Benjamin Nebgen

List of Publications by Year
in descending order

28 papers	1,852 citations	430874 18 h-index	552781 26 g-index
34 all docs	34 docs citations	34 times ranked	1765 citing authors

#	Article	IF	Citations
1	Less is more: Sampling chemical space with active learning. Journal of Chemical Physics, 2018, 148, 241733.	3.0	426
2	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. Nature Communications, 2019, 10, 2903.	12.8	399
3	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. Chemical Reviews, 2020, 120, 2215-2287.	47.7	231
4	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. Scientific Data, 2020, 7, 134.	5.3	104
5	Discovering a Transferable Charge Assignment Model Using Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 4495-4501.	4.6	88
6	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 4687-4698.	5.3	81
7	Dynamics of a Myoglobin Mutant Enzyme: 2D IR Vibrational Echo Experiments and Simulations. Journal of the American Chemical Society, 2010, 132, 18367-18376.	13.7	64
8	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5771-5783.	5.3	56
9	Automated discovery of a robust interatomic potential for aluminum. Nature Communications, 2021, 12, 1257.	12.8	47
10	Teaching a neural network to attach and detach electrons from molecules. Nature Communications, 2021, 12, 4870.	12.8	46
11	Photoexcited Nonadiabatic Dynamics of Solvated Pushâ€“Pull Ï€-Conjugated Oligomers with the NEXMD Software. Journal of Chemical Theory and Computation, 2018, 14, 3955-3966.	5.3	39
12	The Rise of Neural Networks for Materials and Chemical Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6227-6243.	4.6	39
13	Machine learned HÃ¼ckel theory: Interfacing physics and deep neural networks. Journal of Chemical Physics, 2021, 154, 244108.	3.0	25
14	The Mystery of Perpendicular Fivefold Axes and the Fourth Dimension in Intermetallic Structures. Chemistry - A European Journal, 2008, 14, 3908-3930.	3.3	24
15	Vibronic coupling in asymmetric bichromophores: Theory and application to diphenylmethane. Journal of Chemical Physics, 2012, 137, 084112.	3.0	24
16	Graphics Processing Unit-Accelerated Semiempirical Born Oppenheimer Molecular Dynamics Using PyTorch. Journal of Chemical Theory and Computation, 2020, 16, 4951-4962.	5.3	24
17	Fragment Molecular Orbital Nonadiabatic Molecular Dynamics for Condensed Phase Systems. Journal of Physical Chemistry A, 2016, 120, 7205-7212.	2.5	20
18	Deep learning of dynamically responsive chemical Hamiltonians with semiempirical quantum mechanics. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	19

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19	Jet-Cooled Spectroscopy of the Î±-Methylbenzyl Radical: Probing the State-Dependent Effects of Methyl Rocking Against a Radical Site. Journal of Physical Chemistry A, 2013, 117, 13465-13480.	2.5	17
20	Laves Phases, Î³â€Brass, and 2Ã—2Ã—2 Superstructures: A New Class of Quasicrystal Approximants and the Suggestion of a New Quasicrystal. Chemistry - A European Journal, 2008, 14, 6627-6639.	3.3	16
21	Predicting phosphorescence energies and inferring wavefunction localization with machine learning. Chemical Science, 2021, 12, 10207-10217.	7.4	14
22	Vibronic coupling in asymmetric bichromophores: Experimental investigation of diphenylmethane-d5. Journal of Chemical Physics, 2014, 141, 064316.	3.0	13
23	Vibronic coupling in asymmetric bichromophores: Theory and application to diphenylmethane-d5. Journal of Chemical Physics, 2014, 141, 134119.	3.0	9
24	Design principles from multiscale simulations to predict nanostructure in self-assembling ionic liquids. Faraday Discussions, 2018, 206, 159-181.	3.2	9
25	Bond order predictions using deep neural networks. Journal of Applied Physics, 2021, 129, .	2.5	8
26	A neural network for determination of latent dimensionality in Nonnegative Matrix Factorization. Machine Learning: Science and Technology, 0, , .	5.0	7
27	The effects of site asymmetry on near-degenerate state-to-state vibronic mixing in flexible bichromophores. Journal of Chemical Physics, 2019, 151, 084313.	3.0	3
28	Weak matching of temporal interval graphs of sensors for robust multi-modal event detection in noise. , 2020, , .		0