Franz Saija

List of Publications by Year in descending order

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112 papers	2,642 citations	159585 30 h-index	223800 46 g-index
116 all docs	116 docs citations	116 times ranked	1868 citing authors

#	Article	IF	Citations
1	Ab InitioMolecular Dynamics Study of Dissociation of Water under an Electric Field. Physical Review Letters, 2012, 108, 207801.	7.8	181
2	Miller experiments in atomistic computer simulations. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 13768-13773.	7.1	146
3	Phase diagram of the Gaussian-core model. Physical Review E, 2005, 71, 050102.	2.1	142
4	Unusual phase behavior of one-component systems with two-scale isotropic interactions. Journal of Physics Condensed Matter, 2009, 21, 504106.	1.8	91
5	Phase diagram of softly repulsive systems: The Gaussian and inverse-power-law potentials. Journal of Chemical Physics, 2005, 123, 144110.	3.0	90
6	Hexatic Phase in the Two-Dimensional Gaussian-Core Model. Physical Review Letters, 2011, 106, 235701.	7.8	77
7	Evaluation of phenomenological one-phase criteria for the melting and freezing of softly repulsive particles. Journal of Chemical Physics, 2006, 124, 244504.	3.0	58
8	One-step electric-field driven methane and formaldehyde synthesis from liquid methanol. Chemical Science, 2017, 8, 2329-2336.	7.4	56
9	Fourth virial coefficient of hard-body mixtures in two and three dimensions. Molecular Physics, 1996, 87, 991-998.	1.7	55
10	Synthesis of (<scp>d</scp>)-erythrose from glycolaldehyde aqueous solutions under electric field. Chemical Communications, 2018, 54, 3211-3214.	4.1	50
11	Raman scattering measurements on a floating water bridge. Journal Physics D: Applied Physics, 2010, 43, 175405.	2.8	48
12	Prebiotic synthesis of nucleic acids and their building blocks at the atomic level â€“ merging models and mechanisms from advanced computations and experiments. Physical Chemistry Chemical Physics, 2016, 18, 20047-20066.	2.8	48
13	The zero-temperature phase diagram of soft-repulsive particle fluids. Soft Matter, 2009, 5, 2795.	2.7	47
14	Anomalous phase behavior of a soft-repulsive potential with a strictly monotonic force. Physical Review E, 2009, 80, 031502.	2.1	46
15	Hexatic phase and water-like anomalies in a two-dimensional fluid of particles with a weakly softened core. Journal of Chemical Physics, 2012, 137, 104503.	3.0	46
16	Ab initio spectroscopy of water under electric fields. Physical Chemistry Chemical Physics, 2019, 21, 21205-21212.	2.8	44
17	Anomalous phase behavior in a model fluid with only one type of local structure. Journal of Chemical Physics, 2010, 133, 144504.	3.0	43
18	Proton Conduction in Water Ices under an Electric Field. Journal of Physical Chemistry B, 2014, 118, 4419-4424.	2.6	41

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19	Entropy-based measure of structural order in water. Physical Review E, 2006, 73, 040502.	2.1	40
20	Ionic diffusion and proton transfer in aqueous solutions of alkali metal salts. Physical Chemistry Chemical Physics, 2017, 19, 20420-20429.	2.8	40
21	High-pressure phase diagram of the exp-6 model: The case of Xe. Physical Review B, 2005, 72, .	3.2	39
22	Ab initio molecular dynamics study of an aqueous NaCl solution under an electric field. Physical Chemistry Chemical Physics, 2016, 18, 23164-23173.	2.8	36
23	Statistical entropy and density maximum anomaly in liquid water. Journal of Chemical Physics, 2003, 119, 3587-3589.	3.0	34
24	Virial expansion of a non-additive hard-sphere mixture. Journal of Chemical Physics, 1998, 108, 9098-9101.	3.0	33
25	Entropy, correlations, and ordering in two dimensions. Journal of Chemical Physics, 2000, 113, 2806-2813.	3.0	33
26	Anomalous melting behavior under extreme conditions: Hard matter turning â€œsoftâ€• Journal of Chemical Physics, 2008, 129, 241101.	3.0	33
27	Re-entrant Melting in the Gaussian-Core Model: The Entropy Imprint. ChemPhysChem, 2005, 6, 1768-1771.	2.1	32
28	Liquid methanol under a static electric field. Journal of Chemical Physics, 2015, 142, 054502.	3.0	32
29	Hexatic phase and cluster crystals of two-dimensional GEM4 spheres. Journal of Chemical Physics, 2014, 141, 184502.	3.0	31
30	Entropy and Fluidâ˜Fluid Separation in Nonadditive Hard-Sphere Mixtures. Journal of Physical Chemistry B, 1998, 102, 10368-10371.	2.6	30
31	Scaling of local density correlations in a fluid close to freezing. Journal of Chemical Physics, 2001, 115, 7586-7591.	3.0	30
32	Monte Carlo simulation and phase behavior of nonadditive hard-core mixtures in two dimensions. Journal of Chemical Physics, 2002, 117, 5780-5784.	3.0	30
33	Stability of hydrolytic arsenic species in aqueous solutions: As³⁺vs. As⁵⁺. Physical Chemistry Chemical Physics, 2018, 20, 23272-23280.	2.8	30
34	Communication: An extended model of liquid bridging. Journal of Chemical Physics, 2010, 133, 081104.	3.0	27
35	Excess Thermodynamic Properties in Mixtures of a Representative Room-Temperature Ionic Liquid and Acetonitrile. Journal of Physical Chemistry B, 2007, 111, 10202-10207.	2.6	26
36	SERS and DFT study of indigo adsorbed on silver nanostructured surface. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 205, 465-469.	3.9	24

