Valeria Molinero

List of Publications by Citations

119 papers	8,022 citations	51 h-index	88 g-index
125 ext. papers	9,040 ext. citations	7.9 avg, IF	6.75 L-index

#	Paper	IF	Citations
119	Water modeled as an intermediate element between carbon and silicon. *Journal of Physical Chemistry B*, **2009**, 113, 4008-16	3.4	648
118	Structural transformation in supercooled water controls the crystallization rate of ice. *Nature*, **2011** , 479, 506-8	50.4	477
117	Nanophase-Segregation and Transport in Nafion 117 from Molecular Dynamics Simulations: Effect of Monomeric Sequence. *Journal of Physical Chemistry B*, **2004**, 108, 3149-3157	3.4	375
116	Amorphous precursors in the nucleation of clathrate hydrates. *Journal of the American Chemical Society*, **2010**, 132, 11806-11	16.4	306
115	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. *Chemical Reviews*, **2016**, 116, 7501-28	68.1	234
114	Freezing, melting and structure of ice in a hydrophilic nanopore. *Physical Chemistry Chemical Physics* , **2010**, 12, 4124-34	3.6	223
113	Thermodynamic stability and growth of guest-free clathrate hydrates: a low-density crystal phase of water. *Journal of Physical Chemistry B*, **2009**, 113, 10298-307	3.4	220
112	Heterogeneous nucleation of ice on carbon surfaces. *Journal of the American Chemical Society*, **2014** , 136, 3156-64	16.4	202
111	Homogeneous nucleation of methane hydrates: unrealistic under realistic conditions. *Journal of the American Chemical Society*, **2012**, 134, 19544-7	16.4	188
110	Is it cubic? Ice crystallization from deeply supercooled water. *Physical Chemistry Chemical Physics*, **2011**, 13, 20008-16	3.6	175
109	Stacking disorder in ice I. *Physical Chemistry Chemical Physics*, **2015**, 17, 60-76	3.6	169
108	Nucleation pathways of clathrate hydrates: effect of guest size and solubility. *Journal of Physical Chemistry B*, **2010**, 114, 13796-807	3.4	149
107	Growing correlation length in supercooled water. *Journal of Chemical Physics*, **2009**, 130, 244505	3.9	148
106	Ice crystallization in waterRs "no-manRs land". *Journal of Chemical Physics*, **2010**, 132, 244504	3.9	146
105	Role of stacking disorder in ice nucleation. *Nature*, **2017**, 551, 218-222	50.4	132
104	Can amorphous nuclei grow crystalline clathrates? The size and crystallinity of critical clathrate nuclei. *Journal of the American Chemical Society*, **2011**, 133, 6458-63	16.4	127
103	A methane-water model for coarse-grained simulations of solutions and clathrate hydrates. *Journal of Physical Chemistry B*, **2010**, 114, 7302-11	3.4	121

