Yanting Wang

List of Publications by Citations

83 papers	4,476 citations	30 h-index	66 g-index
90 ext. papers	4,915 ext. citations	4.3 avg, IF	5.81 L-index

#	Paper	IF	Citations
83	Unique spatial heterogeneity in ionic liquids. *Journal of the American Chemical Society*, **2005**, 127, 12192-3	16.4	853
82	Molecular dynamics simulation of nanostructural organization in ionic liquid/water mixtures. *Journal of Physical Chemistry B*, **2007**, 111, 4812-8	3.4	395
81	Tail aggregation and domain diffusion in ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 18601-8	3.4	365
80	Understanding ionic liquids through atomistic and coarse-grained molecular dynamics simulations. *Accounts of Chemical Research*, **2007**, 40, 1193-9	24.3	285
79	The multiscale coarse-graining method. II. Numerical implementation for coarse-grained molecular models. *Journal of Chemical Physics*, **2008**, 128, 244115	3.9	284
78	Melting of icosahedral gold nanoclusters from molecular dynamics simulations. *Journal of Chemical Physics*, **2005**, 122, 214722	3.9	171
77	Multiscale coarse-graining of ionic liquids. *Journal of Physical Chemistry B*, **2006**, 110, 3564-75	3.4	158
76	Real-time mass spectrometric characterization of the solid-electrolyte interphase of a lithium-ion battery. *Nature Nanotechnology*, **2020**, 15, 224-230	28.7	156
75	Effect of the chain length on the structure of ionic liquids: from spatial heterogeneity to ionic liquid crystals. *Journal of Physical Chemistry B*, **2013**, 117, 1104-9	3.4	117
74	Tuning the self-assembly of short peptides via sequence variations. *Langmuir*, **2013**, 29, 13457-64	4	103
73	A Multiscale Coarse-Graining Study of the Liquid/Vacuum Interface of Room-Temperature Ionic Liquids with Alkyl Substituents of Different Lengths. *Journal of Physical Chemistry C*, **2008**, 112, 1132-1139	3.8	100
72	Effective force coarse-graining. *Physical Chemistry Chemical Physics*, **2009**, 11, 2002-15	3.6	97
71	Dual Ionic and Organic Nature of Ionic Liquids. *Scientific Reports*, **2016**, 6, 19644	4.9	76
70	Molecular dynamics simulation of the energetic room-temperature ionic liquid, 1-hydroxyethyl-4-amino-1,2,4-triazolium nitrate (HEATN). *Journal of Physical Chemistry B*, **2008**, 112, 3121-31	3.4	74
69	Melting and equilibrium shape of icosahedral gold nanoparticles. *Chemical Physics Letters*, **2004**, 394, 257-261	2.5	69
68	Transferable Coarse-Grained Models for Ionic Liquids. *Journal of Chemical Theory and Computation*, **2009**, 5, 1091-8	6.4	66
67	Surface-driven bulk reorganization of gold nanorods. *Nano Letters*, **2005**, 5, 2174-8	11.5	65

66	On the structure of ionic liquids: comparisons between electronically polarizable and nonpolarizable models I. *Journal of Physical Chemistry B*, **2010**, 114, 6905-21	3.4	61
65	Atomic origins of water-vapour-promoted alloy oxidation. *Nature Materials*, **2018**, 17, 514-518	27	59
64	Template-based and free modeling of I-TASSER and QUARK pipelines using predicted contact maps in CASP12. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86 Suppl 1, 136-151	4.2	58
63	Structural and Morphological Transitions in Gold Nanorods: A Computer Simulation Study. *Journal of Physical Chemistry B*, **2003**, 107, 9214-9219	3.4	57
62	On the dynamics of ionic liquids: comparisons between electronically polarizable and nonpolarizable models II. *Journal of Physical Chemistry B*, **2010**, 114, 6886-904	3.4	55
61	NeBcon: protein contact map prediction using neural network training coupled with naïve Bayes classifiers. *Bioinformatics*, **2017**, 33, 2296-2306	7.2	52
60	Molecular dynamics simulations of polyglutamine aggregation using solvent-free multiscale coarse-grained models. *Journal of Physical Chemistry B*, **2010**, 114, 8735-43	3.4	46
59	Ion-cage interpretation for the structural and dynamic changes of ionic liquids under an external electric field. *Journal of Physical Chemistry B*, **2013**, 117, 5102-12	3.4	41
58	Disordering and reordering of ionic liquids under an external electric field. *Journal of Physical Chemistry B*, **2009**, 113, 11058-60	3.4	41
57	Insights on the isotropic-to-smectic A transition in ionic liquid crystals from coarse-grained molecular dynamics simulations: the role of microphase segregation. *Journal of Physical Chemistry B* , **2015**, 119, 3829-36	3.4	40
56	Structures and Energetics of Silver and Gold Nanoparticles. *Journal of Physical Chemistry C*, **2011**, 115, 11374-11381	3.8	34
55	Intrinsic electric fields in ionic liquids determined by vibrational Stark effect spectroscopy and molecular dynamics simulation. *Chemistry - A European Journal*, **2012**, 18, 11904-8	4.8	31
54	Different nanostructures caused by competition of intra- and inter-β-sheet interactions in hierarchical self-assembly of short peptides. *Journal of Colloid and Interface Science*, **2016**, 464, 219-28	9.3	30
53	Diffusion mechanisms in smectic ionic liquid crystals: insights from coarse-grained MD simulations. *Soft Matter*, **2013**, 9, 5716	3.6	30
52	Structural, dynamic, and transport properties of concentrated aqueous sodium chloride solutions under an external static electric field. *Journal of Physical Chemistry B*, **2014**, 118, 4404-11	3.4	24
51	Spatial Heterogeneity in Ionic Liquids. *ACS Symposium Series*, **2007**, 272-307	0.4	23
50	Role of the Electrostatic Interactions in the Stabilization of Ionic Liquid Crystals: Insights from Coarse-Grained MD Simulations of an Imidazolium Model. *Journal of Physical Chemistry B*, **2016**, 120, 9152-60	3.4	22
49	Molecular origin of the self-assembled morphological difference caused by varying the order of charged residues in short peptides. *Journal of Physical Chemistry B*, **2014**, 118, 12501-10	3.4	21

