Weiwei Zhang

List of Publications by Year
in descending order

29	1,268	361045 20	476904 29
papers	citations	h-index	g-index

29	29	29	1668
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Effects of hydroxylation on the acidic and basic strengths of anatase TiO₂ surfaces. Molecular Simulation, 2022, 48, 829-843.	0.9	2
2	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.	1.3	55
3	Investigating the Accuracy of Water Models through the Van Hove Correlation Function. Journal of Chemical Theory and Computation, 2021, 17, 5992-6005.	2.3	9
4	Theoretical characterization of zeolite encapsulated platinum clusters in the presence of water molecules. Physical Chemistry Chemical Physics, 2021, 23, 23360-23371.	1.3	5
5	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.	3.2	27
6	Reactive molecular dynamics simulation for isotope-exchange reactions in H/D systems: ReaxFFHD development. Journal of Chemical Physics, 2020, 152, 224111.	1.2	2
7	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.	1.5	31
8	Laboratory formation and photo-chemistry of ionic HBC/anthracene clusters in the gas phase. Monthly Notices of the Royal Astronomical Society, 2019, 486, 3259-3265.	1.6	6
9	Mechanical size effects of amorphous polymer-derived ceramics at the nanoscale: experiments and ReaxFF simulations. Nanoscale, 2019, 11, 7447-7456.	2.8	34
10	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.	5.2	39
11	Development of the ReaxFF Methodology for Electrolyteâ€“Water Systems. Journal of Physical Chemistry A, 2019, 123, 2125-2141.	1.1	48
12	Cathodic Corrosion at the Bismuthâ€“Ionic Liquid Electrolyte Interface under Conditions for CO₂ Reduction. Chemistry of Materials, 2018, 30, 2362-2373.	3.2	38
13	Improvement of the ReaxFF Description for Functionalized Hydrocarbon/Water Weak Interactions in the Condensed Phase. Journal of Physical Chemistry B, 2018, 122, 4083-4092.	1.2	83
14	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.	2.1	68
15	Multiscale Modeling of Structure, Transport and Reactivity in Alkaline Fuel Cell Membranes: Combined Coarse-Grained, Atomistic and Reactive Molecular Dynamics Simulations. Polymers, 2018, 10, 1289.	2.0	26
16	Si/C/H ReaxFF Reactive Potential for Silicon Surfaces Grafted with Organic Molecules. Journal of Physical Chemistry C, 2018, 122, 23515-23527.	1.5	33
17	Isotope Effects in Water: Differences of Structure, Dynamics, Spectrum, and Proton Transport between Heavy and Light Water from ReaxFF Reactive Force Field Simulations. Journal of Physical Chemistry Letters, 2018, 9, 5445-5452.	2.1	22
18	Benchmark of ReaxFF force field for subcritical and supercritical water. Journal of Chemical Physics, 2018, 148, 234503.	1.2	34

#	Article	IF	Citations
19	Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers. Journal of Physical Chemistry A, 2018, 122, 6633-6642.	1.1	96
20	Photophysical/Chemistry Properties of Distyryl-BODIPY Derivatives: An Experimental and Density Functional Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 5574-5579.	1.1	19
21	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.	1.1	27
22	Atomistic mechanisms of Si chemical mechanical polishing in aqueous H2O2: ReaxFF reactive molecular dynamics simulations. Computational Materials Science, 2017, 131, 230-238.	1.4	68
23	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.	1.2	87
24	Thermal Stability of Organic Monolayers Grafted to Si(111): Insights from ReaxFF Reactive Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2017, 9, 30969-30981.	4.0	19
25	Modified Random Sequential Adsorption Model for Understanding Kinetics of Proteins Adsorption at a Liquidâ€“Solid Interface. Langmuir, 2017, 33, 7215-7224.	1.6	12
26	Atomic insight into tribochemical wear mechanism of silicon at the Si/SiO2 interface in aqueous environment: Molecular dynamics simulations using ReaxFF reactive force field. Applied Surface Science, 2016, 390, 216-223.	3.1	89
27	ReaxFF Reactive Molecular Dynamics Simulation of Functionalized Poly(phenylene oxide) Anion Exchange Membrane. Journal of Physical Chemistry C, 2015, 119, 27727-27736.	1.5	68
28	Aqueous proton transfer across single-layer graphene. Nature Communications, 2015, 6, 6539.	5.8	214
29	An Efficient and Green Oneâ€pot Synthesis of 12â€Arylâ€8,9,10,12â€tetrahydrobenzo[a]xanthenâ€11â€one Derivatives Promoted by Sulfamic Acid in [BMIM]BF₄ Ionic Liquid. Chinese Journal of Chemistry, 2012, 30, 362-366.	2.6	7