Feng Wang

List of Publications by Year
in descending order

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78 papers	3,241 citations	218677 26 h-index	149698 56 g-index
80 all docs	80 docs citations	80 times ranked	4883 citing authors

#	Article	IF	Citations
1	Fragmentation Method for Computing Quantum Mechanics and Molecular Mechanics Gradients for Force Matching: Validation with Hydration Free Energy Predictions Using Adaptive Force Matching. Journal of Physical Chemistry A, 2022, 126, 2609-2617.	2.5	2
2	Development and Validation of a DFT-Based Force Field for a Hydrated Homoalanine Polypeptide. Journal of Physical Chemistry B, 2021, 125, 1568-1581.	2.6	6
3	Study of Thermal Expansion Coefficient of Graphene via Raman Microâ€Spectroscopy: Revisited. Small, 2021, 17, e2006146.	10.0	7
4	Determining the hydration free energies of selected small molecules with MP2 and local MP2 through adaptive force matching. Journal of Chemical Physics, 2021, 154, 104113.	3.0	2
5	Real-Time Imaging of Laser-Induced Nanowelding of Silver Nanoparticles in Solution. Journal of Physical Chemistry C, 2021, 125, 10422-10430.	3.1	5
6	Performing Molecular Dynamics Simulations and Computing Hydration Free Energies on the B3LYP-D3(BJ) Potential Energy Surface with Adaptive Force Matching: A Benchmark Study with Seven Alcohols and One Amine. ACS Physical Chemistry Au, 2021, 1, 14-24.	4.0	9
7	A comparison of three DFT exchangeâ€“correlation functionals and two basis sets for the prediction of the conformation distribution of hydrated polyglycine. Journal of Chemical Physics, 2021, 155, 094104.	3.0	6
8	Altering the Solubility of the Antibiotic Candidate Nisinâ€”A Computational Study. ACS Omega, 2020, 5, 24854-24863.	3.5	9
9	A Metal-on-Metal Growth Approach to Metalâ€“Metal Oxide Coreâ€“Shell Nanostructures with Plasmonic Properties. Journal of Physical Chemistry C, 2020, 124, 17191-17203.	3.1	3
10	Comparing Alchemical Free Energy Estimates to Experimental Values Based on the Ben-Naim Formula: How Much Agreement Can We Expect?. Journal of Physical Chemistry B, 2020, 124, 840-847.	2.6	2
11	Accurate MP2-based force fields predict hydration free energies for simple alkanes and alcohols in good agreement with experiments. Journal of Chemical Physics, 2020, 153, 244505.	3.0	5
12	From a Liquid to a Crystal without Going through a First-Order Phase Transition: Determining the Free Energy of Melting with Glassy Intermediates. Journal of Physical Chemistry B, 2019, 123, 7740-7747.	2.6	3
13	Surface Penetration without Enrichment: Simulations Show Ion Surface Propensities Consistent with Both Elevated Surface Tension and Surface Sensitive Spectroscopy. Journal of Physical Chemistry B, 2019, 123, 7197-7203.	2.6	6
14	Leveraging local MP2 to reduce basis set superposition errors: An efficient first-principles based force-field for carbon dioxide. Journal of Chemical Physics, 2019, 151, 184501.	3.0	4
15	Self-Assembled Responsive Bilayered Vesicles with Adjustable Oxidative Stress for Enhanced Cancer Imaging and Therapy. Journal of the American Chemical Society, 2019, 141, 8158-8170.	13.7	132
16	On approximating a weak Markovian process as Markovian: Are we justified when discarding longtime correlations. Journal of Chemical Physics, 2019, 150, 085101.	3.0	0
17	Evaluating hydrophobic galactonoamidines as transition state analogs for enzymatic Î²-galactoside hydrolysis. Bioorganic Chemistry, 2018, 77, 144-151.	4.1	4
18	A molecular dynamics investigation of the surface tension of water nanodroplets and a new technique for local pressure determination through density correlation. Journal of Chemical Physics, 2018, 148, 144503.	3.0	10

