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 Initio Molecular Dynamics Studies of the Electric-Field-Induced Catalytic Effects on Liquids. Topics in Catalysis, 2022, 65, 40-58.	2.8	19
2	Hydrolysis of Al3+ in Aqueous Solutions: Experiments and Ab Initio Simulations. Liquids, 2022, 2, 26-38.	2.5	6
3	Binding of Arsenic by Common Functional Groups: An Experimental and Quantum-Mechanical Study. Applied Sciences (Switzerland), 2022, 12, 3210.	2.5	3
4	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
5	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
6	Electric Field and Temperature Effects on the Ab Initio Spectroscopy of Liquid Methanol. Applied Sciences (Switzerland), 2021, 11, 5457.	2.5	1
7	Interstellar chemical reactions toward the synthesis of the life's building blocks. Physics of Life Reviews, 2021, 38, 140-142.	2.8	1
8	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
9	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
10	Molecular dissociation and proton transfer in aqueous methane solution under an electric field. Physical Chemistry Chemical Physics, 2021, 23, 25649-25657.	2.8	2
11	Evidence of Structural Inhomogeneities in Hard-Soft Dimeric Particles without Attractive Interactions. Materials, 2020, 13, 84.	2.9	2
12	Ariel â€“ a window to the origin of life on early earth?. Experimental Astronomy, 2020, , 1.	3.7	1
13	Ab Initio Molecular Dynamics Study of Methanol-Water Mixtures under External Electric Fields. Molecules, 2020, 25, 3371.	3.8	15
14	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
15	Removal of As(III) from Biological Fluids: Mono- versus Dithiolic Ligands. Chemical Research in Toxicology, 2020, 33, 967-974.	3.3	14
16	Arsenicâ€“nucleotides interactions: an experimental and computational investigation. Dalton Transactions, 2020, 49, 6302-6311.	3.3	10
17	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
18	Ab initio spectroscopy of water under electric fields. Physical Chemistry Chemical Physics, 2019, 21, 21205-21212.	2.8	44

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19	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
20	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
21	Free Energy Calculations of Electric Field-Induced Chemistry. Challenges and Advances in Computational Chemistry and Physics, 2019, , 95-126.	0.6	3
22	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
23	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
24	Synthesis of (<scp>d</scp>)-erythrose from glycolaldehyde aqueous solutions under electric field. Chemical Communications, 2018, 54, 3211-3214.	4.1	50
25	Residual Multiparticle Entropy for a Fractal Fluid of Hard Spheres. Entropy, 2018, 20, 544.	2.2	5
26	Dust Motions in Magnetized Turbulence: Source of Chemical Complexity. Astrophysical Journal Letters, 2018, 866, L23.	8.3	17
27	Stability of hydrolytic arsenic species in aqueous solutions: As³⁺vs. As⁵⁺. Physical Chemistry Chemical Physics, 2018, 20, 23272-23280.	2.8	30
28	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
29	Integral equation study of soft-repulsive dimeric fluids. Journal of Physics Condensed Matter, 2017, 29, 115101.	1.8	2
30	One-step electric-field driven methane and formaldehyde synthesis from liquid methanol. Chemical Science, 2017, 8, 2329-2336.	7.4	56
31	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
32	Virial coefficients, equation of state, and demixing of binary asymmetric nonadditive hard-disk mixtures. Journal of Chemical Physics, 2017, 147, 164502.	3.0	4
33	Ionic diffusion and proton transfer in aqueous solutions of alkali metal salts. Physical Chemistry Chemical Physics, 2017, 19, 20420-20429.	2.8	40
34	Novel electrochemical route to cleaner fuel dimethyl ether. Scientific Reports, 2017, 7, 6901.	3.3	22
35	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
36	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

