Md Mahbubul Islam

List of Publications by Year
in descending order

43 papers	2,561 citations	331670 21 h-index	265206 42 g-index
43 all docs	43 docs citations	43 times ranked	2644 citing authors

#	Article	IF	Citations
1	The ReaxFF reactive force-field: development, applications and future directions. Npj Computational Materials, 2016, 2, .	8.7	1,319
2	ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials. Physical Chemistry Chemical Physics, 2015, 17, 3383-3393.	2.8	143
3	eReaxFF: A Pseudoclassical Treatment of Explicit Electrons within Reactive Force Field Simulations. Journal of Chemical Theory and Computation, 2016, 12, 3463-3472.	5.3	91
4	ReaxFF Reactive Force Field Simulations on the Influence of Teflon on Electrolyte Decomposition during Li/SWCNT Anode Discharge in Lithium-Sulfur Batteries. Journal of the Electrochemical Society, 2014, 161, E3009-E3014.	2.9	88
5	Reductive Decomposition Reactions of Ethylene Carbonate by Explicit Electron Transfer from Lithium: An eReaxFF Molecular Dynamics Study. Journal of Physical Chemistry C, 2016, 120, 27128-27134.	3.1	67
6	Interactions of hydrogen with the iron and iron carbide interfaces: a ReaxFF molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 761-771.	2.8	61
7	Mechanical properties of stanene under uniaxial and biaxial loading: A molecular dynamics study. Journal of Applied Physics, 2015, 118, .	2.5	55
8	Single-Atom Catalysts for Improved Cathode Performance in Naâ€“S Batteries: A Density Functional Theory (DFT) Study. Journal of Physical Chemistry C, 2021, 125, 4458-4467.	3.1	45
9	Decomposition and Reaction of Polyvinyl Nitrate under Shock and Thermal Loading: A ReaxFF Reactive Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 22452-22464.	3.1	42
10	Functionalized MXenes as effective polyselenide immobilizers for lithiumâ€“selenium batteries: a density functional theory (DFT) study. Nanoscale, 2020, 12, 14087-14095.	5.6	41
11	Recent Advances for Improving the Accuracy, Transferability, and Efficiency of Reactive Force Fields. Journal of Chemical Theory and Computation, 2021, 17, 3237-3251.	5.3	41
12	Neural network reactive force field for C, H, N, and O systems. Npj Computational Materials, 2021, 7, .	8.7	39
13	Sensitivity of the Shock Initiation Threshold of 1,3,5-Triamino-2,4,6-trinitrobenzene (TATB) to Nuclear Quantum Effects. Journal of Physical Chemistry C, 2019, 123, 21969-21981.	3.1	35
14	Reactive Molecular Dynamics Simulations to Investigate the Shock Response of Liquid Nitromethane. Journal of Physical Chemistry C, 2019, 123, 2613-2626.	3.1	31
15	First-Principles Investigation of the Anchoring Behavior of Pristine and Defect-Engineered Tungsten Disulfide for Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2020, 124, 27323-27332.	3.1	28
16	Investigation of the mechanical properties and fracture mechanisms of graphene/WSe2 vertical heterostructure: A molecular dynamics study. Computational Materials Science, 2021, 188, 110231.	3.0	28
17	Mechanistic Insights into Interactions of Polysulfides at VS₂ Interfaces in Naâ€“S Batteries: A DFT Study. ACS Applied Materials & Interfaces, 2021, 13, 35848-35855.	8.0	28
18	Role of Molecular Disorder on the Reactivity of RDX. Journal of Physical Chemistry C, 2018, 122, 27032-27043.	3.1	27