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19	Molecular-scale processes affecting growth rates of ice at moderate supercooling. Frontiers of Physics, 2018, 13, 1.	5.0	8
20	The strengths and limitations of effective centroid force models explored by studying isotopic effects in liquid water. Journal of Chemical Physics, 2018, 148, 184102.	3.0	4
21	Synthesis of Copperâ€“Silica Coreâ€“Shell Nanostructures with Sharp and Stable Localized Surface Plasmon Resonance. Journal of Physical Chemistry C, 2017, 121, 5684-5692.	3.1	35
22	Water graphene contact surface investigated by pairwise potentials from force-matching PAW-PBE with dispersion correction. Journal of Chemical Physics, 2017, 146, 054702.	3.0	28
23	Performing the Millikan experiment at the molecular scale: Determination of atomic Millikan-Thomson charges by computationally measuring atomic forces. Journal of Chemical Physics, 2017, 147, 161726.	3.0	5
24	Accurate Prediction of the Hydration Free Energies of 20 Salts through Adaptive Force Matching and the Proper Comparison with Experimental References. Journal of Physical Chemistry B, 2017, 121, 6637-6645.	2.6	28
25	Picomolar inhibition of Î²-galactosidase (bovine liver) attributed to loop closure. Bioorganic and Medicinal Chemistry, 2017, 25, 5194-5202.	3.0	7
26	Self-Assembly of Semiconducting-Plasmonic Gold Nanoparticles with Enhanced Optical Property for Photoacoustic Imaging and Photothermal Therapy. Theranostics, 2017, 7, 2177-2185.	10.0	79
27	The effects of replacing the water model while decoupling water-water and water-solute interactions on computed properties of simple salts. Journal of Chemical Physics, 2016, 145, 044501.	3.0	5
28	Gold Nanoparticle Coated Carbon Nanotube Ring with Enhanced Raman Scattering and Photothermal Conversion Property for Theranostic Applications. Journal of the American Chemical Society, 2016, 138, 7005-7015.	13.7	208
29	The Effect of Core Correlation on the MP2 Hydration Free Energies of Li+, Na+, and K+. Journal of Physical Chemistry B, 2016, 120, 9088-9096.	2.6	4
30	Possible Evidence for a New Form of Liquid Buried in the Surface Tension of Supercooled Water. Scientific Reports, 2016, 6, 33284.	3.3	13
31	Pairwise-additive force fields for selected aqueous monovalent ions from adaptive force matching. Journal of Chemical Physics, 2015, 143, 194505.	3.0	38
32	Raman-Active Modes of Even-Numbered Cycloparaphenylenes: Comparisons between Experiments and Density Functional Theory (DFT) Calculations with Group Theory Arguments. Journal of Physical Chemistry C, 2015, 119, 2879-2887.	3.1	19
33	Rapid determination of plasmonic nanoparticle agglomeration status in blood. Biomaterials, 2015, 51, 226-237.	11.4	37
34	Continuous and Discontinuous Dynamic Crossover in Supercooled Water in Computer Simulations. Journal of Physical Chemistry Letters, 2015, 6, 3170-3174.	4.6	8
35	The liquid-vapor equilibria of TIP4P/2005 and BLYPSP-4F water models determined through direct simulations of the liquid-vapor interface. Journal of Chemical Physics, 2015, 142, 214507.	3.0	18
36	Mask-Assisted Seeded Growth of Segmented Metallic Heteronanostructures. Journal of Physical Chemistry C, 2014, 118, 28134-28142.	3.1	23

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37	On the Transferability of Three Water Models Developed by Adaptive Force Matching. Annual Reports in Computational Chemistry, 2014, 10, 25-43.	1.7	9
38	Graphene: A partially ordered non-periodic solid. Journal of Chemical Physics, 2014, 141, 144701.	3.0	9
39	Stable Saltâ€“Water Cluster Structures Reflect the Delicate Competition between Ionâ€“Water and Waterâ€“Water Interactions. Journal of Physical Chemistry B, 2014, 118, 743-751.	2.6	39
40	Raman spectroscopy of carbon nanohoops. Carbon, 2014, 67, 203-213.	10.3	70
41	Accurate ranking of CH4Â·(H2O)20 clusters with the density functional theory supplemental potential approach. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	8
42	Liquidâ€“liquid transition in supercooled water suggested by microsecond simulations. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 12209-12212.	7.1	71
43	Static dielectric constants and molecular dipole distributions of liquid water and ice-Ih investigated by the PAW-PBE exchange-correlation functional. Journal of Chemical Physics, 2012, 137, 034510.	3.0	22
44	Predicting the melting temperature of ice-Ih with only electronic structure information as input. Journal of Chemical Physics, 2012, 137, 014510.	3.0	27
45	Achieving fast convergence of ab initio free energy perturbation calculations with the adaptive force-matching method. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	25
46	Relative stability of armchair, zigzag and reczag graphene edges on the Ru(0001) surface. Surface Science, 2012, 606, 485-489.	1.9	10
47	Studies of iron(ii) and iron(iii) complexes with fac-N2O, cis-N2O2 and N2O3 donor ligands: models for the 2-His 1-carboxylate motif of non-heme iron monooxygenases. Dalton Transactions, 2012, 41, 5662.	3.3	16
48	The effect of varying carboxylate ligation on the electronic environment of N2Ox(x = 1â€“3) nonheme iron: A DFT analysis. Dalton Transactions, 2012, 41, 474-483.	3.3	3
49	Theoretical Analysis of [5.7]_nCyclacenes: Closed-Shell Cyclacene Isomers. Organic Letters, 2011, 13, 6220-6223.	4.6	33
50	Effects of the dispersion interaction in liquid water. Chemical Physics Letters, 2011, 513, 59-62.	2.6	20
51	Doxorubicin-Tethered Responsive Gold Nanoparticles Facilitate Intracellular Drug Delivery for Overcoming Multidrug Resistance in Cancer Cells. ACS Nano, 2011, 5, 3679-3692.	14.6	722
52	The quest for the best nonpolarizable water model from the adaptive force matching method. Journal of Computational Chemistry, 2011, 32, 453-462.	3.3	53
53	The extraordinary stability imparted to silver monolayers by chloride. Electrochimica Acta, 2011, 56, 1652-1661.	5.2	17
54	Approaching post-Hartreeâ€“Fock quality potential energy surfaces with simple pair-wise expressions: parameterising point-charge-based force fields for liquid water using the adaptive force matching method. Molecular Simulation, 2011, 37, 591-605.	2.0	41

