. *Current Opinion in Green and Sustainable Chemistry*, **2020**, 25, 100370	7.9	28
70	Quantum computational chemistry. *Reviews of Modern Physics*, **2020**, 92,	40.5	256
69	Machine learning for analysing ab initio molecular dynamics simulations. *Journal of Physics: Conference Series*, **2020**, 1412, 042003	0.3	1
68	Team-Based Learning for Scientific Computing and Automated Experimentation: Visualization of Colored Reactions. *Journal of Chemical Education*, **2020**, 97, 689-694	2.4	4
67	Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems. *Advanced Materials*, **2020**, 32, e1907801	24	66
66	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
65	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
64	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. *ACS Nano*, **2020**, 14, 6589-6598	16.7	8
63	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. *Machine Learning: Science and Technology*, **2020**, 1, 045024	5.1	85
62	When robotics met fluidics. *Lab on A Chip*, **2020**, 20, 709-716	7.2	16
61	Resource-efficient digital quantum simulation of d-level systems for photonic, vibrational, and spin-s Hamiltonians. *Npj Quantum Information*, **2020**, 6,	8.6	27
60	Designing and understanding light-harvesting devices with machine learning. *Nature Communications*, **2020**, 11, 4587	17.4	21
59	ChemOS: An orchestration software to democratize autonomous discovery. *PLoS ONE*, **2020**, 15, e0229862	3.7	35

58	Oscillatory Active-site Motions Correlate with Kinetic Isotope Effects in Formate Dehydrogenase. *ACS Catalysis*, **2019**, 9, 11199-11206	13.1	13
57	Quantum Chemistry in the Age of Quantum Computing. *Chemical Reviews*, **2019**, 119, 10856-10915	68.1	288
56	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. *Nature Biotechnology*, **2019**, 37, 1038-1040	44.5	338
55	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
54	Next-Generation Experimentation with Self-Driving Laboratories. *Trends in Chemistry*, **2019**, 1, 282-291	14.8	91
53	Autonomous Molecular Design: Then and Now. *ACS Applied Materials & Interfaces*, **2019**, 11, 24825-24836	9.5	48
52	Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. *Quantum Science and Technology*, **2019**, 4, 014008	5.5	189
51	A Bayesian Approach to Predict Solubility Parameters. *Advanced Theory and Simulations*, **2019**, 2, 1800069	3.5	36
50	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
49	The Matter Simulation (R)evolution. *ACS Central Science*, **2018**, 4, 144-152	16.8	66
48	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. *ACS Central Science*, **2018**, 4, 268-276	16.8	950
47	Accelerating the discovery of materials for clean energy in the era of smart automation. *Nature Reviews Materials*, **2018**, 3, 5-20	73.3	308
46	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
45	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
44	Inverse molecular design using machine learning: Generative models for matter engineering. *Science*, **2018**, 361, 360-365	33.3	624
43	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartree-Fock. *ACS Central Science*, **2018**, 4, 559-566	16.8	35
42	Phoenics: A Bayesian Optimizer for Chemistry. *ACS Central Science*, **2018**, 4, 1134-1145	16.8	126
41	ChemOS: Orchestrating autonomous experimentation. *Science Robotics*, **2018**, 3,	18.6	73

40	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. *Chemical Science*, **2018**, 9, 7642-7655	9.4	53
39	Using coherence to enhance function in chemical and biophysical systems. *Nature*, **2017**, 543, 647-656	50.4	367
38	Machine learning for quantum dynamics: deep learning of excitation energy transfer properties. *Chemical Science*, **2017**, 8, 8419-8426	9.4	55
37	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
36	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
35	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. *Joule*, **2017**, 1, 857-870	27.8	120
34	Quantum autoencoders for efficient compression of quantum data. *Quantum Science and Technology*, **2017**, 2, 045001	5.5	154
33	Neural Networks for the Prediction of Organic Chemistry Reactions. *ACS Central Science*, **2016**, 2, 725-732	16.8	234
32	The Harvard organic photovoltaic dataset. *Scientific Data*, **2016**, 3, 160086	8.2	57
31	The theory of variational hybrid quantum-classical algorithms. *New Journal of Physics*, **2016**, 18, 023023	2.9	615
30	Machine learning exciton dynamics. *Chemical Science*, **2016**, 7, 5139-5147	9.4	90
29	Efficiency of energy funneling in the photosystem II supercomplex of higher plants. *Chemical Science*, **2016**, 7, 4174-4183	9.4	21
28	Free energy analysis and mechanism of base pair stacking in nicked DNA. *Nucleic Acids Research*, **2016**, 44, 7100-8	20.1	35
27	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
26	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
25	Computational design of molecules for an all-quinone redox flow battery. *Chemical Science*, **2015**, 6, 885-893	9.4	245
24	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
23	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

22	A compact native 24-residue supersecondary structure derived from the villin headpiece subdomain. *Biophysical Journal*, **2015**, 108, 678-86	2.9	5
21	A metal-free organic-inorganic aqueous flow battery. *Nature*, **2014**, 505, 195-8	50.4	1025
20	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
19	A variational eigenvalue solver on a photonic quantum processor. *Nature Communications*, **2014**, 5, 4213	17.4	1030
18	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
17	Disentangling electronic and vibronic coherences in two-dimensional echo spectra. *Journal of Physical Chemistry B*, **2013**, 117, 9380-5	3.4	54
16	Atomistic study of the long-lived quantum coherences in the Fenna-Matthews-Olson complex. *Biophysical Journal*, **2012**, 102, 649-60	2.9	178
15	Probing biological light-harvesting phenomena by optical cavities. *Physical Review B*, **2012**, 85,	3.3	24
14	On the alternatives for bath correlators and spectral densities from mixed quantum-classical simulations. *Journal of Chemical Physics*, **2012**, 137, 224103	3.9	107
13	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
12	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
11	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
10	Characterization and quantification of the role of coherence in ultrafast quantum biological experiments using quantum master equations, atomistic simulations, and quantum process tomography. *Procedia Chemistry*, **2011**, 3, 332-346		6
9	Communication: Exciton-phonon information flow in the energy transfer process of photosynthetic complexes. *Journal of Chemical Physics*, **2011**, 134, 101103	3.9	89
8	Role of quantum coherence and environmental fluctuations in chromophoric energy transport. *Journal of Physical Chemistry B*, **2009**, 113, 9942-7	3.4	268
7	Environment-assisted quantum transport. *New Journal of Physics*, **2009**, 11, 033003	2.9	606
6	Environment-assisted quantum walks in photosynthetic energy transfer. *Journal of Chemical Physics* , **2008**, 129, 174106	3.9	820
5	Simulated quantum computation of molecular energies. *Science*, **2005**, 309, 1704-7	33.3	555

List of Publications

4	Data-science driven autonomous process optimization		2
3	Data-science driven autonomous process optimization		4
2	Self-Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. *Advanced Functional Materials*,2106725	15.6	11
1	Parallel tempered genetic algorithm guided by deep neural networks for inverse molecular design		3