Bernhardt L Trout

List of Publications by Year in Descending Order

152 papers	8,288 citations	50 h-index	86 g-index
156 ext. papers	9,172 ext. citations	4.9 avg, IF	6.24 L-index

#	Paper	IF	Citations
152	Machine learning prediction of antibody aggregation and viscosity for high concentration formulation development of protein therapeutics.. *MAbs*, **2022**, 14, 2026208	6.6	4
151	Differences in human IgG1 and IgG4 S228P monoclonal antibodies viscosity and self-interactions: Experimental assessment and computational predictions of domain interactions. *MAbs*, **2021**, 13, 1991256	6.6	4
150	Machine Learning Feature Selection for Predicting High Concentration Therapeutic Antibody Aggregation. *Journal of Pharmaceutical Sciences*, **2021**, 110, 1583-1591	3.9	7
149	Calculation of therapeutic antibody viscosity with coarse-grained models, hydrodynamic calculations and machine learning-based parameters. *MAbs*, **2021**, 13, 1907882	6.6	9
148	Machine Learning Applied to Determine the Molecular Descriptors Responsible for the Viscosity Behavior of Concentrated Therapeutic Antibodies. *Molecular Pharmaceutics*, **2021**, 18, 1167-1175	5.6	15
147	In Silico Engineering of Hydrate Anti-agglomerant Molecules Using Bias-Exchange Metadynamics Simulations. *Journal of Physical Chemistry C*, **2020**, 124, 18983-18992	3.8	6
146	Computational Modeling of the Disulfide Cross-Linking Reaction. *Journal of Physical Chemistry B*, **2020**, 124, 9840-9851	3.4	3
145	Molecular computations of preferential interactions of proline, arginine.HCl, and NaCl with IgG1 antibodies and their impact on aggregation and viscosity. *MAbs*, **2020**, 12, 1816312	6.6	7
144	Machine Learning Models of Antibody-Excipient Preferential Interactions for Use in Computational Formulation Design. *Molecular Pharmaceutics*, **2020**, 17, 3589-3599	5.6	5
143	Challenges and Directions for Green Chemical Engineering: Role of Nanoscale Materials **2020**, 1-18		7
142	Why We Need Continuous Pharmaceutical Manufacturing and How to Make It Happen. *Journal of Pharmaceutical Sciences*, **2019**, 108, 3521-3523	3.9	37
141	The use of biocompatible crystalline substrates for the heterogeneous nucleation and polymorphic selection of indomethacin. *CrystEngComm*, **2019**, 21, 2193-2202	3.3	5
140	Achieving continuous manufacturing in lyophilization: Technologies and approaches. *European Journal of Pharmaceutics and Biopharmaceutics*, **2019**, 142, 265-279	5.7	29
139	Understanding the Role of Preferential Exclusion of Sugars and Polyols from Native State IgG1 Monoclonal Antibodies and its Effect on Aggregation and Reversible Self-Association. *Pharmaceutical Research*, **2019**, 36, 109	4.5	13
138	On computing the solubility of molecular systems subject to constraints using the extended Einstein crystal method. *Journal of Chemical Physics*, **2019**, 150, 201104	3.9	1
137	Solubility of paracetamol in ethanol by molecular dynamics using the extended Einstein crystal method and experiments. *Journal of Chemical Physics*, **2019**, 150, 094107	3.9	13
136	In Silico Analysis of the Effect of Alkyl Tail Length on Antiagglomerant Adsorption to Natural Gas Hydrates in Brine. *Journal of Physical Chemistry C*, **2019**, 123, 17239-17248	3.8	9

135	Molecular Computations of Preferential Interaction Coefficients of IgG1 Monoclonal Antibodies with Sorbitol, Sucrose, and Trehalose and the Impact of These Excipients on Aggregation and Viscosity. *Molecular Pharmaceutics*, **2019**, 16, 3657-3664	5.6	12
134	From Batch to Continuous: Freeze-Drying of Suspended Vials for Pharmaceuticals in Unit-Doses. *Industrial & Engineering Chemistry Research*, **2019**, 58, 1635-1649	3.9	27