102	Tuning of tetrahedrality in a silicon potential yields a series of monatomic (metal-like) glass formers of very high fragility. *Physical Review Letters*, **2006**, 97, 075701	7.4	118
101	Does hydrophilicity of carbon particles improve their ice nucleation ability?. *Journal of Physical Chemistry A*, **2014**, 118, 7330-7	2.8	116
100	Crystallization, melting, and structure of water nanoparticles at atmospherically relevant temperatures. *Journal of the American Chemical Society*, **2012**, 134, 6650-9	16.4	112
99	Identification of Clathrate Hydrates, Hexagonal Ice, Cubic Ice, and Liquid Water in Simulations: the CHILL+ Algorithm. *Journal of Physical Chemistry B*, **2015**, 119, 9369-76	3.4	107
98	M3B: A Coarse Grain Force Field for Molecular Simulations of Malto-Oligosaccharides and Their Water Mixtures. *Journal of Physical Chemistry B*, **2004**, 108, 1414-1427	3.4	103
97	Ice Nucleation Efficiency of Hydroxylated Organic Surfaces Is Controlled by Their Structural Fluctuations and Mismatch to Ice. *Journal of the American Chemical Society*, **2017**, 139, 3052-3064	16.4	97
96	Liquid-Ice Coexistence below the Melting Temperature for Water Confined in Hydrophilic and Hydrophobic Nanopores. *Journal of Physical Chemistry C*, **2012**, 116, 7507-7514	3.8	91
95	Liquid to quasicrystal transition in bilayer water. *Journal of Chemical Physics*, **2010**, 133, 154516	3.9	91
94	Nature of the anomalies in the supercooled liquid state of the mW model of water. *Journal of Chemical Physics*, **2013**, 138, 174501	3.9	88
93	Coarse-Graining of TIP4P/2005, TIP4P-Ew, SPC/E, and TIP3P to Monatomic Anisotropic Water Models Using Relative Entropy Minimization. *Journal of Chemical Theory and Computation*, **2014**, 10, 4104-20	6.4	86
92	Antifreeze Glycoproteins Bind Reversibly to Ice via Hydrophobic Groups. *Journal of the American Chemical Society*, **2018**, 140, 4803-4811	16.4	81
91	Low-density liquid water is the mother of ice: on the relation between mesostructure, thermodynamics and ice crystallization in solutions. *Faraday Discussions*, **2013**, 167, 371-88	3.6	77
90	Nanophase segregation in supercooled aqueous solutions and their glasses driven by the polyamorphism of water. *Journal of Physical Chemistry A*, **2011**, 115, 5900-7	2.8	75
89	The anomalously high melting temperature of bilayer ice. *Journal of Chemical Physics*, **2010**, 132, 124511	3.9	74
88	Order parameters for the multistep crystallization of clathrate hydrates. *Journal of Chemical Physics*, **2011**, 135, 074501	3.9	74
87	Ice-Nucleating and Antifreeze Proteins Recognize Ice through a Diversity of Anchored Clathrate and Ice-like Motifs. *Journal of the American Chemical Society*, **2018**, 140, 4905-4912	16.4	73
86	Pore condensation and freezing is responsible for ice formation below water saturation for porous particles. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 8184-8189	11.5	72
85	Free energy contributions and structural characterization of stacking disordered ices. *Physical Chemistry Chemical Physics*, **2016**, 18, 9544-53	3.6	70

84	A coarse-grained model of DNA with explicit solvation by water and ions. *Journal of Physical Chemistry B*, **2011**, 115, 132-42	3.4	69
83	Melting and crystallization of ice in partially filled nanopores. *Journal of Physical Chemistry B*, **2011**, 115, 14196-204	3.4	68
82	Vapor pressure of water nanodroplets. *Journal of the American Chemical Society*, **2014**, 136, 4508-14	16.4	66
81	Microscopic mechanism of water diffusion in glucose glasses. *Physical Review Letters*, **2005**, 95, 045701	7.4	66
80	Structure of the Clathrate/Solution Interface and Mechanism of Cross-Nucleation of Clathrate Hydrates. *Journal of Physical Chemistry C*, **2012**, 116, 19828-19838	3.8	62
79	Coarse-grained ions without charges: reproducing the solvation structure of NaCl in water using short-ranged potentials. *Journal of Chemical Physics*, **2009**, 131, 034107	3.9	61
78	The Rise and Fall of Anomalies in Tetrahedral Liquids. *Journal of Statistical Physics*, **2011**, 145, 293-312	1.5	60
77	Structure of the Ice□Clathrate Interface. *Journal of Physical Chemistry C*, **2015**, 119, 4104-4117	3.8	55
76	Vapor deposition of water on graphitic surfaces: formation of amorphous ice, bilayer ice, ice I, and liquid water. *Journal of Chemical Physics*, **2014**, 141, 18C508	3.9	54
75	Ice crystallization in ultrafine water-salt aerosols: nucleation, ice-solution equilibrium, and internal structure. *Journal of the American Chemical Society*, **2014**, 136, 8081-93	16.4	53
74	Molecular Recognition of Ice by Fully Flexible Molecules. *Journal of Physical Chemistry C*, **2017**, 121, 26949-26957	3.8	53
73	Preordering of water is not needed for ice recognition by hyperactive antifreeze proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 8266-8271	11.5	52
72	The Quasi-Liquid Layer of Ice under Conditions of Methane Clathrate Formation. *Journal of Physical Chemistry C*, **2012**, 116, 12172-12180	3.8	52
71	How Size and Aggregation of Ice-Binding Proteins Control Their Ice Nucleation Efficiency. *Journal of the American Chemical Society*, **2019**, 141, 7439-7452	16.4	51
70	How short is too short for the interactions of a water potential? Exploring the parameter space of a coarse-grained water model using uncertainty quantification. *Journal of Physical Chemistry B*, **2014**, 118, 8190-202	3.4	51
69	Structure, Dynamics, and Phase Behavior of Water in TiO2 Nanopores. *Journal of Physical Chemistry C*, **2013**, 117, 3330-3342	3.8	51
68	Morphology of Liquid-Liquid Phase Separated Aerosols. *Journal of the American Chemical Society*, **2015**, 137, 10642-51	16.4	49
67	Pre-ordering of interfacial water in the pathway of heterogeneous ice nucleation does not lead to a two-step crystallization mechanism. *Journal of Chemical Physics*, **2016**, 145, 211910	3.9	49