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37	On entropy and ordering in binary hard-sphere mixtures. Journal of Physics Condensed Matter, 1994, 6, 9853-9865.	1.8	23
38	Entropy from Correlations in TIP4P Water. Journal of Chemical Theory and Computation, 2010, 6, 625-636.	5.3	22
39	Novel electrochemical route to cleaner fuel dimethyl ether. Scientific Reports, 2017, 7, 6901.	3.3	22
40	Mobilities of iodide anions in aqueous solutions for applications in natural dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2018, 20, 13038-13046.	2.8	22
41	Phase diagram of Gaussian-core nematics. Journal of Chemical Physics, 2007, 126, 194902.	3.0	21
42	Excess compressibility in binary liquid mixtures. Journal of Chemical Physics, 2007, 126, 224508.	3.0	21
43	Effect of Electric Field Orientation on the Mechanical and Electrical Properties of Water Ices: An Ab-initio Study. Journal of Physical Chemistry B, 2014, 118, 12717-12724.	2.6	21
44	Entropy and Correlations in a Fluid of Hard Spherocylinders:Â The Onset of Nematic and Smectic Order. Journal of Physical Chemistry B, 2002, 106, 12297-12306.	2.6	20
45	Structure of bulk water from Raman measurements of supercooled pure liquid and LiCl solutions. Physical Review B, 2012, 86, .	3.2	20
46	Statistical entropy of a binary hard-sphere mixture: the low-density limit. Journal of Physics Condensed Matter, 1996, 8, 8137-8144.	1.8	19
47	Ab Initio Molecular Dynamics Studies of the Electric-Field-Induced Catalytic Effects on Liquids. Topics in Catalysis, 2022, 65, 40-58.	2.8	19
48	Stability of 2â€²,3â€² and 3â€²,5â€² cyclic nucleotides in formamide and in water: a theoretical insight into the factors controlling the accumulation of nucleic acid building blocks in a prebiotic pool. Physical Chemistry Chemical Physics, 2017, 19, 1817-1825.	2.8	18
49	Electric-Field-Induced Effects on the Dipole Moment and Vibrational Modes of the Centrosymmetric Indigo Molecule. Journal of Physical Chemistry A, 2020, 124, 10856-10869.	2.5	18
50	Anomalous melting and solid polymorphism of a modified inverse-power potential. Molecular Physics, 2011, 109, 2837-2844.	1.7	17
51	Dust Motions in Magnetized Turbulence: Source of Chemical Complexity. Astrophysical Journal Letters, 2018, 866, L23.	8.3	17
52	Simulation and reference interaction site model theory of methanol and carbon tetrachloride mixtures. Journal of Chemical Physics, 2010, 132, 084506.	3.0	16
53	A Criterion for Anomalous Melting in Systems with Isotropic Interactions. Journal of Physical Chemistry B, 2011, 115, 14091-14098.	2.6	16
54	Entropy and Fluidâ"Fluid Separation in Nonadditive Hard-Sphere Mixtures:Â The Asymmetric Case. Journal of Physical Chemistry B, 2002, 106, 2035-2040.	2.6	15