133	Low Energy Nanoemulsions as Templates for the Formulation of Hydrophobic Drugs. *Advanced Therapeutics*, **2018**, 1, 1700020	4.9	17
132	Nucleation of Molecular Crystals Driven by Relative Information Entropy. *Journal of Chemical Theory and Computation*, **2018**, 14, 959-972	6.4	19
131	Molecular Dynamics Analysis of Anti-Agglomerant Surface Adsorption in Natural Gas Hydrates. *Journal of Physical Chemistry C*, **2018**, 122, 2673-2683	3.8	34
130	Tablet coating by injection molding technology - Optimization of coating formulation attributes and coating process parameters. *European Journal of Pharmaceutics and Biopharmaceutics*, **2018**, 122, 25-36	5.7	8
129	General Method for the Identification of Crystal Faces Using Raman Spectroscopy Combined with Machine Learning and Application to the Epitaxial Growth of Acetaminophen. *Langmuir*, **2018**, 34, 9836-9846	4	2
128	Demonstration of pharmaceutical tablet coating process by injection molding technology. *International Journal of Pharmaceutics*, **2018**, 535, 106-112	6.5	6
127	Kirkwood-Buff-Derived Alcohol Parameters for Aqueous Carbohydrates and Their Application to Preferential Interaction Coefficient Calculations of Proteins. *Journal of Physical Chemistry B*, **2018**, 122, 9350-9360	3.4	11
126	Effect of Salt on Antiagglomerant Surface Adsorption in Natural Gas Hydrates. *Journal of Physical Chemistry C*, **2018**, 122, 12839-12849	3.8	24
125	Lack of a synergistic effect of arginine-glutamic acid on the physical stability of spray-dried bovine serum albumin. *Pharmaceutical Development and Technology*, **2017**, 22, 785-791	3.4	10
124	Continuous Crystallization of Cyclosporine: Effect of Operating Conditions on Yield and Purity. *Crystal Growth and Design*, **2017**, 17, 1000-1007	3.5	34
123	A New Phenomenon: Sub-T, Solid-State, Plasticity-Induced Bonding in Polymers. *Scientific Reports*, **2017**, 7, 46405	4.9	5
122	Angle-Directed Nucleation of Paracetamol on Biocompatible Nanoimprinted Polymers. *Crystal Growth and Design*, **2017**, 17, 2955-2963	3.5	16
121	Continuous Heterogeneous Crystallization on Excipient Surfaces. *Crystal Growth and Design*, **2017**, 17, 3321-3330	3.5	26
120	Experimental and Mechanistic Study of the Heterogeneous Nucleation and Epitaxy of Acetaminophen with Biocompatible Crystalline Substrates. *Crystal Growth and Design*, **2017**, 17, 3783-3793	3.5	20
119	Rational design of rabies vaccine formulation for enhanced stability. *Turkish Journal of Medical Sciences*, **2017**, 47, 987-995	2.7	2
118	Integrated hot-melt extrusion - injection molding continuous tablet manufacturing platform: Effects of critical process parameters and formulation attributes on product robustness and dimensional stability. *International Journal of Pharmaceutics*, **2017**, 531, 332-342	6.5	17

117	Preferential interactions of trehalose, L-arginine.HCl and sodium chloride with therapeutically relevant IgG1 monoclonal antibodies. *MAbs*, **2017**, 9, 1155-1168	6.6	17
116	Development of Maltodextrin-Based Immediate-Release Tablets Using an Integrated Twin-Screw Hot-Melt Extrusion and Injection-Molding Continuous Manufacturing Process. *Journal of Pharmaceutical Sciences*, **2017**, 106, 3328-3336	3.9	18
115	Molecular Investigation of the Mechanism of Non-Enzymatic Hydrolysis of Proteins and the Predictive Algorithm for Susceptibility. *Biochemistry*, **2016**, 55, 3315-28	3.2	4
114	Novel Technique for Filtration Avoidance in Continuous Crystallization. *Crystal Growth and Design*, **2016**, 16, 285-296	3.5	20
113	Quantitative determination of the surfactant-induced split ratio of influenza virus by fluorescence spectroscopy. *Human Vaccines and Immunotherapeutics*, **2016**, 12, 1757-65	4.4	7
