Robert Horst MeiÃner

List of Publications by Year
in descending order

29	900	567281 15	477307 29
papers	citations	h-index	g-index

30	30	30	1312
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	7.5	220
2	Deep water formation, the subpolar gyre, and the meridional overturning circulation in the subpolar North Atlantic. Deep-Sea Research Part II: Topical Studies in Oceanography, 2011, 58, 1819-1832.	1.4	116
3	Ab initio derived forceâ€field parameters for molecular dynamics simulations of deprotonated amorphousâ€SiO₂/water interfaces. Physica Status Solidi (B): Basic Research, 2012, 249, 292-305.	1.5	71
4	Recognizing Local and Global Structural Motifs at the Atomic Scale. Journal of Chemical Theory and Computation, 2018, 14, 486-498.	5.3	43
5	In silico screening of modulators of magnesium dissolution. Corrosion Science, 2020, 163, 108245.	6.6	38
6	A first-principles analysis of the charge transfer in magnesium corrosion. Scientific Reports, 2020, 10, 15006.	3.3	37
7	ATR-FTIR in Kretschmann configuration integrated with electrochemical cell as in situ interfacial sensitive tool to study corrosion inhibitors for magnesium substrates. Electrochimica Acta, 2020, 345, 136166.	5.2	37
8	Computational Prediction of Circular Dichroism Spectra and Quantification of Helicity Loss upon Peptide Adsorption on Silica. Langmuir, 2014, 30, 3487-3494.	3.5	35
9	Data Science Based Mg Corrosion Engineering. Frontiers in Materials, 2019, 6, .	2.4	34
10	Estimation of the free energy of adsorption of a polypeptide on amorphous SiO₂ from molecular dynamics simulations and force spectroscopy experiments. Soft Matter, 2015, 11, 6254-6265.	2.7	30
11	Exploring key ionic interactions for magnesium degradation in simulated body fluid â€“ A data-driven approach. Corrosion Science, 2021, 182, 109272.	6.6	22
12	Osmotic Transport at the Aqueous Graphene and hBN Interfaces: Scaling Laws from a Unified, First-Principles Description. ACS Nano, 2021, 15, 15249-15258.	14.6	21
13	Exploring structure-property relationships in magnesium dissolution modulators. Npj Materials Degradation, 2021, 5, .	5.8	17
14	Predicting the inhibition efficiencies of magnesium dissolution modulators using sparse machine learning models. Npj Computational Materials, 2021, 7, .	8.7	17
15	Molecular Modeling of Microporous Structures of Carbide-Derived Carbon-Based Supercapacitors. Journal of Physical Chemistry C, 2017, 121, 7221-7231.	3.1	16
16	Combined Computational and Experimental Study on the Influence of Surface Chemistry of Carbon-Based Electrodes on Electrodeâ€“Electrolyte Interactions in Supercapacitors. Journal of Physical Chemistry C, 2019, 123, 2716-2727.	3.1	15
17	A Molecular Simulation Approach to Bond Reorganization in Epoxy Resins: From Curing to Deformation and Fracture. ACS Polymers Au, 2021, 1, 165-174.	4.1	15
18	Electrical Double Layer Capacitance of Curved Graphite Electrodes. Journal of Physical Chemistry C, 2020, 124, 5515-5521.	3.1	14

#	Article	IF	Citations
19	Elucidating Curvature-Capacitance Relationships in Carbon-Based Supercapacitors. Physical Review Letters, 2022, 128, 086001.	7.8	14
20	Modeling Charge Redistribution at Magnetite Interfaces in Empirical Force Fields. Journal of Physical Chemistry C, 2021, 125, 4794-4805.	3.1	13
21	Mutual Influence Between Adhesion and Molecular Conformation: Molecular Geometry is a Key Issue in Interphase Formation. Journal of Adhesion, 2013, 89, 77-95.	3.0	12
22	Weak adhesion detection â€“ Enhancing the analysis of vibroacoustic modulation by machine learning. Composite Structures, 2021, 273, 114233.	5.8	12
23	Molecular Simulation of Thermosetting Polymer Hardening: Reactive Events Enabled by Controlled Topology Transfer. Macromolecules, 2020, 53, 9698-9705.	4.8	11
24	Constant potential simulations on a mesh. Journal of Chemical Physics, 2021, 155, 104104.	3.0	11
25	Atomistic Insight into the Hydration States of Layered Double Hydroxides. ACS Omega, 2022, 7, 12412-12423.	3.5	9
26	Impact of the Conformational Variability of Oligopeptides on the Computational Prediction of Their CD Spectra. Journal of Physical Chemistry B, 2019, 123, 6694-6704.	2.6	7
27	Impact of confinement and polarizability on dynamics of ionic liquids. Journal of Chemical Physics, 2022, 156, 064703.	3.0	7
28	Mechanical degradation estimation of thermosets by peak shift assessment: General approach using infrared spectroscopy. Polymer, 2021, 221, 123585.	3.8	5
29	How water wets and self-hydrophilizes nanopatterns of physisorbed hydrocarbons. Journal of Colloid and Interface Science, 2022, 606, 57-66.	9.4	1