Florian HÃ¤se

List of Publications by Year
in descending order

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94	25,008	23567 58	40979 93
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	Routescore: Punching the Ticket to More Efficient Materials Development. ACS Central Science, 2022, 8, 122-131.	11.3	8
2	A quantum computing view on unitary coupled cluster theory. Chemical Society Reviews, 2022, 51, 1659-1684.	38.1	83
3	Noisy intermediate-scale quantum algorithms. Reviews of Modern Physics, 2022, 94, .	45.6	521
4	Optimized low-depth quantum circuits for molecular electronic structure using a separable-pair approximation. Physical Review A, 2022, 105, .	2.5	19
5	Parallel tempered genetic algorithm guided by deep neural networks for inverse molecular design. , 2022, 1, 390-404.		22
6	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.	2.8	12
7	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.	4.6	33
8	A feasible approach for automatically differentiable unitary coupled-cluster on quantum computers. Chemical Science, 2021, 12, 3497-3508.	7.4	43
9	Inverse design of nanoporous crystalline reticular materials with deep generative models. Nature Machine Intelligence, 2021, 3, 76-86.	16.0	172
10	Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning. Trends in Chemistry, 2021, 3, 96-110.	8.5	39
11	Data-Driven Strategies for Accelerated Materials Design. Accounts of Chemical Research, 2021, 54, 849-860.	15.6	168
12	Automated design of superconducting circuits and its application to 4-local couplers. Npj Quantum Information, 2021, 7, .	6.7	17
13	TEQUILA: a platform for rapid development of quantum algorithms. Quantum Science and Technology, 2021, 6, 024009.	5.8	36
14	Machine-learned potentials for next-generation matter simulations. Nature Materials, 2021, 20, 750-761.	27.5	214
15	Meta-Variational Quantum Eigensolver: Learning Energy Profiles of Parameterized Hamiltonians for Quantum Simulation. PRX Quantum, 2021, 2, .	9.2	33
16	Nanoparticle synthesis assisted by machine learning. Nature Reviews Materials, 2021, 6, 701-716.	48.7	179
17	Quantum computer-aided design of quantum optics hardware. Quantum Science and Technology, 2021, 6, 035010.	5.8	13
18	Olympus: a benchmarking framework for noisy optimization and experiment planning. Machine Learning: Science and Technology, 2021, 2, 035021.	5.0	31

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19	Data-science driven autonomous process optimization. Communications Chemistry, 2021, 4, .	4.5	94
20	Machine learning directed drug formulation development. Advanced Drug Delivery Reviews, 2021, 175, 113806.	13.7	99
21	Selfâ€Driving Platform for Metal Nanoparticle Synthesis: Combining Microfluidics and Machine Learning. Advanced Functional Materials, 2021, 31, 2106725.	14.9	57
22	G<scp>ryffin</scp>: An algorithm for Bayesian optimization of categorical variables informed by expert knowledge. Applied Physics Reviews, 2021, 8, .	11.3	61
23	Beyond generative models: superfast traversal, optimization, novelty, exploration and discovery (STONED) algorithm for molecules using SELFIES. Chemical Science, 2021, 12, 7079-7090.	7.4	64
24	Quantum computation of eigenvalues within target intervals. Quantum Science and Technology, 2021, 6, 015004.	5.8	7
25	Golem: an algorithm for robust experiment and process optimization. Chemical Science, 2021, 12, 14792-14807.	7.4	12
26	When robotics met fluidics. Lab on A Chip, 2020, 20, 709-716.	6.0	27
27	Resource-efficient digital quantum simulation of d-level systems for photonic, vibrational, and spin-s Hamiltonians. Npj Quantum Information, 2020, 6, .	6.7	74
28	Designing and understanding light-harvesting devices with machine learning. Nature Communications, 2020, 11, 4587.	12.8	57
29	Self-driving laboratory for accelerated discovery of thin-film materials. Science Advances, 2020, 6, eaaz8867.	10.3	306
30	Materials Acceleration Platforms: On the way to autonomous experimentation. Current Opinion in Green and Sustainable Chemistry, 2020, 25, 100370.	5.9	67
31	Quantum computational chemistry. Reviews of Modern Physics, 2020, 92, .	45.6	726
32	Machine learning for analysing ab initio molecular dynamics simulations. Journal of Physics: Conference Series, 2020, 1412, 042003.	0.4	6
33	Team-Based Learning for Scientific Computing and Automated Experimentation: Visualization of Colored Reactions. Journal of Chemical Education, 2020, 97, 689-694.	2.3	15
34	Beyond Ternary OPV: Highâ€Throughput Experimentation and Selfâ€Driving Laboratories Optimize Multicomponent Systems. Advanced Materials, 2020, 32, e1907801.	21.0	138
35	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
36	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.	21.0	2