112	Advancing Product Quality: a Summary of the Second FDA/PQRI Conference. *AAPS Journal*, **2016**, 18, 528-43	3.7	12
111	Multistage Continuous Mixed-Suspension, Mixed-Product Removal (MSMPR) Crystallization with Solids Recycle. *Organic Process Research and Development*, **2016**, 20, 510-516	3.9	55
110	Rational design of therapeutic mAbs against aggregation through protein engineering and incorporation of glycosylation motifs applied to bevacizumab. *MAbs*, **2016**, 8, 99-112	6.6	50
109	Computational tool for the early screening of monoclonal antibodies for their viscosities. *MAbs*, **2016**, 8, 43-8	6.6	59
108	Core-Shell Composite Hydrogels for Controlled Nanocrystal Formation and Release of Hydrophobic Active Pharmaceutical Ingredients. *Advanced Healthcare Materials*, **2016**, 5, 1960-8	10.1	33
107	Enhancing the performance of the T-peel test for thin and flexible adhered laminates. *Review of Scientific Instruments*, **2016**, 87, 085111	1.7	16
106	Mechanistic Insights into Radical-Mediated Oxidation of Tryptophan from ab Initio Quantum Chemistry Calculations and QM/MM Molecular Dynamics Simulations. *Journal of Physical Chemistry A*, **2016**, 120, 2926-39	2.8	6
105	Conformational and Colloidal Stabilities of Isolated Constant Domains of Human Immunoglobulin G and Their Impact on Antibody Aggregation under Acidic Conditions. *Molecular Pharmaceutics*, **2015**, 12, 1443-55	5.6	28
104	Effect of Pore Size and Interactions on Paracetamol Aggregation in Porous Polyethylene Glycol Diacrylate Polymers. *Journal of Physical Chemistry B*, **2015**, 119, 8135-45	3.4	7
103	Control of Polymorphism in Continuous Crystallization via Mixed Suspension Mixed Product Removal Systems Cascade Design. *Crystal Growth and Design*, **2015**, 15, 3374-3382	3.5	70
102	Control of Heterogeneous Nucleation via Rationally Designed Biocompatible Polymer Surfaces with Nanoscale Features. *Crystal Growth and Design*, **2015**, 15, 2176-2186	3.5	31
101	Rational Design of Biobetters with Enhanced Stability. *Journal of Pharmaceutical Sciences*, **2015**, 104, 2433-40	3.9	27
100	A general method for molecular modeling of nucleation from the melt. *Journal of Chemical Physics*, **2015**, 143, 174109	3.9	14

99	On the connection between nonmonotonic taste behavior and molecular conformation in solution: The case of rebaudioside-A. *Journal of Chemical Physics*, **2015**, 143, 244301	3.9	8
98	Achieving continuous manufacturing for final dosage formation: challenges and how to meet them. May 20-21, 2014 Continuous Manufacturing Symposium. *Journal of Pharmaceutical Sciences*, **2015**, 104, 792-802	3.9	98
97	A Process for the Formation of Nanocrystals of Active Pharmaceutical Ingredients with Poor Aqueous Solubility in a Nanoporous Substrate. *Organic Process Research and Development*, **2015**, 19, 1109-1118	3.9	17
96	Composite Hydrogels Laden with Crystalline Active Pharmaceutical Ingredients of Controlled Size and Loading. *Chemistry of Materials*, **2014**, 26, 6213-6220	9.6	32
95	Continuous Crystallization and Polymorph Dynamics in the l-Glutamic Acid System. *Organic Process Research and Development*, **2014**, 18, 1382-1390	3.9	52
94	Regulating Nucleation Kinetics through Molecular Interactions at the Polymer□Solute Interface. *Crystal Growth and Design*, **2014**, 14, 678-686	3.5	40
93	Use of Continuous MSMPR Crystallization with Integrated Nanofiltration Membrane Recycle for Enhanced Yield and Purity in API Crystallization. *Crystal Growth and Design*, **2014**, 14, 617-627	3.5	79
92	Application of Continuous Crystallization in an Integrated Continuous Pharmaceutical Pilot Plant. *Crystal Growth and Design*, **2014**, 14, 2148-2157	3.5	60
