Jim Pfaendtner

List of Publications by Citations

119 papers	3,264 citations	31 h-index	52 g-index
139 ext. papers	3,866 ext. citations	5.4 avg, IF	5.92 L-index

#	Paper	IF	Citations
119	The general AMBER force field (GAFF) can accurately predict thermodynamic and transport properties of many ionic liquids. *Journal of Physical Chemistry B*, **2015**, 119, 5882-95	3.4	185
118	The 1-D hindered rotor approximation. *Theoretical Chemistry Accounts*, **2007**, 118, 881-898	1.9	149
117	Ice-nucleating bacteria control the order and dynamics of interfacial water. *Science Advances*, **2016**, 2, e1501630	14.3	128
116	A systematic methodology for defining coarse-grained sites in large biomolecules. *Biophysical Journal*, **2008**, 95, 5073-83	2.9	124
115	Efficient Sampling of High-Dimensional Free-Energy Landscapes with Parallel Bias Metadynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 5062-7	6.4	112
114	Systematic multiscale parameterization of heterogeneous elastic network models of proteins. *Biophysical Journal*, **2008**, 95, 4183-92	2.9	112
113	Nucleotide-dependent conformational states of actin. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 12723-8	11.5	97
112	Efficient Simulation of Explicitly Solvated Proteins in the Well-Tempered Ensemble. *Journal of Chemical Theory and Computation*, **2012**, 8, 2189-92	6.4	94
111	Exhaustively sampling peptide adsorption with metadynamics. *Langmuir*, **2013**, 29, 7999-8009	4	93
110	Lexicography of kinetic modeling of complex reaction networks. *AICHE Journal*, **2005**, 51, 2112-2121	3.6	82
109	Trimethylamine -oxide-derived zwitterionic polymers: A new class of ultralow fouling bioinspired materials. *Science Advances*, **2019**, 5, eaaw9562	14.3	81
108	Actin filament remodeling by actin depolymerization factor/cofilin. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 7299-304	11.5	81
107	Structure, dynamics, and activity of xylanase solvated in binary mixtures of ionic liquid and water. *ACS Chemical Biology*, **2013**, 8, 1179-86	4.9	77
106	Structure and dynamics of the actin filament. *Journal of Molecular Biology*, **2010**, 396, 252-63	6.5	74
105	Defining coarse-grained representations of large biomolecules and biomolecular complexes from elastic network models. *Biophysical Journal*, **2009**, 97, 2327-37	2.9	70
104	Ab initio study of acrylate polymerization reactions: methyl methacrylate and methyl acrylate propagation. *Journal of Physical Chemistry A*, **2008**, 112, 6772-82	2.8	68
103	Millisecond Pulsed Films Unify the Mechanisms of Cellulose Fragmentation. *Chemistry of Materials*, **2016**, 28, 3108-3114	9.6	63