66	Hydrogen-Bonding and Hydrophobic Groups Contribute Equally to the Binding of Hyperactive Antifreeze and Ice-Nucleating Proteins to Ice. *Journal of the American Chemical Society*, **2019**, 141, 7887-7898	16.4	47
65	Sorption Isotherms of Water in Nanopores: Relationship Between Hydropohobicity, Adsorption Pressure, and Hysteresis. *Journal of Physical Chemistry C*, **2014**, 118, 16290-16300	3.8	47
64	Thermodynamic and structural signatures of water-driven methane-methane attraction in coarse-grained mW water. *Journal of Chemical Physics*, **2013**, 139, 054511	3.9	45
63	Is there a liquid-liquid transition in confined water?. *Journal of Physical Chemistry B*, **2011**, 115, 14210-6	3.4	42
62	Water-Driven Cavity-Ligand Binding: Comparison of Thermodynamic Signatures from Coarse-Grained and Atomic-Level Simulations. *Journal of Chemical Theory and Computation*, **2012**, 8, 3696-704	6.4	41
61	Liquid-vapor oscillations of water nanoconfined between hydrophobic disks: thermodynamics and kinetics. *Journal of Physical Chemistry B*, **2010**, 114, 7320-8	3.4	41
60	Mechanisms of Nucleation and Stationary States of Electrochemically Generated Nanobubbles. *Journal of the American Chemical Society*, **2019**, 141, 10801-10811	16.4	39
59	Cross-nucleation between clathrate hydrate polymorphs: assessing the role of stability, growth rate, and structure matching. *Journal of Chemical Physics*, **2014**, 140, 084506	3.9	38
58	What Determines the Ice Polymorph in Clouds?. *Journal of the American Chemical Society*, **2016**, 138, 8958-67	16.4	38
57	Triplet correlations dominate the transition from simple to tetrahedral liquids. *Physical Review Letters*, **2014**, 112, 147801	7.4	37
56	Water filling of hydrophilic nanopores. *Journal of Chemical Physics*, **2010**, 133, 034513	3.9	37
55	Why Is It So Difficult to Identify the Onset of Ice Premelting?. *Journal of Physical Chemistry Letters*, **2018**, 9, 5179-5182	6.4	34
54	The end of ice I. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 24413-24419	11.5	32
53	Water and other tetrahedral liquids: order, anomalies and solvation. *Journal of Physics Condensed Matter*, **2012**, 24, 284116	1.8	31
52	Comparison of liquid-state anomalies in Stillinger-Weber models of water, silicon, and germanium. *Journal of Chemical Physics*, **2016**, 145, 214502	3.9	31
51	The enhancement mechanism of glycolic acid on the formation of atmospheric sulfuric acid[illegible]mmonia molecular clusters. *Journal of Chemical Physics*, **2017**, 146, 184308	3.9	30
50	How Do Surfactants Control the Agglomeration of Clathrate Hydrates?. *ACS Central Science*, **2019**, 5, 428-439	16.8	30
49	Ice nucleation by particles containing long-chain fatty acids of relevance to freezing by sea spray aerosols. *Environmental Sciences: Processes and Impacts*, **2018**, 20, 1559-1569	4.3	30

