

# Yanting Wang

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Conservation of the Stokes-Einstein relation in supercooled water. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 24541-24544	3.6	0
82	Basics of Molecular Modeling and Molecular Simulation. <i>Soft and Biological Matter</i> , <b>2021</b> , 197-240	0.8	
81	Multiscale computational prediction of $\beta$ -sheet peptide self-assembly morphology. <i>Molecular Simulation</i> , <b>2021</b> , 47, 428-438	2	1
80	Folding nucleus and unfolding dynamics of protein 2GB1*. <i>Chinese Physics B</i> , <b>2021</b> , 30, 028703	1.2	0
79	A brief review of continuous models for ionic solutions: the Poisson-Boltzmann and related theories. <i>Communications in Theoretical Physics</i> , <b>2020</b> , 72, 067601	2.4	7
78	Real-time mass spectrometric characterization of the solid-electrolyte interphase of a lithium-ion battery. <i>Nature Nanotechnology</i> , <b>2020</b> , 15, 224-230	28.7	156
77	Modeling Elastically Mediated Liquid-Liquid Phase Separation. <i>Physical Review Letters</i> , <b>2020</b> , 125, 268001	7.4	10
76	Statistical mechanics of a nonequilibrium steady-state classical particle system driven by a constant external force. <i>Communications in Theoretical Physics</i> , <b>2020</b> , 72, 115601	2.4	
75	Influence of the ion size on the stability of the smectic phase of ionic liquid crystals. <i>Soft Matter</i> , <b>2020</b> , 16, 411-420	3.6	19
74	Liquid-Liquid Phase Separation of Viologen Bistriflimide/Benzene Mixtures: Role of the Dual Ionic and Organic Nature of Ionic Liquids. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 7929-7937	3.4	3
73	Percolation Phase Transition from Ionic Liquids to Ionic Liquid Crystals. <i>Scientific Reports</i> , <b>2019</b> , 9, 13169	4.9	4
72	Poisson-Boltzmann theory with non-linear ion correlations. <i>Journal of Physics Condensed Matter</i> , <b>2019</b> , 31, 355101	1.8	3
71	Phase Behaviors of Ionic Liquids Heating from Different Crystal Polymorphs toward the Same Smectic-A Ionic Liquid Crystal by Molecular Dynamics Simulation. <i>Crystals</i> , <b>2019</b> , 9, 26	2.3	6
70	Investigation of Ion-Solvent Interactions in Nonaqueous Electrolytes Using in Situ Liquid SIMS. <i>Analytical Chemistry</i> , <b>2018</b> , 90, 3341-3348	7.8	19
69	Solution structure of extracellular loop of human $\beta$ subunit of BK channel and its biological implication on ChTX sensitivity. <i>Scientific Reports</i> , <b>2018</b> , 8, 4571	4.9	3
68	Dynamic heterogeneity in aqueous ionic solutions. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 21313-21324	3.1	5
67	Atomic origins of water-vapour-promoted alloy oxidation. <i>Nature Materials</i> , <b>2018</b> , 17, 514-518	27	59