91	B□ier curve string method for the study of rare events in complex chemical systems. *Journal of Chemical Physics*, **2014**, 141, 074110	3.9	3
90	Properties of reactive oxygen species by quantum Monte Carlo. *Journal of Chemical Physics*, **2014**, 141, 014305	3.9	12
89	A computational tool to predict the evolutionarily conserved protein-protein interaction hot-spot residues from the structure of the unbound protein. *FEBS Letters*, **2014**, 588, 326-33	3.8	16
88	Geometric Design of Heterogeneous Nucleation Sites on Biocompatible Surfaces. *Crystal Growth and Design*, **2013**, 13, 3835-3841	3.5	27
87	End-to-end continuous manufacturing of pharmaceuticals: integrated synthesis, purification, and final dosage formation. *Angewandte Chemie - International Edition*, **2013**, 52, 12359-63	16.4	426
86	Mathematical modeling and design of layer crystallization in a concentric annulus with and without recirculation. *AICHE Journal*, **2013**, 59, 1308-1321	3.6	16
85	Protein-associated cation clusters in aqueous arginine solutions and their effects on protein stability and size. *ACS Chemical Biology*, **2013**, 8, 416-22	4.9	51
84	Electrospun formulations containing crystalline active pharmaceutical ingredients. *Pharmaceutical Research*, **2013**, 30, 238-46	4.5	41
83	Understanding the Role of Arginine and Citrate as Eluents in Affinity Chromatography. *ACS Symposium Series*, **2013**, 67-86	0.4	1
82	Templated nucleation of acetaminophen on spherical excipient agglomerates. *Langmuir*, **2013**, 29, 3292-300	4	26

81	End-to-End Continuous Manufacturing of Pharmaceuticals: Integrated Synthesis, Purification, and Final Dosage Formation. *Angewandte Chemie*, **2013**, 125, 12585-12589	3.6	56
80	Developability index: a rapid in silico tool for the screening of antibody aggregation propensity. *Journal of Pharmaceutical Sciences*, **2012**, 101, 102-15	3.9	126
79	Production and characterization of carbamazepine nanocrystals by electrospraying for continuous pharmaceutical manufacturing. *Journal of Pharmaceutical Sciences*, **2012**, 101, 1178-88	3.9	72
78	A screening tool for therapeutic monoclonal antibodies: Identifying the most stable protein and its best formulation based on thioflavin T binding. *Biotechnology Journal*, **2012**, 7, 127-32	5.6	13
77	Free surface electrospinning of fibers containing microparticles. *Langmuir*, **2012**, 28, 9714-21	4	54
76	Continuous Crystallization of Aliskiren Hemifumarate. *Crystal Growth and Design*, **2012**, 12, 3036-3044	3.5	112
75	Development of Continuous Crystallization Processes Using a Single-Stage Mixed-Suspension, Mixed-Product Removal Crystallizer with Recycle. *Crystal Growth and Design*, **2012**, 12, 5701-5707	3.5	100
74	Nucleation under Soft Confinement: Role of Polymer–Solute Interactions. *Crystal Growth and Design*, **2012**, 12, 508-517	3.5	48
73	Gel-induced selective crystallization of polymorphs. *Journal of the American Chemical Society*, **2012**, 134, 673-84	16.4	113
72	Toward the Rational Design of Crystalline Surfaces for Heteroepitaxy: Role of Molecular Functionality. *Crystal Growth and Design*, **2012**, 12, 1159-1166	3.5	54
71	Computational methods to predict therapeutic protein aggregation. *Methods in Molecular Biology*, **2012**, 899, 425-51	1.4	48
70	Arginine and the Hofmeister Series: the role of ion-ion interactions in protein aggregation suppression. *Journal of Physical Chemistry B*, **2011**, 115, 7447-58	3.4	99
69	Understanding the synergistic effect of arginine and glutamic acid mixtures on protein solubility. *Journal of Physical Chemistry B*, **2011**, 115, 11831-9	3.4	53
