Anders Steen Christensen

List of Publications by Year
in descending order

27	1,486	471509 17	552781 26
papers	citations	h-index	g-index

45	45	45	1542
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum Machine Learning Approach for Studying Atmospheric Cluster Formation. Environmental Science and Technology Letters, 2022, 9, 239-244.	8.7	18
2	An assessment of the structural resolution of various fingerprints commonly used in machine learning. Machine Learning: Science and Technology, 2021, 2, 015018.	5.0	37
3	OrbNet Denali: A machine learning potential for biological and organic chemistry with semi-empirical cost and DFT accuracy. Journal of Chemical Physics, 2021, 155, 204103.	3.0	40
4	Machine Learning Models of Vibrating H₂CO: Comparing Reproducing Kernels, FCHL, and PhysNet. Journal of Physical Chemistry A, 2020, 124, 8853-8865.	2.5	24
5	Neural networks and kernel ridge regression for excited states dynamics of CH₂NH 2+ : From single-state to multi-state representations and multi-property machine learning models. Machine Learning: Science and Technology, 2020, 1, 025009.	5.0	47
6	Charge and Exciton Transfer Simulations Using Machine-Learned Hamiltonians. Journal of Chemical Theory and Computation, 2020, 16, 4061-4070.	5.3	30
7	FCHL revisited: Faster and more accurate quantum machine learning. Journal of Chemical Physics, 2020, 152, 044107.	3.0	192
8	Quantum Machine Learning with Response Operators in Chemical Compound Space. Lecture Notes in Physics, 2020, , 155-169.	0.7	3
9	On the role of gradients for machine learning of molecular energies and forces. Machine Learning: Science and Technology, 2020, 1, 045018.	5.0	63
10	A universal density matrix functional from molecular orbital-based machine learning: Transferability across organic molecules. Journal of Chemical Physics, 2019, 150, 131103.	3.0	88
11	Operators in quantum machine learning: Response properties in chemical space. Journal of Chemical Physics, 2019, 150, 064105.	3.0	90
12	Operator Quantum Machine Learning: Navigating the Chemical Space of Response Properties. Chimia, 2019, 73, 1028.	0.6	9
13	Random versus Systematic Errors in Reaction Enthalpies Computed Using Semiempirical and Minimal Basis Set Methods. ACS Omega, 2018, 3, 4372-4377.	3.5	12
14	Alchemical and structural distribution based representation for universal quantum machine learning. Journal of Chemical Physics, 2018, 148, 241717.	3.0	272
15	Intermolecular interactions in the condensed phase: Evaluation of semi-empirical quantum mechanical methods. Journal of Chemical Physics, 2017, 147, 161704.	3.0	9
16	Towards a barrier height benchmark set for biologically relevant systems. PeerJ, 2016, 4, e1994.	2.0	22
17	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. Chemical Reviews, 2016, 116, 5301-5337.	47.7	312
18	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. Journal of Chemical Physics, 2015, 143, 084123.	3.0	47

#	Article	IF	Citations
19	DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters. Journal of Chemical Theory and Computation, 2015, 11, 4205-4219.	5.3	30
20	ProCS15: a DFT-based chemical shift predictor for backbone and CÎ²atoms in proteins. PeerJ, 2015, 3, e1344.	2.0	13
21	Bayesian inference of protein structure from chemical shift data. PeerJ, 2015, 3, e861.	2.0	11
22	A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+. PeerJ, 2014, 2, e449.	2.0	46
23	Hybrid RHF/MP2 Geometry Optimizations with the Effective Fragment Molecular Orbital Method. PLoS ONE, 2014, 9, e88800.	2.5	11
24	FragBuilder: an efficient Python library to setup quantum chemistry calculations on peptides models. PeerJ, 2014, 2, e277.	2.0	6
25	Protein Structure Validation and Refinement Using Amide Proton Chemical Shifts Derived from Quantum Mechanics. PLoS ONE, 2013, 8, e84123.	2.5	21
26	Definitive Benchmark Study of Ring Current Effects on Amide Proton Chemical Shifts. Journal of Chemical Theory and Computation, 2011, 7, 2078-2084.	5.3	16
27	High throughput virtual screening of 230 billion molecular solar heat battery candidates. PeerJ Physical Chemistry, 0, 3, e16.	0.0	15