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37	Density and structural anomalies in soft-repulsive dimeric fluids. Physical Chemistry Chemical Physics, 2016, 18, 9484-9489.	2.8	8
38	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
39	Liquid methanol under a static electric field. Journal of Chemical Physics, 2015, 142, 054502.	3.0	32
40	Virial coefficients and demixing in the Asakuraâ€“Oosawa model. Journal of Chemical Physics, 2015, 142, 014902.	3.0	7
41	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
42	Hexatic phase and cluster crystals of two-dimensional GEM4 spheres. Journal of Chemical Physics, 2014, 141, 184502.	3.0	31
43	Theoretical and computer simulation study of phase coexistence of nonadditive hard-disk mixtures. Journal of Chemical Physics, 2014, 141, 214508.	3.0	7
44	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
45	Proton Conduction in Water Ices under an Electric Field. Journal of Physical Chemistry B, 2014, 118, 4419-4424.	2.6	41
46	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
47	Supercooled water escaping from metastability. Scientific Reports, 2014, 4, 7230.	3.3	12
48	Minimum-density anomaly and spatial ordering of softly repulsive particles in a narrow channel. Soft Matter, 2013, 9, 9876.	2.7	6
49	High-frequency propagating density fluctuations in deeply supercooled water: Evidence of a single viscous relaxation. Physical Review E, 2013, 87, 022303.	2.1	3
50	Volume crossover in deeply supercooled water adiabatically freezing under isobaric conditions. Journal of Chemical Physics, 2013, 138, 184504.	3.0	3
51	Fourth virial coefficients of asymmetric nonadditive hard-disk mixtures. Journal of Chemical Physics, 2012, 136, 184505.	3.0	5
52	Structure of bulk water from Raman measurements of supercooled pure liquid and LiCl solutions. Physical Review B, 2012, 86, .	3.2	20
53	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
54	Ab InitioMolecular Dynamics Study of Dissociation of Water under an Electric Field. Physical Review Letters, 2012, 108, 207801.	7.8	181

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55	The fourth virial coefficient of a nonadditive hard-disc mixture. Physical Chemistry Chemical Physics, 2011, 13, 11885.	2.8	7
56	Application of phenomenological freezing and melting indicators to the exp-6 and Gaussian core potentials. Molecular Physics, 2011, 109, 2417-2421.	1.7	10
57	A Criterion for Anomalous Melting in Systems with Isotropic Interactions. Journal of Physical Chemistry B, 2011, 115, 14091-14098.	2.6	16
58	Hexatic Phase in the Two-Dimensional Gaussian-Core Model. Physical Review Letters, 2011, 106, 235701.	7.8	77
59	Anomalous melting and solid polymorphism of a modified inverse-power potential. Molecular Physics, 2011, 109, 2837-2844.	1.7	17
60	Relaxation dynamics and evidence of scaling behaviours in aqueous polymer solutions. Journal of Molecular Liquids, 2011, 159, 105-111.	4.9	0
61	Collective acoustic modes in liquids: A comparison between the generalized-hydrodynamics and memory-function approaches. Physical Review E, 2011, 84, 051202.	2.1	8
62	Anomalous phase behavior in a model fluid with only one type of local structure. Journal of Chemical Physics, 2010, 133, 144504.	3.0	43
63	Raman scattering measurements on a floating water bridge. Journal Physics D: Applied Physics, 2010, 43, 175405.	2.8	48
64	Brillouin scattering investigation of ME6N liquid crystal in CCl4. Journal of Molecular Liquids, 2010, 153, 67-71.	4.9	1
65	Communication: An extended model of liquid bridging. Journal of Chemical Physics, 2010, 133, 081104.	3.0	27
66	Simulation and reference interaction site model theory of methanol and carbon tetrachloride mixtures. Journal of Chemical Physics, 2010, 132, 084506.	3.0	16
67	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
68	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
69	Entropy from Correlations in TIP4P Water. Journal of Chemical Theory and Computation, 2010, 6, 625-636.	5.3	22
70	Unusual phase behavior of one-component systems with two-scale isotropic interactions. Journal of Physics Condensed Matter, 2009, 21, 504106.	1.8	91
71	The zero-temperature phase diagram of soft-repulsive particle fluids. Soft Matter, 2009, 5, 2795.	2.7	47
72	Anomalous phase behavior of a soft-repulsive potential with a strictly monotonic force. Physical Review E, 2009, 80, 031502.	2.1	46