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55	A mean field analysis of the static dielectric behavior of linear lower alcohols. Journal of Chemical Physics, 2004, 121, 3191-3196.	3.0	15
56	Ab Initio Molecular Dynamics Study of Methanol-Water Mixtures under External Electric Fields. Molecules, 2020, 25, 3371.	3.8	15
57	Short length-scale dynamics of polyisobutylene by molecular dynamics simulations. Physica B: Condensed Matter, 2001, 301, 119-125.	2.7	14
58	Evidence of Heterogeneous Aggregation in Methanol/CCl4Mixtures:Â A Brillouin Scattering Investigation. Journal of Physical Chemistry B, 2004, 108, 12972-12977.	2.6	14
59	Reference interaction site model and molecular dynamics study of structure and thermodynamics of methanol. Journal of Chemical Physics, 2007, 127, 224501.	3.0	14
60	Removal of As(III) from Biological Fluids: Mono- versus Dithiolic Ligands. Chemical Research in Toxicology, 2020, 33, 967-974.	3.3	14
61	Virial Coefficients and Demixing of Athermal Nonadditive Mixtures. Journal of Physical Chemistry B, 2007, 111, 4503-4509.	2.6	13
62	Smectic Ordering of Parallel Hard Spherocylinders:Â An Entropy-Based Monte Carlo Study. Journal of Physical Chemistry B, 2003, 107, 9514-9519.	2.6	12
63	Thermodynamic Stability of Fluidâ^'Fluid Phase Separation in Binary Athermal Mixtures:Â The Role of Nonadditivity. Journal of Physical Chemistry B, 2006, 110, 4359-4364.	2.6	12
64	Supercooled water escaping from metastability. Scientific Reports, 2014, 4, 7230.	3.3	12
65	The effective colloid interaction in the Asakuraâ€“Oosawa model. Assessment of non-pairwise terms from the virial expansion. Journal of Chemical Physics, 2015, 142, 224903.	3.0	12
66	Enhanced conductivity of water at the electrified airâ€“water interface: a DFT-MD characterization. Physical Chemistry Chemical Physics, 2020, 22, 10438-10446.	2.8	12
67	Angular correlations and statistical entropy of hard spherocylinders: the isotropicâ€“nematic transition. Chemical Physics Letters, 1998, 283, 86-90.	2.6	11
68	A ground level interpretation of the dielectric behavior of diluted alcohol-in-carbon tetrachloride mixtures. Journal of Chemical Physics, 2003, 119, 10771-10776.	3.0	11
69	Fifth virial coefficient of a two-component mixture of hard discs. Molecular Physics, 1997, 90, 679-682.	1.7	10
70	The role of association in the dielectric behaviour of methanol/carbon tetrachloride mixtures. Chemical Physics Letters, 2003, 382, 523-527.	2.6	10
71	Application of phenomenological freezing and melting indicators to the exp-6 and Gaussian core potentials. Molecular Physics, 2011, 109, 2417-2421.	1.7	10
72	Interaction between As(III) and Simple Thioacids in Water: An Experimental and ab Initio Molecular Dynamics Investigation. Journal of Physical Chemistry B, 2019, 123, 6090-6098.	2.6	10

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73	Arsenicâ€“nucleotides interactions: an experimental and computational investigation. Dalton Transactions, 2020, 49, 6302-6311.	3.3	10
74	Some Evidence of Scaling Behavior in the Relaxation Dynamics of Aqueous Polymer Solutions. Journal of Physical Chemistry B, 2010, 114, 1614-1620.	2.6	9
75	RESEARCH NOTE Fifth virial coefficient of hard sphere mixtures. Molecular Physics, 1998, 94, 877-879.	1.7	8
76	Collective acoustic modes in liquids: A comparison between the generalized-hydrodynamics and memory-function approaches. Physical Review E, 2011, 84, 051202.	2.1	8
77	Density and structural anomalies in soft-repulsive dimeric fluids. Physical Chemistry Chemical Physics, 2016, 18, 9484-9489.	2.8	8
78	Ionic diffusion and proton transfer of MgCl₂ and CaCl₂ aqueous solutions: an ab initio study under electric field. Molecular Simulation, 2019, 45, 373-380.	2.0	8
79	RESEARCH NOTE Fifth virial coefficient of a hard-sphere mixture. Molecular Physics, 1996, 89, 1181-1186.	1.7	7
80	Re-entrant melting of the exp-6 fluid: the role of the repulsion softness. Physics and Chemistry of Liquids, 2010, 48, 477-487.	1.2	7
81	The fourth virial coefficient of a nonadditive hard-disc mixture. Physical Chemistry Chemical Physics, 2011, 13, 11885.	2.8	7
82	Theoretical and computer simulation study of phase coexistence of nonadditive hard-disk mixtures. Journal of Chemical Physics, 2014, 141, 214508.	3.0	7
83	Virial coefficients and demixing in the Asakuraâ€“Oosawa model. Journal of Chemical Physics, 2015, 142, 014902.	3.0	7
84	Monte Carlo simulation and integral equation study of Hertzian spheres in the low-temperature regime. Journal of Chemical Physics, 2019, 151, 134901.	3.0	7
85	Understanding the behaviour of carnosine in aqueous solution: an experimental and quantum-based computational investigation on acidâ€“base properties and complexation mechanisms with Ca²⁺and Mg²⁺. New Journal of Chemistry, 2021, 45, 20352-20364.	2.8	7
86	ERRATUM Fourth virial coefficient of hard-body mixtures in two and three dimensions. Molecular Physics, 1997, 92, 1089-1089.	1.7	6
87	Minimum-density anomaly and spatial ordering of softly repulsive particles in a narrow channel. Soft Matter, 2013, 9, 9876.	2.7	6
88	Reply to Bada and Cleaves: Ab initio free-energy landscape of Miller-like prebiotic reactions. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E343-4.	7.1	6
89	Atomistic simulations of the free-energy landscapes of interstellar chemical reactions: the case of methyl isocyanate. Monthly Notices of the Royal Astronomical Society, 2021, 504, 1565-1570.	4.4	6
90	Hydrolysis of Al3+ in Aqueous Solutions: Experiments and Ab Initio Simulations. Liquids, 2022, 2, 26-38.	2.5	6