102	Quantum chemical investigation of low-temperature intramolecular hydrogen transfer reactions of hydrocarbons. *Journal of Physical Chemistry A*, **2006**, 110, 10863-71	2.8	54
101	Comparison of three ionic liquid-tolerant cellulases by molecular dynamics. *Biophysical Journal*, **2015**, 108, 880-892	2.9	53
100	Diatom mimics: directing the formation of biosilica nanoparticles by controlled folding of lysine-leucine peptides. *Journal of the American Chemical Society*, **2014**, 136, 15134-7	16.4	50
99	Structural and dynamic features of Candida rugosa lipase 1 in water, octane, toluene, and ionic liquids BMIM-PF6 and BMIM-NO3. *Journal of Physical Chemistry B*, **2013**, 117, 2662-70	3.4	49
98	Mechanistic Modeling of Lubricant Degradation. 2. The Autoxidation of Decane and Octane. *Industrial & Engineering Chemistry Research*, **2008**, 47, 2897-2904	3.9	46
97	Mechanistic Modeling of Lubricant Degradation. 1. Structure□Reactivity Relationships for Free-Radical Oxidation. *Industrial & Engineering Chemistry Research*, **2008**, 47, 2886-2896	3.9	46
96	Data science: Accelerating innovation and discovery in chemical engineering. *AICHE Journal*, **2016**, 62, 1402-1416	3.6	44
95	Molecular dynamics investigation of the ionic liquid/enzyme interface: application to engineering enzyme surface charge. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 670-80	4.2	43
94	Application of machine learning to pyrolysis reaction networks: Reducing model solution time to enable process optimization. *Computers and Chemical Engineering*, **2017**, 104, 56-63	4	39
93	New Approach for Investigating Reaction Dynamics and Rates with Ab Initio Calculations. *Journal of Physical Chemistry A*, **2016**, 120, 299-305	2.8	37
92	Enhanced sampling of chemical and biochemical reactions with metadynamics. *Molecular Simulation* , **2015**, 41, 55-72	2	34
91	Fast Pyrolysis of Wood for Biofuels: Spatiotemporally Resolved Diffuse Reflectance In situ Spectroscopy of Particles. *ChemSusChem*, **2014**, 7, 765	8.3	34
90	Detailed Kinetic Modeling of Lignin Pyrolysis for Process Optimization. *Industrial & Engineering Chemistry Research*, **2016**, 55, 9147-9153	3.9	31
89	Strong Electrostatic Interactions Lead to Entropically Favorable Binding of Peptides to Charged Surfaces. *Langmuir*, **2016**, 32, 5690-701	4	31
88	Car□Parrinello Molecular Dynamics + Metadynamics Study of High-Temperature Methanol Oxidation Reactions Using Generic Collective Variables. *Journal of Physical Chemistry C*, **2014**, 118, 10764-10770	4.8	30
87	Free energy of solvated salt bridges: a simulation and experimental study. *Journal of Physical Chemistry B*, **2013**, 117, 7254-9	3.4	30
86	The Structure of the Diatom Silaffin Peptide R5 within Freestanding Two-Dimensional Biosilica Sheets. *Angewandte Chemie - International Edition*, **2017**, 56, 8277-8280	16.4	29
85	Kinetics and mechanism of ionic-liquid induced protein unfolding: application to the model protein HP35. *Molecular Systems Design and Engineering*, **2016**, 1, 382-390	4.6	29

84	Folding and insertion thermodynamics of the transmembrane WALP peptide. *Journal of Chemical Physics*, **2015**, 143, 243127	3.9	29
83	Biomimetic Growth of Ultrathin Silica Sheets Using Artificial Amphiphilic Peptides. *Advanced Materials Interfaces*, **2015**, 2, 1500282	4.6	29
82	Structural effects of methionine oxidation on isolated subdomains of human fibrin D and E regions. *PLoS ONE*, **2014**, 9, e86981	3.7	28
81	Key structural features of the actin filament Arp2/3 complex branch junction revealed by molecular simulation. *Journal of Molecular Biology*, **2012**, 416, 148-61	6.5	25
80	Trp-Cage Folding on Organic Surfaces. *Journal of Physical Chemistry B*, **2015**, 119, 10417-25	3.4	24
79	Solvatochromism and conformational changes in fully dissolved poly(3-alkylthiophene)s. *Langmuir*, **2015**, 31, 458-68	4	24
78	Investigating the Role of Phosphorylation in the Binding of Silaffin Peptide R5 to Silica with Molecular Dynamics Simulations. *Langmuir*, **2018**, 34, 1199-1207	4	23
77	Ultrafast Reorientational Dynamics of Leucine at the Air-Water Interface. *Journal of the American Chemical Society*, **2016**, 138, 5226-9	16.4	23
76	Statistical models are able to predict ionic liquid viscosity across a wide range of chemical functionalities and experimental conditions. *Molecular Systems Design and Engineering*, **2018**, 3, 253-263	4.6	22
75	Essential slow degrees of freedom in protein-surface simulations: A metadynamics investigation. *Biochemical and Biophysical Research Communications*, **2018**, 498, 274-281	3.4	22
74	Deconstruction of high-density polyethylene into liquid hydrocarbon fuels and lubricants by hydrogenolysis over Ru catalyst. *Chem Catalysis*, **2021**, 1, 437-455		22
73	Destabilization of Human Serum Albumin by Ionic Liquids Studied Using Enhanced Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 12079-12087	3.4	21
72	Ionic Liquids Can Selectively Change the Conformational Free-Energy Landscape of Sugar Rings. *Journal of Chemical Theory and Computation*, **2014**, 10, 507-10	6.4	20
71	Elucidating sequence and solvent specific design targets to protect and stabilize enzymes for biocatalysis in ionic liquids. *Physical Chemistry Chemical Physics*, **2017**, 19, 17426-17433	3.6	20
70	Effect of Hydrophobic and Hydrophilic Surfaces on the Stability of Double-Stranded DNA. *Biomacromolecules*, **2015**, 16, 1862-9	6.9	20
69	Characterizing the catalyzed hydrolysis of β1,4 glycosidic bonds using density functional theory. *Journal of Physical Chemistry A*, **2013**, 117, 14200-8	2.8	19
68	Mechanism of Competitive Inhibition and Destabilization of Acidothermus cellulolyticus Endoglucanase 1 by Ionic Liquids. *Journal of Physical Chemistry B*, **2017**, 121, 10793-10803	3.4	19
67	Chain Flexibility in Self-Assembled Monolayers Affects Protein Adsorption and Surface Hydration: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2016**, 120, 10423-10432	3.4	19