66	Aggregation behavior of dihexadecylviologen bistriflimide ionic liquid crystal in different solvents: influence of polarity and concentration. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 22730-22738	3.6	7
65	Metastable State during Melting and Solid-Solid Phase Transition of [CMim][NO] (n = 4-12) Ionic Liquids by Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 229-239	3.4	15
64	Template-based and free modeling of I-TASSER and QUARK pipelines using predicted contact maps in CASP12. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2018</b> , 86 Suppl 1, 136-151	4.2	58
63	Molecular Origin of Donor- and Acceptor-Rich Domain Formation in Bulk-Heterojunction Solar Cells with an Enhanced Charge Transport Efficiency. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 5864-5870	3.8	16
62	Surface structure of ionic liquids under an external electric field. <i>Molecular Simulation</i> , <b>2017</b> , 43, 1295-1299		4
61	NeBcon: protein contact map prediction using neural network training coupled with naïve Bayes classifiers. <i>Bioinformatics</i> , <b>2017</b> , 33, 2296-2306	7.2	52
60	Anisotropic formation mechanism and nanomechanics for the self-assembly process of cross- $\beta$ peptides. <i>Chinese Physics B</i> , <b>2017</b> , 26, 128701	1.2	1
59	Thermal properties of a two-dimensional intrinsically curved semiflexible biopolymer. <i>Chinese Physics B</i> , <b>2017</b> , 26, 038701	1.2	0
58	Moderate point: Balanced entropy and enthalpy contributions in soft matter. <i>Chinese Physics B</i> , <b>2017</b> , 26, 030506	1.2	
57	Role of the Electrostatic Interactions in the Stabilization of Ionic Liquid Crystals: Insights from Coarse-Grained MD Simulations of an Imidazolium Model. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 9152-60	3.4	22
56	Jarzynski matrix equality: Calculating the free-energy difference by nonequilibrium simulations with an arbitrary initial distribution. <i>Physical Review E</i> , <b>2016</b> , 93, 043312	2.4	4
55	Equilibrium sampling by reweighting nonequilibrium simulation trajectories. <i>Physical Review E</i> , <b>2016</b> , 93, 033309	2.4	5
54	Dual Ionic and Organic Nature of Ionic Liquids. <i>Scientific Reports</i> , <b>2016</b> , 6, 19644	4.9	76
53	Communication: Probing the existence of partially arrested states in ionic liquids. <i>Journal of Chemical Physics</i> , <b>2016</b> , 145, 191101	3.9	8
52	Effect of Ion Rigidity on Physical Properties of Ionic Liquids Studied by Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , <b>2016</b> , 120, 5678-90	3.4	12
51	Different nanostructures caused by competition of intra- and inter-sheet interactions in hierarchical self-assembly of short peptides. <i>Journal of Colloid and Interface Science</i> , <b>2016</b> , 464, 219-28	9.3	30
50	Modulation of intra- and inter-sheet interactions in short peptide self-assembly by acetonitrile in aqueous solution. <i>Chinese Physics B</i> , <b>2016</b> , 25, 128700	1.2	
49	Modulation of intra- and inter-sheet interactions in short peptide self-assembly by acetonitrile in aqueous solution. <i>Chinese Physics B</i> , <b>2016</b> , 25, 128704	1.2	2

48	Interplay between Intrinsic Conformational Propensities and Intermolecular Interactions in the Self-Assembly of Short Surfactant-like Peptides Composed of Leucine/Isoleucine. <i>Langmuir</i> , <b>2016</b> , 32, 4662-72	4	10
47	Fast adaptive flat-histogram ensemble to enhance the sampling in large systems. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2015</b> , 58, 1	3.6	1
46	Saturated sodium chloride solution under an external static electric field: A molecular dynamics study. <i>Chinese Physics B</i> , <b>2015</b> , 24, 126402	1.2	3
45	Intrinsic defect formation in peptide self-assembly. <i>Applied Physics Letters</i> , <b>2015</b> , 107, 043701	3.4	3
44	The Evidence for Fullerene Aggregation in High-Performance Small-Molecule Solar Cells by Molecular Dynamics Simulation. <i>Advanced Electronic Materials</i> , <b>2015</b> , 1, 1500217	6.4	16
43	Insights on the isotropic-to-smectic A transition in ionic liquid crystals from coarse-grained molecular dynamics simulations: the role of microphase segregation. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 3829-36	3.4	40
42	Molecular origin of the self-assembled morphological difference caused by varying the order of charged residues in short peptides. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 12501-10	3.4	21
41	Structural, dynamic, and transport properties of concentrated aqueous sodium chloride solutions under an external static electric field. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 4404-11	3.4	24
40	Effect of side-chain length on structural and dynamic properties of ionic liquids with hydroxyl cationic tails. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 3642-9	3.4	10
39	Formation and dissociation of protonated cytosine-tytosine base pairs in i-motifs by ab initio quantum chemical calculations. <i>Chinese Physics B</i> , <b>2014</b> , 23, 020702	1.2	2
38	Reversible transient nucleation in ionic solutions as the precursor of ion crystallization. <i>Europhysics Letters</i> , <b>2014</b> , 107, 30005	1.6	3
37	Ion-cage interpretation for the structural and dynamic changes of ionic liquids under an external electric field. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 5102-12	3.4	41
36	Effect of the chain length on the structure of ionic liquids: from spatial heterogeneity to ionic liquid crystals. <i>Journal of Physical Chemistry B</i> , <b>2013</b> , 117, 1104-9	3.4	117
35	Nanoparticle-based crystal growth via multistep self-assembly. <i>CrystEngComm</i> , <b>2013</b> , 15, 5114	3.3	21
34	Diffusion mechanisms in smectic ionic liquid crystals: insights from coarse-grained MD simulations. <i>Soft Matter</i> , <b>2013</b> , 9, 5716	3.6	30
33	Hydrogen-bond rich ionic liquids with hydroxyl cationic tails. <i>Chemical Physics Letters</i> , <b>2013</b> , 560, 32-36	2.5	14
32	Tuning the self-assembly of short peptides via sequence variations. <i>Langmuir</i> , <b>2013</b> , 29, 13457-64	4	103
31	Concentration and temperature dependences of polyglutamine aggregation by multiscale coarse-graining molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 10135-44	3.4	19

