Mojtaba Haghighatlari

List of Publications by Year in descending order

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1307594 1372567 11 404 10 7 citations g-index h-index papers 17 17 17 513 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Protein Dynamics to Define and Refine Disordered Protein Ensembles. Journal of Physical Chemistry B, 2022, 126, 1885-1894.	2.6	9
2	NewtonNet: a Newtonian message passing network for deep learning of interatomic potentials and forces., 2022, 1, 333-343.		42
3	A benchmark dataset for Hydrogen Combustion. Scientific Data, 2022, 9, 215.	5.3	6
4	Open Chemistry, <scp>JupyterLab</scp> , <scp>REST</scp> , and quantum chemistry. International Journal of Quantum Chemistry, 2021, 121, .	2.0	7
5	Extended experimental inferential structure determination method in determining the structural ensembles of disordered protein states. Communications Chemistry, 2020, 3, .	4.5	39
6	Learning to Make Chemical Predictions: The Interplay of Feature Representation, Data, and Machine Learning Methods. CheM, 2020, 6, 1527-1542.	11.7	61
7	<i>ChemML</i> : A machine learning and informatics program package for the analysis, mining, and modeling of chemical and materials data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1458.	14.6	41
8	A deep neural network model for packing density predictions and its application in the study of 1.5 million organic molecules. Chemical Science, 2019, 10, 8374-8383.	7.4	30
9	Accelerated Discovery of High-Refractive-Index Polyimides via <i>First-Principles</i> Molecular Modeling, Virtual High-Throughput Screening, and Data Mining. Journal of Physical Chemistry C, 2019, 123, 14610-14618.	3.1	36
10	Advances of machine learning in molecular modeling and simulation. Current Opinion in Chemical Engineering, 2019, 23, 51-57.	7.8	84
11	Building and deploying a cyberinfrastructure for the data-driven design of chemical systems and the exploration of chemical space. Molecular Simulation, 2018, 44, 921-929.	2.0	28