48	The Clathrate-Water Interface Is Oleophilic. *Journal of Physical Chemistry Letters*, **2018**, 9, 3224-3231	6.4	30
47	What Controls the Limit of Supercooling and Superheating of Pinned Ice Surfaces?. *Journal of Physical Chemistry Letters*, **2018**, 9, 1712-1720	6.4	29
46	Excess entropy and crystallization in Stillinger-Weber and Lennard-Jones fluids. *Journal of Chemical Physics*, **2015**, 143, 164512	3.9	28
45	Mechanisms of Nonexponential Relaxation in Supercooled Glucose Solutions: the Role of Water Facilitation. *Journal of Physical Chemistry A*, **2004**, 108, 3699-3712	2.8	28
44	Relationship between the line of density anomaly and the lines of melting, crystallization, cavitation, and liquid spinodal in coarse-grained water models. *Journal of Chemical Physics*, **2016**, 144, 234507	3.9	28
43	Ice-Liquid Oscillations in Nanoconfined Water. *ACS Nano*, **2018**, 12, 8234-8239	16.7	26
42	Promotion of Homogeneous Ice Nucleation by Soluble Molecules. *Journal of the American Chemical Society*, **2017**, 139, 17003-17006	16.4	25
41	Sink or Swim: Ions and Organics at the Ice-Air Interface. *Journal of the American Chemical Society*, **2017**, 139, 10095-10103	16.4	25
40	Self-Assembly of Mesophases from Nanoparticles. *Journal of Physical Chemistry Letters*, **2017**, 8, 5053-5058	6.4	24
39	Slow Propagation of Ice Binding Limits the Ice-Recrystallization Inhibition Efficiency of PVA and Other Flexible Polymers. *Journal of the American Chemical Society*, **2020**, 142, 4356-4366	16.4	24
38	Can Guest Occupancy in Binary Clathrate Hydrates Be Tuned through Control of the Growth Temperature?. *Journal of Physical Chemistry C*, **2014**, 118, 23022-23031	3.8	24
37	Reaction Coordinate for Ice Crystallization on a Soft Surface. *Journal of Physical Chemistry Letters*, **2017**, 8, 4201-4205	6.4	24
36	Is Water at the Graphite Interface Vapor-like or Ice-like?. *Journal of Physical Chemistry B*, **2018**, 122, 3626-3634	3.4	23
35	Strength of AlkaneFluid Attraction Determines the Interfacial Orientation of Liquid Alkanes and Their Crystallization through Heterogeneous or Homogeneous Mechanisms. *Crystals*, **2017**, 7, 86	2.3	23
34	High-Resolution Coarse-Grained Model of Hydrated Anion-Exchange Membranes that Accounts for Hydrophobic and Ionic Interactions through Short-Ranged Potentials. *Journal of Chemical Theory and Computation*, **2017**, 13, 245-264	6.4	22
33	A simple grand canonical approach to compute the vapor pressure of bulk and finite size systems. *Journal of Chemical Physics*, **2014**, 140, 064111	3.9	22
32	Role of Confinement and Surface Affinity on Filling Mechanisms and Sorption Hysteresis of Water in Nanopores. *Journal of Physical Chemistry C*, **2012**, 116, 1833-1840	3.8	22
31	Hydrogen-Bond Heterogeneity Boosts Hydrophobicity of Solid Interfaces. *Journal of the American Chemical Society*, **2015**, 137, 10618-23	16.4	21

