Florian HÃ¤se

List of Publications by Year
in descending order

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94	25,008	24978	40881
papers	citations	57	93
		h-index	g-index

104	104	104	18783
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	A variational eigenvalue solver on a photonic quantum processor. Nature Communications, 2014, 5, 4213.	5.8	2,210
3	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. ACS Central Science, 2018, 4, 268-276.	5.3	1,761
4	A metal-free organicâ€“inorganic aqueous flow battery. Nature, 2014, 505, 195-198.	13.7	1,333
5	The theory of variational hybrid quantum-classical algorithms. New Journal of Physics, 2016, 18, 023023.	1.2	1,186
6	Inverse molecular design using machine learning: Generative models for matter engineering. Science, 2018, 361, 360-365.	6.0	1,055
7	Environment-assisted quantum walks in photosynthetic energy transfer. Journal of Chemical Physics, 2008, 129, 174106.	1.2	939
8	Simulated Quantum Computation of Molecular Energies. Science, 2005, 309, 1704-1707.	6.0	852
9	Quantum Chemistry in the Age of Quantum Computing. Chemical Reviews, 2019, 119, 10856-10915.	23.0	748
10	Quantum computational chemistry. Reviews of Modern Physics, 2020, 92, .	16.4	726
11	Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. Nature Materials, 2016, 15, 1120-1127.	13.3	708
12	Environment-assisted quantum transport. New Journal of Physics, 2009, 11, 033003.	1.2	694
13	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nature Biotechnology, 2019, 37, 1038-1040.	9.4	671
14	Noisy intermediate-scale quantum algorithms. Reviews of Modern Physics, 2022, 94, .	16.4	521
15	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	23.3	489
16	Using coherence to enhance function in chemical and biophysical systems. Nature, 2017, 543, 647-656.	13.7	477
17	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.	2.1	470
18	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427

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19	Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. Quantum Science and Technology, 2019, 4, 014008.	2.6	381
20	Computational design of molecules for an all-quinone redox flow battery. Chemical Science, 2015, 6, 885-893.	3.7	341
21	Neural Networks for the Prediction of Organic Chemistry Reactions. ACS Central Science, 2016, 2, 725-732.	5.3	321
22	Self-driving laboratory for accelerated discovery of thin-film materials. Science Advances, 2020, 6, eaaz8867.	4.7	306
23	Role of Quantum Coherence and Environmental Fluctuations in Chromophoric Energy Transport. Journal of Physical Chemistry B, 2009, 113, 9942-9947.	1.2	300
24	Quantum autoencoders for efficient compression of quantum data. Quantum Science and Technology, 2017, 2, 045001.	2.6	295
25	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. Machine Learning: Science and Technology, 2020, 1, 045024.	2.4	272
26	Phoenics: A Bayesian Optimizer for Chemistry. ACS Central Science, 2018, 4, 1134-1145.	5.3	215
27	Machine-learned potentials for next-generation matter simulations. Nature Materials, 2021, 20, 750-761.	13.3	214
28	Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry â€“ the Harvard Clean Energy Project. Energy and Environmental Science, 2014, 7, 698-704.	15.6	189
29	Atomistic Study of the Long-Lived Quantum Coherences in the Fenna-Matthews-Olson Complex. Biophysical Journal, 2012, 102, 649-660.	0.2	188
30	Nanoparticle synthesis assisted by machine learning. Nature Reviews Materials, 2021, 6, 701-716.	23.3	179
31	Next-Generation Experimentation with Self-Driving Laboratories. Trends in Chemistry, 2019, 1, 282-291.	4.4	175
32	Inverse design of nanoporous crystalline reticular materials with deep generative models. Nature Machine Intelligence, 2021, 3, 76-86.	8.3	172
33	Data-Driven Strategies for Accelerated Materials Design. Accounts of Chemical Research, 2021, 54, 849-860.	7.6	168
34	Learning from the Harvard Clean Energy Project: The Use of Neural Networks to Accelerate Materials Discovery. Advanced Functional Materials, 2015, 25, 6495-6502.	7.8	160
35	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. Joule, 2017, 1, 857-870.	11.7	157
36	Beyond Ternary OPV: Highâ€Throughput Experimentation and Selfâ€Driving Laboratories Optimize Multicomponent Systems. Advanced Materials, 2020, 32, e1907801.	11.1	138