68	Economic Analysis of Integrated Continuous and Batch Pharmaceutical Manufacturing: A Case Study. *Industrial & Engineering Chemistry Research*, **2011**, 50, 10083-10092	3.9	336
67	Conformational stability and aggregation of therapeutic monoclonal antibodies studied with ANS and Thioflavin T binding. *MAbs*, **2011**, 3, 408-11	6.6	36
66	Surface design for controlled crystallization: the role of surface chemistry and nanoscale pores in heterogeneous nucleation. *Langmuir*, **2011**, 27, 5324-34	4	156
65	Preferential interaction coefficients of proteins in aqueous arginine solutions and their molecular origins. *Journal of Physical Chemistry B*, **2011**, 115, 1243-53	3.4	45
64	Complex interactions between molecular ions in solution and their effect on protein stability. *Journal of the American Chemical Society*, **2011**, 133, 18713-8	16.4	31

63	Effects of PAMAM Dendrimer Salt Solutions on Protein Stability. *Journal of Physical Chemistry Letters*, **2011**, 2, 1782-1788	6.4	13
62	Understanding the role of arginine as an eluent in affinity chromatography via molecular computations. *Journal of Physical Chemistry B*, **2011**, 115, 2645-54	3.4	36
61	Effects of solute-solute interactions on protein stability studied using various counterions and dendrimers. *PLoS ONE*, **2011**, 6, e27665	3.7	15
60	Glycosylation influences on the aggregation propensity of therapeutic monoclonal antibodies. *Biotechnology Journal*, **2011**, 6, 38-44	5.6	119
59	A general set of order parameters for molecular crystals. *Journal of Chemical Physics*, **2011**, 134, 064109	3.9	73
58	Molecular level insight into intra-solvent interaction effects on protein stability and aggregation. *Advanced Drug Delivery Reviews*, **2011**, 63, 1074-85	18.5	69
57	Tryptophan-tryptophan energy transfer and classification of tryptophan residues in proteins using a therapeutic monoclonal antibody as a model. *Journal of Fluorescence*, **2011**, 21, 275-88	2.4	16
56	Prediction of protein binding regions. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 888-97	4.2	16
55	Evaluation of a non-Arrhenius model for therapeutic monoclonal antibody aggregation. *Journal of Pharmaceutical Sciences*, **2011**, 100, 2526-42	3.9	81
54	Aggregation in protein-based biotherapeutics: computational studies and tools to identify aggregation-prone regions. *Journal of Pharmaceutical Sciences*, **2011**, 100, 5081-95	3.9	109
53	Binding affinity of a small molecule to an amorphous polymer in a solvent. Part 1: free energy of binding to a binding site. *Langmuir*, **2011**, 27, 12381-95	4	4
52	Computer simulations of homogeneous nucleation of benzene from the melt. *Journal of Physical Chemistry B*, **2011**, 115, 10400-12	3.4	30
51	The role of nanopore shape in surface-induced crystallization. *Nature Materials*, **2011**, 10, 867-71	27	134
50	Computer-Aided Solvent Selection for Improving the Morphology of Needle-like Crystals: A Case Study of 2,6-Dihydroxybenzoic Acid. *Crystal Growth and Design*, **2010**, 10, 4379-4388	3.5	58
49	Design and application of antibody cysteine variants. *Bioconjugate Chemistry*, **2010**, 21, 385-92	6.3	33
48	Interaction of arginine with proteins and the mechanism by which it inhibits aggregation. *Journal of Physical Chemistry B*, **2010**, 114, 13426-38	3.4	153
47	Prediction of aggregation prone regions of therapeutic proteins. *Journal of Physical Chemistry B*, **2010**, 114, 6614-24	3.4	145
46	Design of therapeutic proteins with enhanced stability. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 11937-42	11.5	404

45	Predictive tools for stabilization of therapeutic proteins. *MAbs*, **2009**, 1, 580-2	6.6	46
