Chowdhury M Ashraf

List of Publications by Year
in descending order

17	826	758635 12	887659 17
papers	citations	h-index	g-index

17	17	17	854
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Extension of the ReaxFF Combustion Force Field toward Syngas Combustion and Initial Oxidation Kinetics. Journal of Physical Chemistry A, 2017, 121, 1051-1068.	1.1	204
2	Atomistic Scale Analysis of the Carbonization Process for C/H/O/N-Based Polymers with the ReaxFF Reactive Force Field. Journal of Physical Chemistry B, 2019, 123, 5357-5367.	1.2	123
3	Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers. Journal of Physical Chemistry A, 2018, 122, 6633-6642.	1.1	96
4	ReaxFF Simulations of Laser-Induced Graphene (LIG) Formation for Multifunctional Polymer Nanocomposites. ACS Applied Nano Materials, 2020, 3, 1881-1890.	2.4	76
5	Pyrolysis of binary fuel mixtures at supercritical conditions: A ReaxFF molecular dynamics study. Fuel, 2019, 235, 194-207.	3.4	75
6	Effect of chemical structure on thermo-mechanical properties of epoxy polymers: Comparison of accelerated ReaxFF simulations and experiments. Polymer, 2018, 158, 354-363.	1.8	43
7	ReaxFF based molecular dynamics simulations of ignition front propagation in hydrocarbon/oxygen mixtures under high temperature and pressure conditions. Physical Chemistry Chemical Physics, 2017, 19, 5004-5017.	1.3	40
8	Unveiling Carbon Ring Structure Formation Mechanisms in Polyacrylonitrile-Derived Carbon Fibers. ACS Applied Materials & Interfaces, 2019, 11, 42288-42297.	4.0	36
9	Reactive Molecular Dynamics Simulations of the Atomic Oxygen Impact on Epoxies with Different Chemistries. Journal of Physical Chemistry C, 2019, 123, 15145-15156.	1.5	29
10	Development of a Charge-Implicit ReaxFF Potential for Hydrocarbon Systems. Journal of Physical Chemistry Letters, 2018, 9, 359-363.	2.1	27
11	Converting PBO fibers into carbon fibers by ultrafast carbonization. Carbon, 2020, 159, 432-442.	5.4	25
12	Defect Design of Two-Dimensional MoS₂ Structures by Using a Graphene Layer and Potato Stamp Concept. Journal of Physical Chemistry C, 2018, 122, 11911-11917.	1.5	13
13	Modified Random Sequential Adsorption Model for Understanding Kinetics of Proteins Adsorption at a Liquidâ€“Solid Interface. Langmuir, 2017, 33, 7215-7224.	1.6	12
14	Continuous Molecular Representations of Ionic Liquids. Journal of Physical Chemistry B, 2020, 124, 8347-8357.	1.2	12
15	Data Science in Chemical Engineering: Applications to Molecular Science. Annual Review of Chemical and Biomolecular Engineering, 2021, 12, 15-37.	3.3	9
16	Assessing the Performance of Various Stochastic Optimization Methods on Chemical Kinetic Modeling of Combustion. Industrial & Engineering Chemistry Research, 2020, 59, 19212-19225.	1.8	4
17	Application of ReaxFF-Reactive Molecular Dynamics and Continuum Methods in High-Temperature/Pressure Pyrolysis of Fuel Mixtures. Challenges and Advances in Computational Chemistry and Physics, 2019, , 161-185.	0.6	2