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91	Excess thermodynamic properties in liquid binary mixtures. Journal of Raman Spectroscopy, 2008, 39, 220-226.	2.5	5
92	An entropy-based approach to the freezing of the generalized exponential model. Journal of Chemical Physics, 2008, 128, 136101.	3.0	5
93	Fourth virial coefficients of asymmetric nonadditive hard-disk mixtures. Journal of Chemical Physics, 2012, 136, 184505.	3.0	5
94	Residual Multiparticle Entropy for a Fractal Fluid of Hard Spheres. Entropy, 2018, 20, 544.	2.2	5
95	Virial coefficients, equation of state, and demixing of binary asymmetric nonadditive hard-disk mixtures. Journal of Chemical Physics, 2017, 147, 164502.	3.0	4
96	High-frequency propagating density fluctuations in deeply supercooled water: Evidence of a single viscous relaxation. Physical Review E, 2013, 87, 022303.	2.1	3
97	Volume crossover in deeply supercooled water adiabatically freezing under isobaric conditions. Journal of Chemical Physics, 2013, 138, 184504.	3.0	3
98	Free Energy Calculations of Electric Field-Induced Chemistry. Challenges and Advances in Computational Chemistry and Physics, 2019, , 95-126.	0.6	3
99	Binding of Arsenic by Common Functional Groups: An Experimental and Quantum-Mechanical Study. Applied Sciences (Switzerland), 2022, 12, 3210.	2.5	3
100	On the Origin of Excess Thermodynamic Quantities in Liquid Mixtures. Oil and Gas Science and Technology, 2008, 63, 353-361.	1.4	2
101	Integral equation study of soft-repulsive dimeric fluids. Journal of Physics Condensed Matter, 2017, 29, 115101.	1.8	2
102	Evidence of Structural Inhomogeneities in Hard-Soft Dimeric Particles without Attractive Interactions. Materials, 2020, 13, 84.	2.9	2
103	Ab initio molecular dynamics simulations and experimental speciation study of levofloxacin under different pH conditions. Physical Chemistry Chemical Physics, 2021, 23, 24403-24412.	2.8	2
104	Molecular dissociation and proton transfer in aqueous methane solution under an electric field. Physical Chemistry Chemical Physics, 2021, 23, 25649-25657.	2.8	2
105	Formamide-Based Post-impact Thermal Prebiotic Synthesis in Simulated Craters: Intermediates, Products and Mechanism. Frontiers in Astronomy and Space Sciences, 2022, 9, .	2.8	2
106	Brillouin scattering investigation of ME6N liquid crystal in CCl4. Journal of Molecular Liquids, 2010, 153, 67-71.	4.9	1
107	Ariel â€“ a window to the origin of life on early earth?. Experimental Astronomy, 2020, , 1.	3.7	1
108	Electric Field and Temperature Effects on the Ab Initio Spectroscopy of Liquid Methanol. Applied Sciences (Switzerland), 2021, 11, 5457.	2.5	1

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109	Interstellar chemical reactions toward the synthesis of the life's building blocks. Physics of Life Reviews, 2021, 38, 140-142.	2.8	1
110	Relaxation processes in polymer-salt complexes. Colloid and Polymer Science, 2003, 281, 882-886.	2.1	0
111	Relaxation dynamics and evidence of scaling behaviours in aqueous polymer solutions. Journal of Molecular Liquids, 2011, 159, 105-111.	4.9	0
112	Theory and equation of state of two-component nonadditive hard-disks: an application in the colloidal regime. Physics and Chemistry of Liquids, 0, , 1-22.	1.2	0