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37	On the alternatives for bath correlators and spectral densities from mixed quantum-classical simulations. Journal of Chemical Physics, 2012, 137, 224103.	1.2	121
38	Modified Scaled Hierarchical Equation of Motion Approach for the Study of Quantum Coherence in Photosynthetic Complexes. Journal of Physical Chemistry B, 2011, 115, 1531-1537.	1.2	120
39	ChemOS: Orchestrating autonomous experimentation. Science Robotics, 2018, 3, .	9.9	113
40	Machine learning exciton dynamics. Chemical Science, 2016, 7, 5139-5147.	3.7	112
41	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, 4045-4054.	2.3	103
42	Machine learning directed drug formulation development. Advanced Drug Delivery Reviews, 2021, 175, 113806.	6.6	99
43	Data-science driven autonomous process optimization. Communications Chemistry, 2021, 4, .	2.0	94
44	Communication: Excitonâ€“phonon information flow in the energy transfer process of photosynthetic complexes. Journal of Chemical Physics, 2011, 134, 101103.	1.2	92
45	The Matter Simulation (R)evolution. ACS Central Science, 2018, 4, 144-152.	5.3	88
46	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. Chemical Science, 2018, 9, 7642-7655.	3.7	86
47	The Harvard organic photovoltaic dataset. Scientific Data, 2016, 3, 160086.	2.4	85
48	Absence of Quantum Oscillations and Dependence on Site Energies in Electronic Excitation Transfer in the Fennaâ€“Matthewsâ€“Olson Trimer. Journal of Physical Chemistry Letters, 2011, 2, 2912-2917.	2.1	83
49	A quantum computing view on unitary coupled cluster theory. Chemical Society Reviews, 2022, 51, 1659-1684.	18.7	83
50	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.	1.2	82
51	How machine learning can assist the interpretation of ab initio molecular dynamics simulations and conceptual understanding of chemistry. Chemical Science, 2019, 10, 2298-2307.	3.7	80
52	ChemOS: An orchestration software to democratize autonomous discovery. PLoS ONE, 2020, 15, e0229862.	1.1	77
53	Resource-efficient digital quantum simulation of d-level systems for photonic, vibrational, and spin-s Hamiltonians. Npj Quantum Information, 2020, 6, .	2.8	74
54	Machine learning for quantum dynamics: deep learning of excitation energy transfer properties. Chemical Science, 2017, 8, 8419-8426.	3.7	70

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55	Autonomous Molecular Design: Then and Now. ACS Applied Materials & Interfaces, 2019, 11, 24825-24836.	4.0	69
56	Materials Acceleration Platforms: On the way to autonomous experimentation. Current Opinion in Green and Sustainable Chemistry, 2020, 25, 100370.	3.2	67
57	Beyond generative models: superfast traversal, optimization, novelty, exploration and discovery (STONED) algorithm for molecules using SELFIES. Chemical Science, 2021, 12, 7079-7090.	3.7	64
58	A Bayesian Approach to Predict Solubility Parameters. Advanced Theory and Simulations, 2019, 2, 1800069.	1.3	62
59	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.	3.3	61
60	A Mixed Quantum Chemistry/Machine Learning Approach for the Fast and Accurate Prediction of Biochemical Redox Potentials and Its Large-Scale Application to 315â€¯000 Redox Reactions. ACS Central Science, 2019, 5, 1199-1210.	5.3	61
61	G<scp>ryffin</scp>: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. Applied Physics Reviews, 2021, 8, .	5.5	61
62	Free energy analysis and mechanism of base pair stacking in nicked DNA. Nucleic Acids Research, 2016, 44, gkw607.	6.5	60
63	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.	1.3	57
64	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartreeâ€“Fock. ACS Central Science, 2018, 4, 559-566.	5.3	57
65	Designing and understanding light-harvesting devices with machine learning. Nature Communications, 2020, 11, 4587.	5.8	57
66	Selfâ€Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. Advanced Functional Materials, 2021, 31, 2106725.	7.8	57
67	Disentangling Electronic and Vibronic Coherences in Two-Dimensional Echo Spectra. Journal of Physical Chemistry B, 2013, 117, 9380-9385.	1.2	55
68	A feasible approach for automatically differentiable unitary coupled-cluster on quantum computers. Chemical Science, 2021, 12, 3497-3508.	3.7	43
69	Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning. Trends in Chemistry, 2021, 3, 96-110.	4.4	39
70	Closed-loop discovery platform integration is needed for artificial intelligence to make an impact in drug discovery. Expert Opinion on Drug Discovery, 2019, 14, 1-4.	2.5	37
71	TEQUILA: a platform for rapid development of quantum algorithms. Quantum Science and Technology, 2021, 6, 024009.	2.6	36
72	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.	2.1	33

