

# Florian Hse

## List of Publications by Citations

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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.

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	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , <b>2015</b> , 113, 184-215	1.7	2068
92	A variational eigenvalue solver on a photonic quantum processor. <i>Nature Communications</i> , <b>2014</b> , 5, 4213	17.4	1030
91	A metal-free organic-inorganic aqueous flow battery. <i>Nature</i> , <b>2014</b> , 505, 195-8	50.4	1025
90	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. <i>ACS Central Science</i> , <b>2018</b> , 4, 268-276	16.8	950
89	Environment-assisted quantum walks in photosynthetic energy transfer. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 174106	3.9	820
88	Inverse molecular design using machine learning: Generative models for matter engineering. <i>Science</i> , <b>2018</b> , 361, 360-365	33.3	624
87	The theory of variational hybrid quantum-classical algorithms. <i>New Journal of Physics</i> , <b>2016</b> , 18, 023023	2.9	615
86	Environment-assisted quantum transport. <i>New Journal of Physics</i> , <b>2009</b> , 11, 033003	2.9	606
85	Simulated quantum computation of molecular energies. <i>Science</i> , <b>2005</b> , 309, 1704-7	33.3	555
84	Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. <i>Nature Materials</i> , <b>2016</b> , 15, 1120-7	27	492
83	Using coherence to enhance function in chemical and biophysical systems. <i>Nature</i> , <b>2017</b> , 543, 647-656	50.4	367
82	The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 2241-2251	6.4	367
81	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. <i>Nature Biotechnology</i> , <b>2019</b> , 37, 1038-1040	44.5	338
80	Accelerating the discovery of materials for clean energy in the era of smart automation. <i>Nature Reviews Materials</i> , <b>2018</b> , 3, 5-20	73.3	308
79	Quantum Chemistry in the Age of Quantum Computing. <i>Chemical Reviews</i> , <b>2019</b> , 119, 10856-10915	68.1	288
78	Role of quantum coherence and environmental fluctuations in chromophoric energy transport. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 9942-7	3.4	268
77	Quantum computational chemistry. <i>Reviews of Modern Physics</i> , <b>2020</b> , 92,	40.5	256

76	Computational design of molecules for an all-quinone redox flow battery. <i>Chemical Science</i> , <b>2015</b> , 6, 885-893	24.5	245
75	Neural Networks for the Prediction of Organic Chemistry Reactions. <i>ACS Central Science</i> , <b>2016</b> , 2, 725-732	26.8	234
74	QSAR without borders. <i>Chemical Society Reviews</i> , <b>2020</b> , 49, 3525-3564	58.5	196
73	Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. <i>Quantum Science and Technology</i> , <b>2019</b> , 4, 014008	5.5	189
72	Atomistic study of the long-lived quantum coherences in the Fenna-Matthews-Olson complex. <i>Biophysical Journal</i> , <b>2012</b> , 102, 649-60	2.9	178
71	Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry [the Harvard Clean Energy Project]. <i>Energy and Environmental Science</i> , <b>2014</b> , 7, 698-704	35.4	158
70	Quantum autoencoders for efficient compression of quantum data. <i>Quantum Science and Technology</i> , <b>2017</b> , 2, 045001	5.5	154
69	Self-driving laboratory for accelerated discovery of thin-film materials. <i>Science Advances</i> , <b>2020</b> , 6, eaaz8867	17.3	138
68	Phoenics: A Bayesian Optimizer for Chemistry. <i>ACS Central Science</i> , <b>2018</b> , 4, 1134-1145	16.8	126
67	Learning from the Harvard Clean Energy Project: The Use of Neural Networks to Accelerate Materials Discovery. <i>Advanced Functional Materials</i> , <b>2015</b> , 25, 6495-6502	15.6	121
66	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. <i>Joule</i> , <b>2017</b> , 1, 857-870	27.8	120
65	Modified scaled hierarchical equation of motion approach for the study of quantum coherence in photosynthetic complexes. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 1531-7	3.4	110
64	On the alternatives for bath correlators and spectral densities from mixed quantum-classical simulations. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 224103	3.9	107
63	Next-Generation Experimentation with Self-Driving Laboratories. <i>Trends in Chemistry</i> , <b>2019</b> , 1, 282-291	14.8	91
62	Machine learning exciton dynamics. <i>Chemical Science</i> , <b>2016</b> , 7, 5139-5147	9.4	90
61	Communication: Exciton-phonon information flow in the energy transfer process of photosynthetic complexes. <i>Journal of Chemical Physics</i> , <b>2011</b> , 134, 101103	3.9	89
60	Scalable High-Performance Algorithm for the Simulation of Exciton Dynamics. Application to the Light-Harvesting Complex II in the Presence of Resonant Vibrational Modes. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 4045-54	6.4	86
59	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. <i>Machine Learning: Science and Technology</i> , <b>2020</b> , 1, 045024	5.1	85