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55	A simple molecular mechanics potential for Î¼m scale graphene simulations from the adaptive force matching method. Journal of Chemical Physics, 2011, 134, 184704.	3.0	51
56	The potential of mean force of nitrous oxide in a 1,2-dimyristoylphosphatidylcholine lipid bilayer. Chemical Physics Letters, 2010, 489, 96-98.	2.6	3
57	Computational investigation of lipid hydration water ofLÎ±1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine at three hydration levels. Molecular Physics, 2010, 108, 2027-2036.	1.7	17
58	Mimicking coarse-grained simulations without coarse-graining: Enhanced sampling by damping short-range interactions. Journal of Chemical Physics, 2010, 133, 084101.	3.0	7
59	Correcting for dispersion interaction and beyond in density functional theory through force matching. Journal of Chemical Physics, 2010, 133, 174115.	3.0	24
60	Understanding the Rotational Mechanism of a Single Molecule: STM and DFT Investigations of Dimethyl Sulfide Molecular Rotors on Au(111). Journal of Physical Chemistry C, 2010, 114, 3152-3155.	3.1	22
61	Improving the Point-Charge Description of Hydrogen Bonds by Adaptive Force Matching. Journal of Physical Chemistry B, 2009, 113, 1237-1240.	2.6	25
62	Effects Of Hydration On The Dynamics Of Water In Lipid Bilayer Systems: A Molecular Dynamics Study. Biophysical Journal, 2009, 96, 152a.	0.5	0
63	Optimizing the switching function for nonequilibrium free-energy calculations: An on-the-fly approach. Journal of Chemical Physics, 2009, 130, 174705.	3.0	8
64	Developing ab initio quality force fields from condensed phase quantum-mechanics/molecular-mechanics calculations through the adaptive force matching method. Journal of Chemical Physics, 2008, 129, 064108.	3.0	106
65	An Improved Multistate Empirical Valence Bond Model for Aqueous Proton Solvation and Transport. Journal of Physical Chemistry B, 2008, 112, 467-482.	2.6	228
66	Unusual â€œAmphiphilicâ€•Association of Hydrated Protons in Strong Acid Solution. Journal of the American Chemical Society, 2008, 130, 3120-3126.	13.7	39
67	Efficient Sampling of Ice Structures by Electrostatic Switching. Journal of Physical Chemistry B, 2008, 112, 6436-6441.	2.6	26
68	Nitrous Oxide Vibrational Energy Relaxation Is a Probe of Interfacial Water in Lipid Bilayers. Journal of Physical Chemistry B, 2008, 112, 12776-12782.	2.6	17
69	Kinetic Monte Carlo modeling of chemical reactions coupled with heat transfer. Journal of Chemical Physics, 2008, 128, 124706.	3.0	6
70	A linear-scaling self-consistent generalization of the multistate empirical valence bond method for multiple excess protons in aqueous systems. Journal of Chemical Physics, 2005, 122, 144105.	3.0	78
71	Excess Proton Solvation and Delocalization in a Hydrophilic Pocket of the Proton Conducting Polymer Membrane Nafion. Journal of Physical Chemistry B, 2005, 109, 3727-3730.	2.6	122
72	Calculation of the photodetachment cross sections of the HCNâ¯ and HNCâ¯ dipole-bound anions as described by a one-electron Drude model. Journal of Chemical Physics, 2004, 121, 1824-1829.	3.0	8

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73	Electron Attachment to (H2O)2ArnClustersâ€. Journal of Physical Chemistry A, 2004, 108, 2912-2921.	2.5	11
74	THEORY OFDIPOLE-BOUNDANIONS. Annual Review of Physical Chemistry, 2003, 54, 367-396.	10.8	273
75	Parallel-tempering Monte Carlo simulations of the finite temperature behavior of (H2O)6â˜. Journal of Chemical Physics, 2003, 119, 11645-11653.	3.0	36
76	Theoretical Calculations of Voltage-Dependent STM Images of Acetylene on the Si(001) Surface. Journal of Physical Chemistry B, 2002, 106, 1316-1321.	2.6	24
77	Application of a Drude model to the binding of excess electrons to water clusters. Journal of Chemical Physics, 2002, 116, 6973-6981.	3.0	67
78	A Drude-model approach to dispersion interactions in dipole-bound anions. Journal of Chemical Physics, 2001, 114, 10717-10724.	3.0	63