30	Stability and metastability of bromine clathrate polymorphs. *Journal of Physical Chemistry B*, **2013**, 117, 6330-8	3.4	21
29	Two-Step to One-Step Nucleation of a Zeolite through a Metastable Gyroid Mesophase. *Journal of Physical Chemistry Letters*, **2018**, 9, 5692-5697	6.4	20
28	Effect of Polymer Architecture on the Nanophase Segregation, Ionic Conductivity, and Electro-Osmotic Drag of Anion Exchange Membranes. *Journal of Physical Chemistry C*, **2019**, 123, 8717-8726	3.8	19
27	Vapor Pressure of Aqueous Solutions of Electrolytes Reproduced with Coarse-Grained Models without Electrostatics. *Journal of Chemical Theory and Computation*, **2016**, 12, 2942-9	6.4	18
26	A Single-Component Silicon Quasicrystal. *Journal of Physical Chemistry Letters*, **2011**, 2, 384-388	6.4	18
25	Parameterization of a coarse-grained model with short-ranged interactions for modeling fuel cell membranes with controlled water uptake. *Physical Chemistry Chemical Physics*, **2017**, 19, 17698-17707	3.6	17
24	Multiscale Modeling of Structure, Transport and Reactivity in Alkaline Fuel Cell Membranes: Combined Coarse-Grained, Atomistic and Reactive Molecular Dynamics Simulations. *Polymers*, **2018** , 10,	4.5	16
23	Could Mesophases Play a Role in the Nucleation and Polymorph Selection of Zeolites?. *Journal of the American Chemical Society*, **2018**, 140, 16071-16086	16.4	15
22	Assessing the Effects of Crowding, Pore Size, and Interactions on Electro-Osmotic Drag Coefficients. *Journal of Physical Chemistry C*, **2014**, 118, 2093-2103	3.8	14
21	Why Is Gyroid More Difficult to Nucleate from Disordered Liquids than Lamellar and Hexagonal Mesophases?. *Journal of Physical Chemistry B*, **2018**, 122, 4758-4770	3.4	11
20	Can clathrates heterogeneously nucleate ice?. *Journal of Chemical Physics*, **2019**, 151, 114707	3.9	8
19	Soluble Oligomeric Nucleants: Simulations of Chain Length, Binding Strength, and Volume Fraction Effects. *Journal of Physical Chemistry Letters*, **2017**, 8, 5815-5820	6.4	7
18	Water-like Anomalies and Phase Behavior of a Pair Potential that Stabilizes Diamond. *Journal of Physical Chemistry B*, **2016**, 120, 1649-59	3.4	6
17	Systematic derivation of implicit solvent models for the study of polymer collapse. *Journal of Computational Chemistry*, **2017**, 38, 1353-1361	3.5	5
16	Electrochemically Generated Nanobubbles: Invariance of the Current with Respect to Electrode Size and Potential. *Journal of Physical Chemistry Letters*, **2020**, 11, 6573-6579	6.4	5
15	Assembly of Zeolitic Crystals From a Model of Mesogenic Patchy Nanoparticles. *Journal of Physical Chemistry C*, **2019**, 123, 971-978	3.8	5
14	Molecular Modeling of Carbohydrates with No Charges, No Hydrogen Bonds, and No Atoms. *ACS Symposium Series*, **2006**, 271-284	0.4	4
13	Width and Clustering of Ion-Conducting Channels in Fuel Cell Membranes Are Insensitive to the Length of Ion Tethers. *Journal of Physical Chemistry C*, **2021**, 125, 27693-27702	3.8	4

12	Coarse-Grained Model for the Hydrothermal Synthesis of Zeolites. *Journal of Physical Chemistry C*,	3.8	3
11	Mechanism of Facilitation of Ion Mobility in Low-Water-Content Fuel Cell Membranes. *Journal of Physical Chemistry C*, **2021**, 125, 27703-27713	3.8	3
10	Stability and Vapor Pressure of Aqueous Aggregates and Aerosols Containing a Monovalent Ion. *Journal of Physical Chemistry A*, **2017**, 121, 2597-2602	2.8	2
9	Following the nucleation pathway from disordered liquid to gyroid mesophase. *Journal of Chemical Physics*, **2019**, 150, 164902	3.9	2
8	Computationally efficient approach for the identification of ice-binding surfaces and how they bind ice. *Journal of Chemical Physics*, **2020**, 153, 174106	3.9	2
7	Preface: special topic on interfacial and confined water. *Journal of Chemical Physics*, **2014**, 141, 18C101	3.9	2
6	What determines the homogeneous freezing temperature of water? **2013**,		2
5	Is Ice Nucleation by Organic Crystals Nonclassical? An Assessment of the Monolayer Hypothesis of Ice Nucleation. *Journal of the American Chemical Society*, **2021**, 143, 4607-4624	16.4	2
4	Unstable and Metastable Mesophases Can Assist in the Nucleation of Porous Crystals. *Journal of Physical Chemistry C*, **2022**, 126, 3776-3786	3.8	2
3	Is It Possible to Follow the Structural Evolution of Water in "No-ManB Land" Using a Pulsed-Heating Procedure?. *Journal of Physical Chemistry Letters*, **2022**, 1085-1089	6.4	1
2	Polymorph Selection in Zeolite Synthesis Occurs after Nucleation.. *Journal of Physical Chemistry Letters*, **2022**, 977-981	6.4	1
1	What Is the Smallest Zeolite That Could Be Synthesized?. *Angewandte Chemie - International Edition* , **2022**, e202205095	16.4	