## 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  | Advances of machine learning in molecular modeling and simulation. Current Opinion in Chemical Engineering, 2019, 23, 51-57.   | 7.8         | 84        |
| 2  | Learning to Make Chemical Predictions: The Interplay of Feature Representation, Data, and Machine Learning Methods. CheM, 2020, 6, 1527-1542.  | 11.7        | 61        |
| 3  | NewtonNet: a Newtonian message passing network for deep learning of interatomic potentials and forces., 2022, 1, 333-343.  |             | 42        |
| 4  | <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        |
| 5  | Extended experimental inferential structure determination method in determining the structural ensembles of disordered protein states. Communications Chemistry, 2020, 3, .  | 4.5         | 39        |
| 6  | 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        |
| 7  | 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        |
| 8  | 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        |
| 9  | Protein Dynamics to Define and Refine Disordered Protein Ensembles. Journal of Physical Chemistry B, 2022, 126, 1885-1894.   | 2.6         | 9         |
| 10 | Open Chemistry, <scp>JupyterLab</scp> , <scp>REST</scp> , and quantum chemistry. International Journal of Quantum Chemistry, 2021, 121, .  | 2.0         | 7         |
| 11 | A benchmark dataset for Hydrogen Combustion. Scientific Data, 2022, 9, 215.  | <b>5.</b> 3 | 6         |