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73	Excess thermodynamic properties in liquid binary mixtures. Journal of Raman Spectroscopy, 2008, 39, 220-226.	2.5	5
74	Anomalous melting behavior under extreme conditions: Hard matter turning â€œsoftâ€• Journal of Chemical Physics, 2008, 129, 241101.	3.0	33
75	An entropy-based approach to the freezing of the generalized exponential model. Journal of Chemical Physics, 2008, 128, 136101.	3.0	5
76	On the Origin of Excess Thermodynamic Quantities in Liquid Mixtures. Oil and Gas Science and Technology, 2008, 63, 353-361.	1.4	2
77	Phase diagram of Gaussian-core nematics. Journal of Chemical Physics, 2007, 126, 194902.	3.0	21
78	Virial Coefficients and Demixing of Athermal Nonadditive Mixtures. Journal of Physical Chemistry B, 2007, 111, 4503-4509.	2.6	13
79	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
80	Reference interaction site model and molecular dynamics study of structure and thermodynamics of methanol. Journal of Chemical Physics, 2007, 127, 224501.	3.0	14
81	Excess compressibility in binary liquid mixtures. Journal of Chemical Physics, 2007, 126, 224508.	3.0	21
82	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
83	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
84	Entropy-based measure of structural order in water. Physical Review E, 2006, 73, 040502.	2.1	40
85	Re-entrant Melting in the Gaussian-Core Model: The Entropy Imprint. ChemPhysChem, 2005, 6, 1768-1771.	2.1	32
86	High-pressure phase diagram of the exp-6 model: The case of Xe. Physical Review B, 2005, 72, .	3.2	39
87	Phase diagram of the Gaussian-core model. Physical Review E, 2005, 71, 050102.	2.1	142
88	Phase diagram of softly repulsive systems: The Gaussian and inverse-power-law potentials. Journal of Chemical Physics, 2005, 123, 144110.	3.0	90
89	A mean field analysis of the static dielectric behavior of linear lower alcohols. Journal of Chemical Physics, 2004, 121, 3191-3196.	3.0	15
90	Evidence of Heterogeneous Aggregation in Methanol/CCl4Mixtures:Â A Brillouin Scattering Investigation. Journal of Physical Chemistry B, 2004, 108, 12972-12977.	2.6	14

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91	Relaxation processes in polymer-salt complexes. Colloid and Polymer Science, 2003, 281, 882-886.	2.1	0
92	The role of association in the dielectric behaviour of methanol/carbon tetrachloride mixtures. Chemical Physics Letters, 2003, 382, 523-527.	2.6	10
93	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
94	Statistical entropy and density maximum anomaly in liquid water. Journal of Chemical Physics, 2003, 119, 3587-3589.	3.0	34
95	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
96	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
97	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
98	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
99	Short length-scale dynamics of polyisobutylene by molecular dynamics simulations. Physica B: Condensed Matter, 2001, 301, 119-125.	2.7	14
100	Scaling of local density correlations in a fluid close to freezing. Journal of Chemical Physics, 2001, 115, 7586-7591.	3.0	30
101	Entropy, correlations, and ordering in two dimensions. Journal of Chemical Physics, 2000, 113, 2806-2813.	3.0	33
102	Angular correlations and statistical entropy of hard spherocylinders: the isotropicâ€“nematic transition. Chemical Physics Letters, 1998, 283, 86-90.	2.6	11
103	RESEARCH NOTE Fifth virial coefficient of hard sphere mixtures. Molecular Physics, 1998, 94, 877-879.	1.7	8
104	Entropy and Fluidâ^'Fluid Separation in Nonadditive Hard-Sphere Mixtures. Journal of Physical Chemistry B, 1998, 102, 10368-10371.	2.6	30
105	Virial expansion of a non-additive hard-sphere mixture. Journal of Chemical Physics, 1998, 108, 9098-9101.	3.0	33
106	Fifth virial coefficient of a two-component mixture of hard discs. Molecular Physics, 1997, 90, 679-682.	1.7	10
107	ERRATUM Fourth virial coefficient of hard-body mixtures in two and three dimensions. Molecular Physics, 1997, 92, 1089-1089.	1.7	6
108	Fourth virial coefficient of hard-body mixtures in two and three dimensions. Molecular Physics, 1996, 87, 991-998.	1.7	55

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109	RESEARCH NOTE Fifth virial coefficient of a hard-sphere mixture. Molecular Physics, 1996, 89, 1181-1186.	1.7	7
110	Statistical entropy of a binary hard-sphere mixture: the low-density limit. Journal of Physics Condensed Matter, 1996, 8, 8137-8144.	1.8	19
111	On entropy and ordering in binary hard-sphere mixtures. Journal of Physics Condensed Matter, 1994, 6, 9853-9865.	1.8	23
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