#	Article	IF	Citations
19	Atomistic Representation of Anomalies in the Failure Behaviour of Nanocrystalline Silicene. Scientific Reports, 2017, 7, 14629.	3.3	26
20	Pulse Dynamics of Electric Double Layer Formation on All-Solid-State Graphene Field-Effect Transistors. ACS Applied Materials & Interfaces, 2018, 10, 43166-43176.	8.0	25
21	Design Principles of Bifunctional Electrocatalysts for Engineered Interfaces in Naâ€“S Batteries. ACS Catalysis, 2021, 11, 15149-15161.	11.2	24
22	Atomic-Scale Insights into Comparative Mechanisms and Kinetics of Naâ€“S and Liâ€“S Batteries. ACS Catalysis, 2022, 12, 7664-7676.	11.2	23
23	Role of surface oxidation on the size dependent mechanical properties of nickel nanowires: a ReaxFF molecular dynamics study. Physical Chemistry Chemical Physics, 2018, 20, 284-298.	2.8	21
24	Engineered defects to modulate the phonon thermal conductivity of Silicene: A nonequilibrium molecular dynamics study. Computational Materials Science, 2021, 191, 110338.	3.0	21
25	Atomistic Insights on the Full Operation Cycle of a HfO₂-Based Resistive Random Access Memory Cell from Molecular Dynamics. ACS Nano, 2021, 15, 12945-12954.	14.6	21
26	Tuning the mechanical properties of silicene nanosheet by auxiliary cracks: a molecular dynamics study. RSC Advances, 2018, 8, 30354-30365.	3.6	20
27	Role of dynamical compressive and shear loading on hotspot criticality in RDX via reactive molecular dynamics. Journal of Applied Physics, 2020, 128, .	2.5	19
28	Atomic-scale analysis of the physical strength and phonon transport mechanisms of monolayer Î²-bismuthene. Physical Chemistry Chemical Physics, 2020, 22, 28238-28255.	2.8	18
29	Elucidating Synergistic Mechanisms of Adsorption and Electrocatalysis of Polysulfides on Double-Transition Metal MXenes for Naâ€“S Batteries. ACS Applied Materials & Interfaces, 2022, 14, 10298-10307.	8.0	18
30	Oxyhydroxide of metallic nanowires in a molecular H2O and H2O2 environment and their effects on mechanical properties. Physical Chemistry Chemical Physics, 2018, 20, 17289-17303.	2.8	17
31	Atomistic investigation on the mechanical properties and failure behavior of zinc-blende cadmium selenide (CdSe) nanowire. Computational Materials Science, 2021, 186, 110001.	3.0	16
32	Nitromethane Decomposition via Automated Reaction Discovery and an Ab Initio Corrected Kinetic Model. Journal of Physical Chemistry A, 2021, 125, 1447-1460.	2.5	16
33	Phonon thermal conductivity of the stanene/hBN van der Waals heterostructure. Physical Chemistry Chemical Physics, 2021, 23, 11028-11038.	2.8	14
34	Understanding mechanical properties and failure mechanism of germanium-silicon alloy at nanoscale. Journal of Nanoparticle Research, 2020, 22, 1.	1.9	13
35	Unveiling the Electrocatalytic Activity of 1Tâ€²-MoSe₂ on Lithium-Polysulfide Conversion Reactions. ACS Applied Materials & Interfaces, 2022, 14, 24486-24496.	8.0	11
36	Firstâ€principles investigation of elastic and electronic properties of double transition metal carbide MXenes. Journal of the American Ceramic Society, 2022, 105, 4400-4413.	3.8	7

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37	Nanomechanics of antimonene allotropes under tensile loading. Physical Chemistry Chemical Physics, 2021, 23, 6241-6251.	2.8	6
38	Atomic-scale perspective of mechanical properties and fracture mechanisms of graphene/WS2/graphene heterostructure. Computational Condensed Matter, 2021, 29, e00612.	2.1	6
39	Atomistic insights on the influence of pre-oxide shell layer and size on the compressive mechanical properties of nickel nanowires. Journal of Applied Physics, 2019, 125, .	2.5	4
40	Phonon thermal transport in encapsulated copper hybrids. Journal of Applied Physics, 2019, 125, 045106.	2.5	3
41	Atomistic elucidation of mechanical properties and fracture phenomenon of defective indium selenide monolayer. Computational Condensed Matter, 2022, 30, e00637.	2.1	2
42	Atomic-scale investigation of the effect of surface carbon coatings on the oxidation and mechanical properties of iron nanowires. New Journal of Chemistry, 2021, 45, 21763-21774.	2.8	1
43	Single-Atom Electrocatalyst for Engineered Cathode Interfaces in Sodium-Sulfur Batteries. ECS Meeting Abstracts, 2022, MA2022-01, 1963-1963.	0.0	0