66	Molecular Driving Forces in Peptide Adsorption to Metal Oxide Surfaces. *Langmuir*, **2019**, 35, 5911-5920	4	18
65	Molecular dynamics simulation and coarse-grained analysis of the Arp2/3 complex. *Biophysical Journal*, **2008**, 95, 5324-33	2.9	18
64	Assessing Generic Collective Variables for Determining Reaction Rates in Metadynamics Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 968-973	6.4	16
63	Generic Biphasic Catalytic Approach for Producing Renewable Diesel from Fatty Acids and Vegetable Oils. *ACS Catalysis*, **2019**, 9, 3753-3763	13.1	16
62	Lifting the Curse of Dimensionality on Enhanced Sampling of Reaction Networks with Parallel Bias Metadynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 2516-2525	6.4	16
61	Peptoid Backbone Flexibilility Dictates Its Interaction with Water and Surfaces: A Molecular Dynamics Investigation. *Biomacromolecules*, **2018**, 19, 1006-1015	6.9	16
60	Elucidation of structure–reactivity relationships in hindered phenols via quantum chemistry and transition state theory. *Chemical Engineering Science*, **2007**, 62, 5232-5239	4.4	16
59	Lytic Polysaccharide Monooxygenases ScLPMO10B and ScLPMO10C Are Stable in Ionic Liquids As Determined by Molecular Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 3863-72	3.4	15
58	Biasing Smarter, Not Harder, by Partitioning Collective Variables into Families in Parallel Bias Metadynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 4985-4990	6.4	14
57	Quantifying the Molecular-Scale Aqueous Response to the Mica Surface. *Journal of Physical Chemistry C*, **2017**, 121, 18496-18504	3.8	14
56	Ice-binding site of surface-bound type III antifreeze protein partially decoupled from water. *Physical Chemistry Chemical Physics*, **2018**, 20, 26926-26933	3.6	14
55	Enhancing the Oxidation of Toluene with External Electric Fields: a Reactive Molecular Dynamics Study. *Scientific Reports*, **2017**, 7, 1710	4.9	13
54	Orientation and Conformation of Proteins at the Air-Water Interface Determined from Integrative Molecular Dynamics Simulations and Sum Frequency Generation Spectroscopy. *Langmuir*, **2020**, 36, 11855-11865	4	13
53	Determining energy barriers and selectivities of a multi-pathway system with infrequent metadynamics. *Journal of Chemical Physics*, **2017**, 146, 014108	3.9	11
52	LK peptide side chain dynamics at interfaces are independent of secondary structure. *Physical Chemistry Chemical Physics*, **2017**, 19, 28507-28511	3.6	11
51	Sequence-Structure-Binding Relationships Reveal Adhesion Behavior of the Car9 Solid-Binding Peptide: An Integrated Experimental and Simulation Study. *Journal of the American Chemical Society*, **2020**, 142, 2355-2363	16.4	11
50	Assessment of molecular dynamics simulations for amorphous poly(3-hexylthiophene) using neutron and X-ray scattering experiments. *Soft Matter*, **2019**, 15, 5067-5083	3.6	10
49	Structure Characterization and Properties of Metal-Surfactant Complexes Dispersed in Organic Solvents. *Langmuir*, **2015**, 31, 9006-16	4	10