44	Mechanisms of protein stabilization and prevention of protein aggregation by glycerol. *Biochemistry*, **2009**, 48, 11084-96	3.2	291
43	Molecular computations of preferential interaction coefficients of proteins. *Journal of Physical Chemistry B*, **2009**, 113, 12546-54	3.4	70
42	Aggregation-prone motifs in human immunoglobulin G. *Journal of Molecular Biology*, **2009**, 391, 404-13	6.5	133
41	Investigation of cosolute-protein preferential interaction coefficients: new insight into the mechanism by which arginine inhibits aggregation. *Journal of Physical Chemistry B*, **2009**, 113, 2050-8	3.4	96
40	Molecular anatomy of preferential interaction coefficients by elucidating protein solvation in mixed solvents: methodology and application for lysozyme in aqueous glycerol. *Journal of Physical Chemistry B*, **2009**, 113, 11743-53	3.4	35
39	Dynamic fluctuations of protein-carbohydrate interactions promote protein aggregation. *PLoS ONE* , **2009**, 4, e8425	3.7	37
38	Path sampling calculation of methane diffusivity in natural gas hydrates from a water-vacancy assisted mechanism. *Journal of the American Chemical Society*, **2008**, 130, 17342-50	16.4	113
37	Interaction of hydrogen chloride with ice surfaces: the effects of grain size, surface roughness, and surface disorder. *Journal of Physical Chemistry A*, **2007**, 111, 6274-84	2.8	48
36	New Insights on the Nanoparticle Growth Mechanism in the Citrate Reduction of Gold(III) Salt: Formation of the Au Nanowire Intermediate and Its Nonlinear Optical Properties. *Journal of Physical Chemistry C*, **2007**, 111, 6281-6287	3.8	235
35	Hydrogen chloride-induced surface disordering on ice. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 9422-7	11.5	79
34	Comparative oxidation studies of methionine residues reflect a structural effect on chemical kinetics in rhG-CSF. *Biochemistry*, **2006**, 45, 15430-43	3.2	41
33	Role of arginine in the stabilization of proteins against aggregation. *Biochemistry*, **2005**, 44, 4919-25	3.2	192
32	Order Parameter Approach to Understanding and Quantifying the Physico-Chemical Behavior of Complex Systems **2005**, 1613-1626		6
31	Properties of inhibitors of methane hydrate formation via molecular dynamics simulations. *Journal of the American Chemical Society*, **2005**, 127, 17852-62	16.4	202
30	Application of the cell potential method to predict phase equilibria of multicomponent gas hydrate systems. *Journal of Physical Chemistry B*, **2005**, 109, 8153-63	3.4	47
29	Effects of excipients on the hydrogen peroxide-induced oxidation of methionine residues in granulocyte colony-stimulating factor. *Pharmaceutical Research*, **2005**, 22, 141-7	4.5	34
28	Order Parameter Approach to Understanding and Quantifying the Physico-Chemical Behavior of Complex Systems **2005**, 1613-1626		

27	Lateral interactions between oxygen atoms adsorbed on platinum (111) by first principles. *Molecular Physics*, **2004**, 102, 273-279	1.7	28
26	Phase diagram of oxygen adsorbed on platinum (111) by first-principles investigation. *Physical Review B*, **2004**, 70,	3.3	99
25	Density-functional theory characterization of acid sites in chabazite. *Journal of Catalysis*, **2004**, 227, 77-89	3.3	65
24	Effects of antioxidants on the hydrogen peroxide-mediated oxidation of methionine residues in granulocyte colony-stimulating factor and human parathyroid hormone fragment 13-34. *Pharmaceutical Research*, **2004**, 21, 2377-83	4.5	34
23	A comprehensive picture of non-site specific oxidation of methionine residues by peroxides in protein pharmaceuticals. *Journal of Pharmaceutical Sciences*, **2004**, 93, 3096-102	3.9	45
