

# Anders Steen Christensen

## List of Publications by Year in descending order

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Version: 2024-02-01

27  
papers

1,486  
citations

471509

17  
h-index

552781

26  
g-index

45  
all docs

45  
docs citations

45  
times ranked

1542  
citing authors

#	ARTICLE	IF	CITATIONS
1	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. <i>Chemical Reviews</i> , 2016, 116, 5301-5337.	47.7	312
2	Alchemical and structural distribution based representation for universal quantum machine learning. <i>Journal of Chemical Physics</i> , 2018, 148, 241717.	3.0	272
3	FCHL revisited: Faster and more accurate quantum machine learning. <i>Journal of Chemical Physics</i> , 2020, 152, 044107.	3.0	192
4	Operators in quantum machine learning: Response properties in chemical space. <i>Journal of Chemical Physics</i> , 2019, 150, 064105.	3.0	90
5	A universal density matrix functional from molecular orbital-based machine learning: Transferability across organic molecules. <i>Journal of Chemical Physics</i> , 2019, 150, 131103.	3.0	88
6	On the role of gradients for machine learning of molecular energies and forces. <i>Machine Learning: Science and Technology</i> , 2020, 1, 045018.	5.0	63
7	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. <i>Journal of Chemical Physics</i> , 2015, 143, 084123.	3.0	47
8	Neural networks and kernel ridge regression for excited states dynamics of CH <sub>2</sub> NH <sub>2</sub> <sup>+</sup> : From single-state to multi-state representations and multi-property machine learning models. <i>Machine Learning: Science and Technology</i> , 2020, 1, 025009.	5.0	47
9	A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+. <i>PeerJ</i> , 2014, 2, e449.	2.0	46
10	OrbNet Denali: A machine learning potential for biological and organic chemistry with semi-empirical cost and DFT accuracy. <i>Journal of Chemical Physics</i> , 2021, 155, 204103.	3.0	40
11	An assessment of the structural resolution of various fingerprints commonly used in machine learning. <i>Machine Learning: Science and Technology</i> , 2021, 2, 015018.	5.0	37
12	DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4205-4219.	5.3	30
13	Charge and Exciton Transfer Simulations Using Machine-Learned Hamiltonians. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4061-4070.	5.3	30
14	Machine Learning Models of Vibrating H <sub>2</sub> CO: Comparing Reproducing Kernels, FCHL, and PhysNet. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8853-8865.	2.5	24
15	Towards a barrier height benchmark set for biologically relevant systems. <i>PeerJ</i> , 2016, 4, e1994.	2.0	22
16	Protein Structure Validation and Refinement Using Amide Proton Chemical Shifts Derived from Quantum Mechanics. <i>PLoS ONE</i> , 2013, 8, e84123.	2.5	21
17	Quantum Machine Learning Approach for Studying Atmospheric Cluster Formation. <i>Environmental Science and Technology Letters</i> , 2022, 9, 239-244.	8.7	18
18	Definitive Benchmark Study of Ring Current Effects on Amide Proton Chemical Shifts. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2078-2084.	5.3	16

#	ARTICLE	IF	CITATIONS
19	High throughput virtual screening of 230 billion molecular solar heat battery candidates. PeerJ Physical Chemistry, 0, 3, e16.	0.0	15
20	ProCS15: a DFT-based chemical shift predictor for backbone and C <sup>13</sup> atoms in proteins. PeerJ, 2015, 3, e1344.	2.0	13
21	Random versus Systematic Errors in Reaction Enthalpies Computed Using Semiempirical and Minimal Basis Set Methods. ACS Omega, 2018, 3, 4372-4377.	3.5	12
22	Hybrid RHF/MP2 Geometry Optimizations with the Effective Fragment Molecular Orbital Method. PLoS ONE, 2014, 9, e88800.	2.5	11
23	Bayesian inference of protein structure from chemical shift data. PeerJ, 2015, 3, e861.	2.0	11
24	Intermolecular interactions in the condensed phase: Evaluation of semi-empirical quantum mechanical methods. Journal of Chemical Physics, 2017, 147, 161704.	3.0	9
25	Operator Quantum Machine Learning: Navigating the Chemical Space of Response Properties. Chimia, 2019, 73, 1028.	0.6	9
26	FragBuilder: an efficient Python library to setup quantum chemistry calculations on peptides models. PeerJ, 2014, 2, e277.	2.0	6
27	Quantum Machine Learning with Response Operators in Chemical Compound Space. Lecture Notes in Physics, 2020, , 155-169.	0.7	3