58	Absence of Quantum Oscillations and Dependence on Site Energies in Electronic Excitation Transfer in the Fenna-Matthews-Olson Trimer. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 2912-2917	6.4	79
57	Influence of Force Fields and Quantum Chemistry Approach on Spectral Densities of BChl a in Solution and in FMO Proteins. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 9995-10004	3.4	74
56	ChemOS: Orchestrating autonomous experimentation. <i>Science Robotics</i> , <b>2018</b> , 3,	18.6	73
55	Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems. <i>Advanced Materials</i> , <b>2020</b> , 32, e1907801	24	66
54	The Matter Simulation (R)evolution. <i>ACS Central Science</i> , <b>2018</b> , 4, 144-152	16.8	66
53	Data-Driven Strategies for Accelerated Materials Design. <i>Accounts of Chemical Research</i> , <b>2021</b> , 54, 849-860	10.3	61
52	How machine learning can assist the interpretation of molecular dynamics simulations and conceptual understanding of chemistry. <i>Chemical Science</i> , <b>2019</b> , 10, 2298-2307	9.4	58
51	Inverse design of nanoporous crystalline reticular materials with deep generative models. <i>Nature Machine Intelligence</i> , <b>2021</b> , 3, 76-86	22.5	58
50	The Harvard organic photovoltaic dataset. <i>Scientific Data</i> , <b>2016</b> , 3, 160086	8.2	57
49	Machine learning for quantum dynamics: deep learning of excitation energy transfer properties. <i>Chemical Science</i> , <b>2017</b> , 8, 8419-8426	9.4	55
48	Disentangling electronic and vibronic coherences in two-dimensional echo spectra. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 9380-5	3.4	54
47	Machine-learned potentials for next-generation matter simulations. <i>Nature Materials</i> , <b>2021</b> , 20, 750-761	27	54
46	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. <i>Chemical Science</i> , <b>2018</b> , 9, 7642-7655	9.4	53
45	Noisy intermediate-scale quantum algorithms. <i>Reviews of Modern Physics</i> , <b>2022</b> , 94,	40.5	49
44	Autonomous Molecular Design: Then and Now. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 24825-24836	24.9	48
43	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> , <b>2018</b> , 115, E3342-E3350	11.5	47
42	Nanoparticle synthesis assisted by machine learning. <i>Nature Reviews Materials</i> , <b>2021</b> , 6, 701-716	73.3	38
41	A Bayesian Approach to Predict Solubility Parameters. <i>Advanced Theory and Simulations</i> , <b>2019</b> , 2, 1800069	5	36

40	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> , <b>2019</b> , 5, 1199-1210	16.8	35
39	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartree-Fock. <i>ACS Central Science</i> , <b>2018</b> , 4, 559-566	16.8	35
38	UV-Vis spectrophotometry of quinone flow battery electrolyte for in situ monitoring and improved electrochemical modeling of potential and quinhydrone formation. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 31684-31691	3.6	35
37	Free energy analysis and mechanism of base pair stacking in nicked DNA. <i>Nucleic Acids Research</i> , <b>2016</b> , 44, 7100-8	20.1	35
36	ChemOS: An orchestration software to democratize autonomous discovery. <i>PLoS ONE</i> , <b>2020</b> , 15, e0229867	6.7	35
35	Materials Acceleration Platforms: On the way to autonomous experimentation. <i>Current Opinion in Green and Sustainable Chemistry</i> , <b>2020</b> , 25, 100370	7.9	28
34	Resource-efficient digital quantum simulation of d-level systems for photonic, vibrational, and spin-s Hamiltonians. <i>Npj Quantum Information</i> , <b>2020</b> , 6,	8.6	27
33	Probing biological light-harvesting phenomena by optical cavities. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	24
32	Designing and understanding light-harvesting devices with machine learning. <i>Nature Communications</i> , <b>2020</b> , 11, 4587	17.4	21
31	Efficiency of energy funneling in the photosystem II supercomplex of higher plants. <i>Chemical Science</i> , <b>2016</b> , 7, 4174-4183	9.4	21
30	Data-science driven autonomous process optimization. <i>Communications Chemistry</i> , <b>2021</b> , 4,	6.3	19
29	A feasible approach for automatically differentiable unitary coupled-cluster on quantum computers. <i>Chemical Science</i> , <b>2021</b> , 12, 3497-3508	9.4	18
28	Machine learning directed drug formulation development. <i>Advanced Drug Delivery Reviews</i> , <b>2021</b> , 175, 113806	18.5	17
27	When robotics met fluidics. <i>Lab on A Chip</i> , <b>2020</b> , 20, 709-716	7.2	16
26	Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning. <i>Trends in Chemistry</i> , <b>2021</b> , 3, 96-110	14.8	16
25	Beyond generative models: superfast traversal, optimization, novelty, exploration and discovery (STONED) algorithm for molecules using SELFIES. <i>Chemical Science</i> , <b>2021</b> , 12, 7079-7090	9.4	16
24	Olympus: a benchmarking framework for noisy optimization and experiment planning. <i>Machine Learning: Science and Technology</i> , <b>2021</b> , 2, 035021	5.1	14
23	Gryffin: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. <i>Applied Physics Reviews</i> , <b>2021</b> , 8, 031406	17.3	14