48	Nanoparticle-based crystal growth via multistep self-assembly. *CrystEngComm*, **2013**, 15, 5114	3.3	21
47	Investigation of Ion-Solvent Interactions in Nonaqueous Electrolytes Using in Situ Liquid SIMS. *Analytical Chemistry*, **2018**, 90, 3341-3348	7.8	19
46	Concentration and temperature dependences of polyglutamine aggregation by multiscale coarse-graining molecular dynamics simulations. *Journal of Physical Chemistry B*, **2012**, 116, 10135-44	3.4	19
45	Influence of the ion size on the stability of the smectic phase of ionic liquid crystals. *Soft Matter*, **2020**, 16, 411-420	3.6	19
44	Molecular Origin of Donor- and Acceptor-Rich Domain Formation in Bulk-Heterojunction Solar Cells with an Enhanced Charge Transport Efficiency. *Journal of Physical Chemistry C*, **2017**, 121, 5864-5870	3.8	16
43	The Evidence for Fullerene Aggregation in High-Performance Small-Molecule Solar Cells by Molecular Dynamics Simulation. *Advanced Electronic Materials*, **2015**, 1, 1500217	6.4	16
42	Metastable State during Melting and Solid-Solid Phase Transition of [CMim][NO] (n = 4-12) Ionic Liquids by Molecular Dynamics Simulation. *Journal of Physical Chemistry B*, **2018**, 122, 229-239	3.4	15
41	Hydrogen-bond rich ionic liquids with hydroxyl cationic tails. *Chemical Physics Letters*, **2013**, 560, 32-36	2.5	14
40	Microscopic structure and dynamics of air/water interface by computer simulations--comparison with sum-frequency generation experiments. *Physical Chemistry Chemical Physics*, **2011**, 13, 5388-93	3.6	14
39	Nanoscale Tail Aggregation in Ionic Liquids: Roles of Electrostatic and van der Waals Interactions. *Communications in Theoretical Physics*, **2011**, 56, 499-503	2.4	14
38	Effect of Ion Rigidity on Physical Properties of Ionic Liquids Studied by Molecular Dynamics Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 5678-90	3.4	12
37	Effect of side-chain length on structural and dynamic properties of ionic liquids with hydroxyl cationic tails. *Journal of Physical Chemistry B*, **2014**, 118, 3642-9	3.4	10
36	Effect of Surface Structure on Shape Transformations of Gold Nanorods. *Journal of Computational and Theoretical Nanoscience*, **2007**, 4, 282-290	0.3	10
35	Modeling Elastically Mediated Liquid-Liquid Phase Separation. *Physical Review Letters*, **2020**, 125, 268001	7.4	10
34	Interplay between Intrinsic Conformational Propensities and Intermolecular Interactions in the Self-Assembly of Short Surfactant-like Peptides Composed of Leucine/Isoleucine. *Langmuir*, **2016**, 32, 4662-72	4	10
33	Communication: Probing the existence of partially arrested states in ionic liquids. *Journal of Chemical Physics*, **2016**, 145, 191101	3.9	8
32	A brief review of continuous models for ionic solutions: the PoissonBoltzmann and related theories. *Communications in Theoretical Physics*, **2020**, 72, 067601	2.4	7
31	Aggregation behavior of dihexadecylviologen bistriflimide ionic liquid crystal in different solvents: influence of polarity and concentration. *Physical Chemistry Chemical Physics*, **2018**, 20, 22730-22738	3.6	7

