Justin S Smith

List of Publications by Year
in descending order

20 papers	3,452 citations	394421 19 h-index	752698 20 g-index
20 all docs	20 docs citations	20 times ranked	2720 citing authors

#	Article	IF	Citations
1	ANI-1: an extensible neural network potential with DFT accuracy at force field computational cost. Chemical Science, 2017, 8, 3192-3203.	7.4	1,111
2	Less is more: Sampling chemical space with active learning. Journal of Chemical Physics, 2018, 148, 241733.	3.0	426
3	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. Nature Communications, 2019, 10, 2903.	12.8	399
4	Hierarchical modeling of molecular energies using a deep neural network. Journal of Chemical Physics, 2018, 148, 241715.	3.0	221
5	ANI-1, A data set of 20 million calculated off-equilibrium conformations for organic molecules. Scientific Data, 2017, 4, 170193.	5.3	178
6	Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens. Journal of Chemical Theory and Computation, 2020, 16, 4192-4202.	5.3	160
7	Accurate and transferable multitask prediction of chemical properties with an atoms-in-molecules neural network. Science Advances, 2019, 5, eaav6490.	10.3	148
8	TorchANI: A Free and Open Source PyTorch-Based Deep Learning Implementation of the ANI Neural Network Potentials. Journal of Chemical Information and Modeling, 2020, 60, 3408-3415.	5.4	143
9	Operative Versus Nonoperative Treatment for Adult Symptomatic Lumbar Scoliosis. Journal of Bone and Joint Surgery - Series A, 2019, 101, 338-352.	3.0	110
10	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
11	Discovering a Transferable Charge Assignment Model Using Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 4495-4501.	4.6	88
12	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 4687-4698.	5.3	81
13	Transforming Computational Drug Discovery with Machine Learning and AI. ACS Medicinal Chemistry Letters, 2018, 9, 1065-1069.	2.8	70
14	Automated discovery of a robust interatomic potential for aluminum. Nature Communications, 2021, 12, 1257.	12.8	47
15	Teaching a neural network to attach and detach electrons from molecules. Nature Communications, 2021, 12, 4870.	12.8	46
16	The Rise of Neural Networks for Materials and Chemical Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6227-6243.	4.6	39
17	Machine learned HÃ¼ckel theory: Interfacing physics and deep neural networks. Journal of Chemical Physics, 2021, 154, 244108.	3.0	25
18	Modeling of Peptides with Classical and Novel Machine Learning Force Fields: A Comparison. Journal of Physical Chemistry B, 2021, 125, 3598-3612.	2.6	22

#	Article	IF	Citations
19	Machine learning for molecular dynamics with strongly correlated electrons. Physical Review B, 2019, 99, .	3.2	20
20	Predicting phosphorescence energies and inferring wavefunction localization with machine learning. Chemical Science, 2021, 12, 10207-10217.	7.4	14