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73	Meta-Variational Quantum Eigensolver: Learning Energy Profiles of Parameterized Hamiltonians for Quantum Simulation. PRX Quantum, 2021, 2, .	3.5	33
74	Olympus: a benchmarking framework for noisy optimization and experiment planning. Machine Learning: Science and Technology, 2021, 2, 035021.	2.4	31
75	Efficiency of energy funneling in the photosystem II supercomplex of higher plants. Chemical Science, 2016, 7, 4174-4183.	3.7	30
76	Oscillatory Active-Site Motions Correlate with Kinetic Isotope Effects in Formate Dehydrogenase. ACS Catalysis, 2019, 9, 11199-11206.	5.5	29
77	Probing biological light-harvesting phenomena by optical cavities. Physical Review B, 2012, 85, .	1.1	28
78	When robotics met fluidics. Lab on A Chip, 2020, 20, 709-716.	3.1	27
79	Parallel tempered genetic algorithm guided by deep neural networks for inverse molecular design. , 2022, 1, 390-404.		22
80	Optimized low-depth quantum circuits for molecular electronic structure using a separable-pair approximation. Physical Review A, 2022, 105, .	1.0	19
81	Automated design of superconducting circuits and its application to 4-local couplers. Npj Quantum Information, 2021, 7, .	2.8	17
82	Team-Based Learning for Scientific Computing and Automated Experimentation: Visualization of Colored Reactions. Journal of Chemical Education, 2020, 97, 689-694.	1.1	15
83	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.	3.7	13
84	Quantum computer-aided design of quantum optics hardware. Quantum Science and Technology, 2021, 6, 035010.	2.6	13
85	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. ACS Nano, 2020, 14, 6589-6598.	7.3	12
86	Golem: an algorithm for robust experiment and process optimization. Chemical Science, 2021, 12, 14792-14807.	3.7	12
87	Improving the accuracy of the variational quantum eigensolver for molecular systems by the explicitly-correlated perturbative [2]_{R12}-correction. Physical Chemistry Chemical Physics, 2022, 24, 13550-13564.	1.3	12
88	Absence of Selection for Quantum Coherence in the Fennaâ€“Matthewsâ€“Olson Complex: A Combined Evolutionary and Excitonic Study. ACS Central Science, 2017, 3, 1086-1095.	5.3	11
89	Routescore: Punching the Ticket to More Efficient Materials Development. ACS Central Science, 2022, 8, 122-131.	5.3	8
90	A Compact Native 24-Residue Supersecondary Structure Derived from the Villin Headpiece Subdomain. Biophysical Journal, 2015, 108, 678-686.	0.2	7

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91	Quantum computation of eigenvalues within target intervals. Quantum Science and Technology, 2021, 6, 015004.	2.6	7
92	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.	0.7	6
93	Machine learning for analysing ab initio molecular dynamics simulations. Journal of Physics: Conference Series, 2020, 1412, 042003.	0.3	6
94	Film Fabrication Techniques: Beyond Ternary OPV: Highâ€Throughput Experimentation and Selfâ€Driving Laboratories Optimize Multicomponent Systems (Adv. Mater. 14/2020). Advanced Materials, 2020, 32, 2070110.	11.1	2