22	A structural and mechanistic study of the oxidation of methionine residues in hPTH(1-34) via experiments and simulations. *Biochemistry*, **2004**, 43, 14139-48	3.2	22
21	Molecular dynamics simulations and oxidation rates of methionine residues of granulocyte colony-stimulating factor at different pH values. *Biochemistry*, **2004**, 43, 1019-29	3.2	45
20	On the mechanisms of oxidation of organic sulfides by H2O2 in aqueous solutions. *Journal of the American Chemical Society*, **2004**, 126, 900-8	16.4	89
19	Methanol coupling in the zeolite chabazite studied via Car□Parrinello molecular dynamics. *Molecular Physics*, **2004**, 102, 281-288	1.7	24
18	Chemistry of Sulfur Oxides on Transition Metals. III. Oxidation of SO2 and Self-Diffusion of O, SO2, and SO3 on Pt(111). *Journal of Physical Chemistry B*, **2004**, 108, 13329-13340	3.4	39
17	Accurate Potentials for Argon□Water and Methane□Water Interactions via ab Initio Methods and Their Application to Clathrate Hydrates. *Journal of Physical Chemistry B*, **2004**, 108, 18705-18715	3.4	71
16	Rational design of solution additives for the prevention of protein aggregation. *Biophysical Journal*, **2004**, 87, 1631-9	2.9	90
15	A consistent and verifiable macroscopic model for the dissolution of liquid CO2 in water under hydrate forming conditions. *Energy Conversion and Management*, **2003**, 44, 771-780	10.6	15
14	Nucleation of crystalline phases of water in homogeneous and inhomogeneous environments. *Physical Review Letters*, **2003**, 90, 158301	7.4	49
13	Proteins in Mixed Solvents: A Molecular-Level Perspective. *Journal of Physical Chemistry B*, **2003**, 107, 14058-14067	3.4	131
12	Computations of diffusivities in ice and CO2 clathrate hydrates via molecular dynamics and Monte Carlo simulations. *Journal of Chemical Physics*, **2002**, 116, 702-709	3.9	89
11	Sensitivity Analysis of Hydrate Thermodynamic Reference Properties Using Experimental Data and ab Initio Methods. *Journal of Physical Chemistry B*, **2002**, 106, 7681-7687	3.4	19
10	A Theoretical Study of the Interaction of HCl with Crystalline NAT. *Journal of Physical Chemistry A*, **2002**, 106, 6972-6981	2.8	11

9	A new approach for studying nucleation phenomena using molecular simulations: Application to CO2 hydrate clathrates. *Journal of Chemical Physics*, **2002**, 117, 1786-1796	3.9	217
8	A method to extract potentials from the temperature dependence of Langmuir constants for clathrate-hydrates. *Physica A: Statistical Mechanics and Its Applications*, **2001**, 300, 139-173	3.3	27
7	The interaction of HCl with the (0001) face of hexagonal ice studied theoretically via Car Parrinello molecular dynamics. *Chemical Physics Letters*, **2001**, 348, 285-292	2.5	47
6	Molecular Computations Using Robust Hydrocarbon Water Potentials for Predicting Gas Hydrate Phase Equilibria. *Journal of Physical Chemistry B*, **2001**, 105, 10950-10960	3.4	65
5	Computation of the methane water potential energy hypersurface via ab initio methods. *Journal of Chemical Physics*, **2001**, 115, 2550-2559	3.9	61
4	First-Principles Theoretical Study of Molecular HCl Adsorption on a Hexagonal Ice (0001) Surface. *Journal of Physical Chemistry A*, **2001**, 105, 7037-7046	2.8	34
3	Thermochemistry of gas phase CF2 reactions: A density functional theory study. *Journal of Chemical Physics*, **2000**, 113, 4103-4108	3.9	29
2	First-principles molecular-dynamics study of surface disordering of the (0001) face of hexagonal ice. *Journal of Chemical Physics*, **2000**, 113, 10733-10743	3.9	45
1	Configurational Properties of Water Clathrates: Monte Carlo and Multidimensional Integration versus the Lennard-Jones and Devonshire Approximation. *Journal of Physical Chemistry B*, **1999**, 103, 6300-6308	3.4	48