

Weiwei Zhang

List of Publications by Year in descending order

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Version: 2024-02-01

29
papers

1,268
citations

361413

20
h-index

477307

29
g-index

29
all docs

29
docs citations

29
times ranked

1668
citing authors

#	ARTICLE	IF	CITATIONS
1	Aqueous proton transfer across single-layer graphene. Nature Communications, 2015, 6, 6539.	12.8	214
2	Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers. Journal of Physical Chemistry A, 2018, 122, 6633-6642.	2.5	96
3	Atomic insight into tribochemical wear mechanism of silicon at the Si/SiO ₂ interface in aqueous environment: Molecular dynamics simulations using ReaxFF reactive force field. Applied Surface Science, 2016, 390, 216-223.	6.1	89
4	Second-Generation ReaxFF Water Force Field: Improvements in the Description of Water Density and OH-Anion Diffusion. Journal of Physical Chemistry B, 2017, 121, 6021-6032.	2.6	87
5	Improvement of the ReaxFF Description for Functionalized Hydrocarbon/Water Weak Interactions in the Condensed Phase. Journal of Physical Chemistry B, 2018, 122, 4083-4092.	2.6	83
6	ReaxFF Reactive Molecular Dynamics Simulation of Functionalized Poly(phenylene oxide) Anion Exchange Membrane. Journal of Physical Chemistry C, 2015, 119, 27727-27736.	3.1	68
7	Atomistic mechanisms of Si chemical mechanical polishing in aqueous H ₂ O ₂ : ReaxFF reactive molecular dynamics simulations. Computational Materials Science, 2017, 131, 230-238.	3.0	68
8	Grotthuss versus Vehicular Transport of Hydroxide in Anion-Exchange Membranes: Insight from Combined Reactive and Nonreactive Molecular Simulations. Journal of Physical Chemistry Letters, 2018, 9, 825-829.	4.6	68
9	ReaxFF reactive molecular dynamics simulations to study the interfacial dynamics between defective h-BN nanosheets and water nanodroplets. Physical Chemistry Chemical Physics, 2021, 23, 10822-10834.	2.8	55
10	Development of the ReaxFF Methodology for Electrolyteâ€“Water Systems. Journal of Physical Chemistry A, 2019, 123, 2125-2141.	2.5	48
11	Hydroxide transport and chemical degradation in anion exchange membranes: a combined reactive and non-reactive molecular simulation study. Journal of Materials Chemistry A, 2019, 7, 5442-5452.	10.3	39
12	Cathodic Corrosion at the Bismuthâ€“Ionic Liquid Electrolyte Interface under Conditions for CO ₂ Reduction. Chemistry of Materials, 2018, 30, 2362-2373.	6.7	38
13	Benchmark of ReaxFF force field for subcritical and supercritical water. Journal of Chemical Physics, 2018, 148, 234503.	3.0	34
14	Mechanical size effects of amorphous polymer-derived ceramics at the nanoscale: experiments and ReaxFF simulations. Nanoscale, 2019, 11, 7447-7456.	5.6	34
15	Si/C/H ReaxFF Reactive Potential for Silicon Surfaces Grafted with Organic Molecules. Journal of Physical Chemistry C, 2018, 122, 23515-23527.	3.1	33
16	Atomistic Insights into Cu Chemical Mechanical Polishing Mechanism in Aqueous Hydrogen Peroxide and Glycine: ReaxFF Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2019, 123, 26467-26474.	3.1	31
17	Surface Orientation and Temperature Effects on the Interaction of Silicon with Water: Molecular Dynamics Simulations Using ReaxFF Reactive Force Field. Journal of Physical Chemistry A, 2017, 121, 587-594.	2.5	27
18	Atomistic-Scale Simulations of the Graphene Growth on a Silicon Carbide Substrate Using Thermal Decomposition and Chemical Vapor Deposition. Chemistry of Materials, 2020, 32, 8306-8317.	6.7	27

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19	Multiscale Modeling of Structure, Transport and Reactivity in Alkaline Fuel Cell Membranes: Combined Coarse-Grained, Atomistic and Reactive Molecular Dynamics Simulations. <i>Polymers</i> , 2018, 10, 1289.	4.5	26
20	Isotope Effects in Water: Differences of Structure, Dynamics, Spectrum, and Proton Transport between Heavy and Light Water from ReaxFF Reactive Force Field Simulations. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5445-5452.	4.6	22
21	Thermal Stability of Organic Monolayers Grafted to Si(111): Insights from ReaxFF Reactive Molecular Dynamics Simulations. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 30969-30981.	8.0	19
22	Photophysical/Chemistry Properties of Distyryl-BODIPY Derivatives: An Experimental and Density Functional Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5574-5579.	2.5	19
23	Modified Random Sequential Adsorption Model for Understanding Kinetics of Proteins Adsorption at a Liquid-Solid Interface. <i>Langmuir</i> , 2017, 33, 7215-7224.	3.5	12
24	Investigating the Accuracy of Water Models through the Van Hove Correlation Function. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5992-6005.	5.3	9
25	An Efficient and Green One-pot Synthesis of 12-Aryl-8,9,10,12-tetrahydrobenzo[<i>a</i>]xanthene Derivatives Promoted by Sulfamic Acid in [BMIM]BF ₄ Ionic Liquid. <i>Chinese Journal of Chemistry</i> , 2012, 30, 362-366.	4.9	7
26	Laboratory formation and photo-chemistry of ionic HBC/anthracene clusters in the gas phase. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 486, 3259-3265.	4.4	6
27	Theoretical characterization of zeolite encapsulated platinum clusters in the presence of water molecules. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23360-23371.	2.8	5
28	Reactive molecular dynamics simulation for isotope-exchange reactions in H/D systems: ReaxFFHD development. <i>Journal of Chemical Physics</i> , 2020, 152, 224111.	3.0	2
29	Effects of hydroxylation on the acidic and basic strengths of anatase TiO ₂ surfaces. <i>Molecular Simulation</i> , 2022, 48, 829-843.	2.0	2