30	Continuous-time Monte Carlo and spatial ordering in driven lattice gases: Application to driven vortices in periodic superconducting networks. *Physical Review B*, **2005**, 72,	3.3	7
29	Phase Behaviors of Ionic Liquids Heating from Different Crystal Polymorphs toward the Same Smectic-A Ionic Liquid Crystal by Molecular Dynamics Simulation. *Crystals*, **2019**, 9, 26	2.3	6
28	Diffusion-Limited Aggregation with Polygon Particles. *Communications in Theoretical Physics*, **2012**, 58, 895-901	2.4	6
27	Equilibrium sampling by reweighting nonequilibrium simulation trajectories. *Physical Review E*, **2016**, 93, 033309	2.4	5
26	Dynamic heterogeneity in aqueous ionic solutions. *Physical Chemistry Chemical Physics*, **2018**, 20, 21313-21324	3.6	5
25	Surface structure of ionic liquids under an external electric field. *Molecular Simulation*, **2017**, 43, 1295-1299	2	4
24	Percolation Phase Transition from Ionic Liquids to Ionic Liquid Crystals. *Scientific Reports*, **2019**, 9, 13169	4.9	4
23	Jarzynski matrix equality: Calculating the free-energy difference by nonequilibrium simulations with an arbitrary initial distribution. *Physical Review E*, **2016**, 93, 043312	2.4	4
22	Heterogeneous Responses of Chinese Cities' Housing Prices to Monetary Policies. *Communications in Theoretical Physics*, **2011**, 56, 791-796	2.4	4
21	Solution structure of extracellular loop of human β4 subunit of BK channel and its biological implication on ChTX sensitivity. *Scientific Reports*, **2018**, 8, 4571	4.9	3
20	Poisson-Boltzmann theory with non-linear ion correlations. *Journal of Physics Condensed Matter*, **2019**, 31, 355101	1.8	3
19	Saturated sodium chloride solution under an external static electric field: A molecular dynamics study. *Chinese Physics B*, **2015**, 24, 126402	1.2	3
18	Intrinsic defect formation in peptide self-assembly. *Applied Physics Letters*, **2015**, 107, 043701	3.4	3
17	Reversible transient nucleation in ionic solutions as the precursor of ion crystallization. *Europhysics Letters*, **2014**, 107, 30005	1.6	3
16	Interaction of gas molecules with crystalline polymer separation membranes: Atomic-scale modeling and first-principles calculations. *Journal of Membrane Science*, **2011**, 384, 176-183	9.6	3
15	Liquid-Liquid Phase Separation of Viologen Bistriflimide/Benzene Mixtures: Role of the Dual Ionic and Organic Nature of Ionic Liquids. *Journal of Physical Chemistry B*, **2020**, 124, 7929-7937	3.4	3
14	Formation and dissociation of protonated cytosine–cytosine base pairs in i-motifs by ab initio quantum chemical calculations. *Chinese Physics B*, **2014**, 23, 020702	1.2	2
13	Melting Phase Transitions and Catalytic Activity of Bilayer Gold Nanoclusters. *Journal of Physical Chemistry C*, **2009**, 113, 10517-10520	3.8	2

12	Modulation of intra- and inter-sheet interactions in short peptide self-assembly by acetonitrile in aqueous solution. *Chinese Physics B*, **2016**, 25, 128704	1.2	2
11	Fast adaptive flat-histogram ensemble to enhance the sampling in large systems. *Science China: Physics, Mechanics and Astronomy*, **2015**, 58, 1	3.6	1
10	Anisotropic formation mechanism and nanomechanics for the self-assembly process of cross- peptides. *Chinese Physics B*, **2017**, 26, 128701	1.2	1
9	Competition between attraction and diffusion in nanoscale non-equilibrium aggregation. *Science China: Physics, Mechanics and Astronomy*, **2012**, 55, 2237-2243	3.6	1
8	Multiscale computational prediction of sheet peptide self-assembly morphology. *Molecular Simulation*, **2021**, 47, 428-438	2	1
7	Thermal properties of a two-dimensional intrinsically curved semiflexible biopolymer. *Chinese Physics B*, **2017**, 26, 038701	1.2	0
6	Conservation of the Stokes-Einstein relation in supercooled water. *Physical Chemistry Chemical Physics*, **2021**, 23, 24541-24544	3.6	0
5	Folding nucleus and unfolding dynamics of protein 2GB1*. *Chinese Physics B*, **2021**, 30, 028703	1.2	0
4	Moderate point: Balanced entropy and enthalpy contributions in soft matter. *Chinese Physics B*, **2017**, 26, 030506	1.2	
3	Statistical mechanics of a nonequilibrium steady-state classical particle system driven by a constant external force. *Communications in Theoretical Physics*, **2020**, 72, 115601	2.4	
2	Basics of Molecular Modeling and Molecular Simulation. *Soft and Biological Matter*, **2021**, 197-240	0.8	
1	Modulation of intra- and inter-sheet interactions in short peptide self-assembly by acetonitrile in aqueous solution. *Chinese Physics B*, **2016**, 25, 128700	1.2	