30	Intrinsic electric fields in ionic liquids determined by vibrational Stark effect spectroscopy and molecular dynamics simulation. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 11904-8	4.8	31
29	Competition between attraction and diffusion in nanoscale non-equilibrium aggregation. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2012</b> , 55, 2237-2243	3.6	1
28	Diffusion-Limited Aggregation with Polygon Particles. <i>Communications in Theoretical Physics</i> , <b>2012</b> , 58, 895-901	2.4	6
27	Microscopic structure and dynamics of air/water interface by computer simulations--comparison with sum-frequency generation experiments. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 5388-93	3.6	14
26	Structures and Energetics of Silver and Gold Nanoparticles. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 11374-11381	3.8	34
25	Interaction of gas molecules with crystalline polymer separation membranes: Atomic-scale modeling and first-principles calculations. <i>Journal of Membrane Science</i> , <b>2011</b> , 384, 176-183	9.6	3
24	Nanoscale Tail Aggregation in Ionic Liquids: Roles of Electrostatic and van der Waals Interactions. <i>Communications in Theoretical Physics</i> , <b>2011</b> , 56, 499-503	2.4	14
23	Heterogeneous Responses of Chinese Cities Housing Prices to Monetary Policies. <i>Communications in Theoretical Physics</i> , <b>2011</b> , 56, 791-796	2.4	4
22	On the structure of ionic liquids: comparisons between electronically polarizable and nonpolarizable models I. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 6905-21	3.4	61
21	Molecular dynamics simulations of polyglutamine aggregation using solvent-free multiscale coarse-grained models. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 8735-43	3.4	46
20	On the dynamics of ionic liquids: comparisons between electronically polarizable and nonpolarizable models II. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 6886-904	3.4	55
19	Melting Phase Transitions and Catalytic Activity of Bilayer Gold Nanoclusters. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 10517-10520	3.8	2
18	Transferable Coarse-Grained Models for Ionic Liquids. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 1091-8	6.4	66
17	Disordering and reordering of ionic liquids under an external electric field. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 11058-60	3.4	41
16	Effective force coarse-graining. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 2002-15	3.6	97
15	The multiscale coarse-graining method. II. Numerical implementation for coarse-grained molecular models. <i>Journal of Chemical Physics</i> , <b>2008</b> , 128, 244115	3.9	284
14	A Multiscale Coarse-Graining Study of the Liquid/Vacuum Interface of Room-Temperature Ionic Liquids with Alkyl Substituents of Different Lengths. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 1132-1139	3.8	100
13	Molecular dynamics simulation of the energetic room-temperature ionic liquid, 1-hydroxyethyl-4-amino-1,2,4-triazolium nitrate (HEATN). <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 3121-31	3.4	74

12	Molecular dynamics simulation of nanostructural organization in ionic liquid/water mixtures. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 4812-8	3.4	395
11	Spatial Heterogeneity in Ionic Liquids. <i>ACS Symposium Series</i> , <b>2007</b> , 272-307	0.4	23
10	Effect of Surface Structure on Shape Transformations of Gold Nanorods. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2007</b> , 4, 282-290	0.3	10
9	Understanding ionic liquids through atomistic and coarse-grained molecular dynamics simulations. <i>Accounts of Chemical Research</i> , <b>2007</b> , 40, 1193-9	24.3	285
8	Multiscale coarse-graining of ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 3564-75	3.4	158
7	Tail aggregation and domain diffusion in ionic liquids. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 18601-8	3.4	365
6	Melting of icosahedral gold nanoclusters from molecular dynamics simulations. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 214722	3.9	171
5	Unique spatial heterogeneity in ionic liquids. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 12192-6	36.4	853
4	Continuous-time Monte Carlo and spatial ordering in driven lattice gases: Application to driven vortices in periodic superconducting networks. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	7
3	Surface-driven bulk reorganization of gold nanorods. <i>Nano Letters</i> , <b>2005</b> , 5, 2174-8	11.5	65
2	Melting and equilibrium shape of icosahedral gold nanoparticles. <i>Chemical Physics Letters</i> , <b>2004</b> , 394, 257-261	2.5	69
1	Structural and Morphological Transitions in Gold Nanorods: A Computer Simulation Study. <i>Journal of Physical Chemistry B</i> , <b>2003</b> , 107, 9214-9219	3.4	57