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37	From Absorption Spectra to Charge Transfer in Nanoaggregates of Oligomers with Machine Learning. ACS Nano, 2020, 14, 6589-6598.	14.6	12
38	ChemOS: An orchestration software to democratize autonomous discovery. PLoS ONE, 2020, 15, e0229862.	2.5	77
39	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. Machine Learning: Science and Technology, 2020, 1, 045024.	5.0	272
40	Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz. Quantum Science and Technology, 2019, 4, 014008.	5.8	381
41	Oscillatory Active-Site Motions Correlate with Kinetic Isotope Effects in Formate Dehydrogenase. ACS Catalysis, 2019, 9, 11199-11206.	11.2	29
42	Quantum Chemistry in the Age of Quantum Computing. Chemical Reviews, 2019, 119, 10856-10915.	47.7	748
43	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nature Biotechnology, 2019, 37, 1038-1040.	17.5	671
44	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.	11.3	61
45	Next-Generation Experimentation with Self-Driving Laboratories. Trends in Chemistry, 2019, 1, 282-291.	8.5	175
46	Autonomous Molecular Design: Then and Now. ACS Applied Materials & Interfaces, 2019, 11, 24825-24836.	8.0	69
47	A Bayesian Approach to Predict Solubility Parameters. Advanced Theory and Simulations, 2019, 2, 1800069.	2.8	62
48	How machine learning can assist the interpretation of ab initio molecular dynamics simulations and conceptual understanding of chemistry. Chemical Science, 2019, 10, 2298-2307.	7.4	80
49	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.	5.0	37
50	The Matter Simulation (R)evolution. ACS Central Science, 2018, 4, 144-152.	11.3	88
51	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. ACS Central Science, 2018, 4, 268-276.	11.3	1,761
52	Accelerating the discovery of materials for clean energy in the era of smart automation. Nature Reviews Materials, 2018, 3, 5-20.	48.7	489
53	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.	7.4	13
54	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.	7.1	61

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55	Chimera: enabling hierarchy based multi-objective optimization for self-driving laboratories. Chemical Science, 2018, 9, 7642-7655.	7.4	86
56	Inverse molecular design using machine learning: Generative models for matter engineering. Science, 2018, 361, 360-365.	12.6	1,055
57	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartreeâ€“Fock. ACS Central Science, 2018, 4, 559-566.	11.3	57
58	Phoenics: A Bayesian Optimizer for Chemistry. ACS Central Science, 2018, 4, 1134-1145.	11.3	215
59	ChemOS: Orchestrating autonomous experimentation. Science Robotics, 2018, 3, .	17.6	113
60	Using coherence to enhance function in chemical and biophysical systems. Nature, 2017, 543, 647-656.	27.8	477
61	Machine learning for quantum dynamics: deep learning of excitation energy transfer properties. Chemical Science, 2017, 8, 8419-8426.	7.4	70
62	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.	11.3	11
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.	2.8	57
64	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. Joule, 2017, 1, 857-870.	24.0	157
65	Quantum autoencoders for efficient compression of quantum data. Quantum Science and Technology, 2017, 2, 045001.	5.8	295
66	Machine learning exciton dynamics. Chemical Science, 2016, 7, 5139-5147.	7.4	112
67	Efficiency of energy funneling in the photosystem II supercomplex of higher plants. Chemical Science, 2016, 7, 4174-4183.	7.4	30
68	Free energy analysis and mechanism of base pair stacking in nicked DNA. Nucleic Acids Research, 2016, 44, gkw607.	14.5	60
69	Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. Nature Materials, 2016, 15, 1120-1127.	27.5	708
70	Neural Networks for the Prediction of Organic Chemistry Reactions. ACS Central Science, 2016, 2, 725-732.	11.3	321
71	The Harvard organic photovoltaic dataset. Scientific Data, 2016, 3, 160086.	5.3	85
72	The theory of variational hybrid quantum-classical algorithms. New Journal of Physics, 2016, 18, 023023.	2.9	1,186

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73	Learning from the Harvard Clean Energy Project: The Use of Neural Networks to Accelerate Materials Discovery. Advanced Functional Materials, 2015, 25, 6495-6502.	14.9	160
74	A Compact Native 24-Residue Supersecondary Structure Derived from the Villin Headpiece Subdomain. Biophysical Journal, 2015, 108, 678-686.	0.5	7
75	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.	2.6	82
76	Computational design of molecules for an all-quinone redox flow battery. Chemical Science, 2015, 6, 885-893.	7.4	341
77	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
78	A metal-free organicâ€“inorganic aqueous flow battery. Nature, 2014, 505, 195-198.	27.8	1,333
79	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.	30.8	189
80	A variational eigenvalue solver on a photonic quantum processor. Nature Communications, 2014, 5, 4213.	12.8	2,210
81	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.	5.3	103
82	Disentangling Electronic and Vibronic Coherences in Two-Dimensional Echo Spectra. Journal of Physical Chemistry B, 2013, 117, 9380-9385.	2.6	55
83	On the alternatives for bath correlators and spectral densities from mixed quantum-classical simulations. Journal of Chemical Physics, 2012, 137, 224103.	3.0	121
84	Atomistic Study of the Long-Lived Quantum Coherences in the Fenna-Matthews-Olson Complex. Biophysical Journal, 2012, 102, 649-660.	0.5	188
85	Probing biological light-harvesting phenomena by optical cavities. Physical Review B, 2012, 85, .	3.2	28
86	Communication: Excitonâ€“phonon information flow in the energy transfer process of photosynthetic complexes. Journal of Chemical Physics, 2011, 134, 101103.	3.0	92
87	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.	4.6	470
88	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.	2.6	120
89	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.	4.6	83
90	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

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91	Role of Quantum Coherence and Environmental Fluctuations in Chromophoric Energy Transport. Journal of Physical Chemistry B, 2009, 113, 9942-9947.	2.6	300
92	Environment-assisted quantum transport. New Journal of Physics, 2009, 11, 033003.	2.9	694
93	Environment-assisted quantum walks in photosynthetic energy transfer. Journal of Chemical Physics, 2008, 129, 174106.	3.0	939
94	Simulated Quantum Computation of Molecular Energies. Science, 2005, 309, 1704-1707.	12.6	852