48	MARTINI-Compatible Coarse-Grained Model for the Mesoscale Simulation of Peptoids. *Journal of Physical Chemistry B*, **2020**, 124, 7745-7764	3.4	10
47	Solid-State NMR and MD Study of the Structure of the Statherin Mutant SNa15 on Mineral Surfaces. *Journal of the American Chemical Society*, **2019**, 141, 1998-2011	16.4	10
46	Acetylation dictates the morphology of nanophase biosilica precipitated by a 14-amino acid leucine-lysine peptide. *Journal of Peptide Science*, **2017**, 23, 141-147	2.1	9
45	Effect of an ionic liquid/air Interface on the structure and dynamics of amphiphilic peptides. *Journal of Molecular Liquids*, **2017**, 236, 404-413	6	8
44	Using Molecular Simulation to Study Biocatalysis in Ionic Liquids. *Methods in Enzymology*, **2016**, 577, 419-441	1.7	8
43	Enhanced Activity and Stability of Acidothermus cellulolyticus Endoglucanase 1 in Ionic Liquids via Engineering Active Site Residues and Non-Native Disulfide Bridges. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 11299-11307	8.3	8
42	Continuous Molecular Representations of Ionic Liquids. *Journal of Physical Chemistry B*, **2020**, 124, 8347-8357	3.4	8
41	Ice-nucleating proteins are activated by low temperatures to control the structure of interfacial water. *Nature Communications*, **2021**, 12, 1183	17.4	8
40	Diagnosing the Impact of External Electric Fields Chemical Kinetics: Application to Toluene Oxidation and Pyrolysis. *Journal of Physical Chemistry A*, **2019**, 123, 3080-3089	2.8	7
39	Design of Polyphosphate Inhibitors: A Molecular Dynamics Investigation on Polyethylene Glycol-Linked Cationic Binding Groups. *Biomacromolecules*, **2018**, 19, 1358-1367	6.9	7
38	Tribological degradation of two vegetable-based lubricants at elevated temperatures. *Journal of Synthetic Lubrication: Research, Development and Application of Synthetic Lubricants and Functional Fluids*, **2007**, 24, 167-179		7
37	Studies of Dynamic Binding of Amino Acids to TiO Nanoparticle Surfaces by Solution NMR and Molecular Dynamics Simulations. *Langmuir*, **2020**, 36, 10341-10350	4	7
36	Solvent oligomerization pathways facilitated by electrolyte additives during solid-electrolyte interphase formation. *Physical Chemistry Chemical Physics*, **2020**, 22, 21494-21503	3.6	7
35	Quantifying the Dynamics of Protein Self-Organization Using Deep Learning Analysis of Atomic Force Microscopy Data. *Nano Letters*, **2021**, 21, 158-165	11.5	7
34	Attention-based generative models for molecular design. *Chemical Science*, **2021**, 12, 8362-8372	9.4	6
33	Effect of Fluoroethylene Carbonate Additives on the Initial Formation of the Solid Electrolyte Interphase on an Oxygen-Functionalized Graphitic Anode in Lithium-Ion Batteries. *ACS Applied Materials & Interfaces*, **2021**, 13, 8169-8180	9.5	6
32	Fantastic Liquids and Where To Find Them: Optimizations of Discrete Chemical Space. *Journal of Chemical Information and Modeling*, **2019**, 59, 2617-2625	6.1	5
31	Elucidating Molecular Design Principles for Charge-Alternating Peptides. *Biomacromolecules*, **2020**, 21, 435-443	6.9	5