22	Oscillatory Active-site Motions Correlate with Kinetic Isotope Effects in Formate Dehydrogenase. <i>ACS Catalysis</i> , <b>2019</b> , 9, 11199-11206	13.1	13
21	Disentanglement of excited-state dynamics with implications for FRET measurements: two-dimensional electronic spectroscopy of a BODIPY-functionalized cavitand. <i>Chemical Science</i> , <b>2018</b> , 9, 3694-3703	9.4	12
20	Self-Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. <i>Advanced Functional Materials</i> , 2106725	15.6	11
19	TEQUILA: a platform for rapid development of quantum algorithms. <i>Quantum Science and Technology</i> , <b>2021</b> , 6, 024009	5.5	10
18	Meta-Variational Quantum Eigensolver: Learning Energy Profiles of Parameterized Hamiltonians for Quantum Simulation. <i>PRX Quantum</i> , <b>2021</b> , 2,	6.1	9
17	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. <i>ACS Nano</i> , <b>2020</b> , 14, 6589-6598	16.7	8
16	Absence of Selection for Quantum Coherence in the Fenna-Matthews-Olson Complex: A Combined Evolutionary and Excitonic Study. <i>ACS Central Science</i> , <b>2017</b> , 3, 1086-1095	16.8	7
15	Characterization and quantification of the role of coherence in ultrafast quantum biological experiments using quantum master equations, atomistic simulations, and quantum process tomography. <i>Procedia Chemistry</i> , <b>2011</b> , 3, 332-346		6
14	Reducing Qubit Requirements while Maintaining Numerical Precision for the Variational Quantum Eigensolver: A Basis-Set-Free Approach. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 663-673	6.4	6
13	A compact native 24-residue supersecondary structure derived from the villin headpiece subdomain. <i>Biophysical Journal</i> , <b>2015</b> , 108, 678-86	2.9	5
12	Quantum computation of eigenvalues within target intervals. <i>Quantum Science and Technology</i> , <b>2021</b> , 6, 015004	5.5	5
11	Team-Based Learning for Scientific Computing and Automated Experimentation: Visualization of Colored Reactions. <i>Journal of Chemical Education</i> , <b>2020</b> , 97, 689-694	2.4	4
10	Data-science driven autonomous process optimization		4
9	Golem: an algorithm for robust experiment and process optimization. <i>Chemical Science</i> , <b>2021</b> , 12, 14792-14807	14.8	4
8	A quantum computing view on unitary coupled cluster theory.. <i>Chemical Society Reviews</i> , <b>2022</b> ,	58.5	4
7	Automated design of superconducting circuits and its application to 4-local couplers. <i>Npj Quantum Information</i> , <b>2021</b> , 7,	8.6	3
6	Parallel tempered genetic algorithm guided by deep neural networks for inverse molecular design		3
5	Film Fabrication Techniques: Beyond Ternary OPV: High-Throughput Experimentation and Self-Driving Laboratories Optimize Multicomponent Systems (Adv. Mater. 14/2020). <i>Advanced Materials</i> , <b>2020</b> , 32, 2070110	24	2

4	Data-science driven autonomous process optimization		2
3	Quantum computer-aided design of quantum optics hardware. <i>Quantum Science and Technology</i> , <b>2021</b> , 6, 035010	5.5	2
2	Machine learning for analysing ab initio molecular dynamics simulations. <i>Journal of Physics: Conference Series</i> , <b>2020</b> , 1412, 042003	0.3	1
1	Routescor: Punching the Ticket to More Efficient Materials Development.. <i>ACS Central Science</i> , <b>2022</b> , 8, 122-131	16.8	1