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	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
2	Bond order predictions using deep neural networks. Journal of Applied Physics, 2021, 129, .	2.5	8
3	Automated discovery of a robust interatomic potential for aluminum. Nature Communications, 2021, 12, 1257.	12.8	47
4	Machine learned HÃ¼ckel theory: Interfacing physics and deep neural networks. Journal of Chemical Physics, 2021, 154, 244108.	3.0	25
5	The Rise of Neural Networks for Materials and Chemical Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6227-6243.	4.6	39
6	Teaching a neural network to attach and detach electrons from molecules. Nature Communications, 2021, 12, 4870.	12.8	46
7	Predicting phosphorescence energies and inferring wavefunction localization with machine learning. Chemical Science, 2021, 12, 10207-10217.	7.4	14
8	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
9	Graphics Processing Unit-Accelerated Semiempirical Born Oppenheimer Molecular Dynamics Using PyTorch. Journal of Chemical Theory and Computation, 2020, 16, 4951-4962.	5.3	24
10	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5771-5783.	5.3	56
11	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
12	Weak matching of temporal interval graphs of sensors for robust multi-modal event detection in noise. , 2020, , .		0
13	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. Nature Communications, 2019, 10, 2903.	12.8	399
14	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
15	Design principles from multiscale simulations to predict nanostructure in self-assembling ionic liquids. Faraday Discussions, 2018, 206, 159-181.	3.2	9
16	Less is more: Sampling chemical space with active learning. Journal of Chemical Physics, 2018, 148, 241733.	3.0	426
17	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 4687-4698.	5.3	81
18	Discovering a Transferable Charge Assignment Model Using Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 4495-4501.	4.6	88

#	Article	IF	Citations
19	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
20	Fragment Molecular Orbital Nonadiabatic Molecular Dynamics for Condensed Phase Systems. Journal of Physical Chemistry A, 2016, 120, 7205-7212.	2.5	20
21	Vibronic coupling in asymmetric bichromophores: Experimental investigation of diphenylmethane-d5. Journal of Chemical Physics, 2014, 141, 064316.	3.0	13
22	Vibronic coupling in asymmetric bichromophores: Theory and application to diphenylmethane-d5. Journal of Chemical Physics, 2014, 141, 134119.	3.0	9
23	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
24	Vibronic coupling in asymmetric bichromophores: Theory and application to diphenylmethane. Journal of Chemical Physics, 2012, 137, 084112.	3.0	24
25	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
26	The Mystery of Perpendicular Fivefold Axes and the Fourth Dimension in Intermetallic Structures. Chemistry - A European Journal, 2008, 14, 3908-3930.	3.3	24
27	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
28	A neural network for determination of latent dimensionality in Nonnegative Matrix Factorization. Machine Learning: Science and Technology, 0, , .	5.0	7