30	Ion-dependent protein-surface interactions from intrinsic solvent response. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	5
29	Determining dominant driving forces affecting controlled protein release from polymeric nanoparticles. *Biointerphases*, **2017**, 12, 02D412	1.8	4
28	Amphiphilic peptide binding on crystalline vs. amorphous silica from molecular dynamics simulations. *Molecular Physics*, **2019**, 117, 3642-3650	1.7	4
27	Density functional tight-binding and infrequent metadynamics can capture entropic effects in intramolecular hydrogen transfer reactions. *Journal of Chemical Physics*, **2018**, 148, 154101	3.9	4
26	Contra-thermodynamic behavior in intermolecular hydrogen transfer of alkylperoxy radicals. *ChemPhysChem*, **2007**, 8, 1969-78	3.2	4
25	Impact of Glutamate Carboxylation in the Adsorption of the Domain of Osteocalcin to Hydroxyapatite and Titania. *Molecular Systems Design and Engineering*, **2020**, 5, 620-631	4.6	4
24	Closing the Gap Between Modeling and Experiments in the Self-Assembly of Biomolecules at Interfaces and in Solution *Chemistry of Materials*, **2020**, 32, 8043-8059	9.6	4
23	Formulation and Efficacy of Catalase-Loaded Nanoparticles for the Treatment of Neonatal Hypoxic-Ischemic Encephalopathy. *Pharmaceutics*, **2021**, 13,	6.4	3
22	Molecular recognition and specificity of biomolecules to titanium dioxide from molecular dynamics simulations. *Npj Computational Materials*, **2020**, 6,	10.9	3
21	IL-Net: Using Expert Knowledge to Guide the Design of Furcated Neural Networks **2018**,		3
20	Metadynamics to Enhance Sampling in Biomolecular Simulations. *Methods in Molecular Biology*, **2019**, 2022, 179-200	1.4	2
19	// Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry B*, **2020**, 124, 9767-9772	3.4	2
18	Trimethylation of the R5 Silica-Precipitating Peptide Increases Silica Particle Size by Redirecting Orthosilicate Binding. *ChemBioChem*, **2020**, 21, 3208-3211	3.8	2
17	Elucidating the Molecular Interactions between Uremic Toxins and the Sudlow II Binding Site of Human Serum Albumin. *Journal of Physical Chemistry B*, **2020**, 124, 3922-3930	3.4	2
16	Assessing the Performance of Various Stochastic Optimization Methods on Chemical Kinetic Modeling of Combustion. *Industrial & Engineering Chemistry Research*, **2020**, 59, 19212-19225	3.9	2
15	Data Science in Chemical Engineering: Applications to Molecular Science. *Annual Review of Chemical and Biomolecular Engineering*, **2021**, 12, 15-37	8.9	2
14	Thiolated Lysine-Leucine Peptides Self-Assemble into Biosilica Nucleation Pits on Gold Surfaces. *Advanced Materials Interfaces*, **2017**, 4, 1700399	4.6	1
13	// Virtual Special Issue on Machine Learning in Physical Chemistry. *Journal of Physical Chemistry A*, **2020**, 124, 9113-9118	2.8	1

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11	Inhibition of the Exoglucanase Cel7A by a Douglas-Fir-Condensed Tannin. *Journal of Physical Chemistry B*, **2018**, 122, 8665-8674	3.4	1
10	Redefining the Protein-Protein Interface: Coarse Graining and Combinatorics for an Improved Understanding of Amino Acid Contributions to the Protein-Protein Binding Affinity. *Langmuir*, **2017** , 33, 11511-11517	4	1
9	Membrane Structure of Aquaporin Observed with Combined Experimental and Theoretical Sum Frequency Generation Spectroscopy. *Langmuir*, **2021**, 37, 13452-13459	4	1
8	Substitution of distal and active site residues reduces product inhibition of E1 from Acidothermus Cellulolyticus.. *Protein Engineering, Design and Selection*, **2021**, 34,	1.9	1
7	Probing the thermodynamics and kinetics of ethylene carbonate reduction at the electrode-electrolyte interface with molecular simulations. *Journal of Chemical Physics*, **2021**, 155, 204703	3.9	1
6	Analyzing the Long Time-Scale Dynamics of Uremic Toxins Bound to Sudlow Site II in Human Serum Albumin. *Journal of Physical Chemistry B*, **2021**, 125, 2910-2920	3.4	1
5	Combining Molecular and Spin Dynamics Simulations with Solid-State NMR: A Case Study of Amphiphilic Lysine-Leucine Repeat Peptide Aggregates. *Journal of Physical Chemistry B*, **2019**, 123, 10915-10929	3.4	1
4	Direct Evidence for Aligned Binding of Cellulase Enzymes to Cellulose Surfaces. *Journal of Physical Chemistry Letters*, **2021**, 12, 10684-10688	6.4	0
3	Effect of graphitic anode surface functionalization on the structure and dynamics of electrolytes at the interface. *Journal of Chemical Physics*, **2021**, 155, 134702	3.9	0
2	Coagulopathy In Trauma Patients Is Accompanied By Oxidation Of a Methionine Residue In The E Domain Of Fibrinogen and Abnormal Fibrin Polymerization. *Blood*, **2013**, 122, 1097-1097	2.2	
1	Efficient Sampling of High-Dimensional Free Energy Landscapes: A Review of Parallel Bias Metadynamics. *Molecular Modeling and Simulation*, **2021**, 123-141		