Bernhardt L Trout

List of Publications by Year
in descending order

152 papers	9,964 citations	36691 53 h-index	46524 93 g-index
156 all docs	156 docs citations	156 times ranked	9931 citing authors

#	Article	IF	Citations
1	Machine learning prediction of antibody aggregation and viscosity for high concentration formulation development of protein therapeutics. MAbs, 2022, 14, 2026208.	2.6	26
2	Calculation of therapeutic antibody viscosity with coarse-grained models, hydrodynamic calculations and machine learning-based parameters. MAbs, 2021, 13, 1907882.	2.6	26
3	Machine Learning Feature Selection for Predicting High Concentration Therapeutic Antibody Aggregation. Journal of Pharmaceutical Sciences, 2021, 110, 1583-1591.	1.6	23
4	Machine Learning Applied to Determine the Molecular Descriptors Responsible for the Viscosity Behavior of Concentrated Therapeutic Antibodies. Molecular Pharmaceutics, 2021, 18, 1167-1175.	2.3	39
5	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.	2.6	14
6	Challenges and Directions for Green Chemical Engineeringâ€"Role of Nanoscale Materials. , 2020, , 1-18.		11
7	In Silico Engineering of Hydrate Anti-agglomerant Molecules Using Bias-Exchange Metadynamics Simulations. Journal of Physical Chemistry C, 2020, 124, 18983-18992.	1.5	11
8	Computational Modeling of the Disulfide Cross-Linking Reaction. Journal of Physical Chemistry B, 2020, 124, 9840-9851.	1.2	9
9	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.	2.6	17
10	Machine Learning Models of Antibodyâ€"Excipient Preferential Interactions for Use in Computational Formulation Design. Molecular Pharmaceutics, 2020, 17, 3589-3599.	2.3	17
11	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.	1.5	13
12	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.	2.3	20
13	Why We Need Continuous Pharmaceutical Manufacturing and How to Make It Happen. Journal of Pharmaceutical Sciences, 2019, 108, 3521-3523.	1.6	75
14	The use of biocompatible crystalline substrates for the heterogeneous nucleation and polymorphic selection of indomethacin. CrystEngComm, 2019, 21, 2193-2202.	1.3	9
15	Achieving continuous manufacturing in lyophilization: Technologies and approaches. European Journal of Pharmaceutics and Biopharmaceutics, 2019, 142, 265-279.	2.0	47
16	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.	1.7	28
17	On computing the solubility of molecular systems subject to constraints using the extended Einstein crystal method. Journal of Chemical Physics, 2019, 150, 201104.	1.2	4
18	Solubility of paracetamol in ethanol by molecular dynamics using the extended Einstein crystal method and experiments. Journal of Chemical Physics, 2019, 150, 094107.	1.2	19

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19	From Batch to Continuous: Freeze-Drying of Suspended Vials for Pharmaceuticals in Unit-Doses. Industrial & Engineering Chemistry Research, 2019, 58, 1635-1649.	1.8	45
20	Low Energy Nanoemulsions as Templates for the Formulation of Hydrophobic Drugs. Advanced Therapeutics, 2018, 1, 1700020.	1.6	22
21	Nucleation of Molecular Crystals Driven by Relative Information Entropy. Journal of Chemical Theory and Computation, 2018, 14, 959-972.	2.3	27
22	Molecular Dynamics Analysis of Anti-Agglomerant Surface Adsorption in Natural Gas Hydrates. Journal of Physical Chemistry C, 2018, 122, 2673-2683.	1.5	51
23	Tablet coating by injection molding technology â€“ Optimization of coating formulation attributes and coating process parameters. European Journal of Pharmaceutics and Biopharmaceutics, 2018, 122, 25-36.	2.0	12
24	Demonstration of pharmaceutical tablet coating process by injection molding technology. International Journal of Pharmaceutics, 2018, 535, 106-112.	2.6	6
25	Kirkwoodâ€“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.	1.2	17
26	Effect of Salt on Antiagglomerant Surface Adsorption in Natural Gas Hydrates. Journal of Physical Chemistry C, 2018, 122, 12839-12849.	1.5	31
27	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.	1.6	3
28	Lack of a synergistic effect of arginineâ€“glutamic acid on the physical stability of spray-dried bovine serum albumin. Pharmaceutical Development and Technology, 2017, 22, 785-791.	1.1	11
29	Continuous Crystallization of Cyclosporine: Effect of Operating Conditions on Yield and Purity. Crystal Growth and Design, 2017, 17, 1000-1007.	1.4	46
30	A New Phenomenon: Sub-Tg, Solid-State, Plasticity-Induced Bonding in Polymers. Scientific Reports, 2017, 7, 46405.	1.6	7
31	Angle-Directed Nucleation of Paracetamol on Biocompatible Nanoimprinted Polymers. Crystal Growth and Design, 2017, 17, 2955-2963.	1.4	18
32	Continuous Heterogeneous Crystallization on Excipient Surfaces. Crystal Growth and Design, 2017, 17, 3321-3330.	1.4	33
33	Experimental and Mechanistic Study of the Heterogeneous Nucleation and Epitaxy of Acetaminophen with Biocompatible Crystalline Substrates. Crystal Growth and Design, 2017, 17, 3783-3795.	1.4	22
34	Integrated hot-melt extrusion â€“ 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.	2.6	23
35	Preferential interactions of trehalose, L-arginine.HCl and sodium chloride with therapeutically relevant IgG1 monoclonal antibodies. MAbs, 2017, 9, 1155-1168.	2.6	29
36	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.	1.6	20

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37	Rational design of rabies vaccine formulation for enhanced stability. Turkish Journal of Medical Sciences, 2017, 47, 987-995.	0.4	4
38	Coreâ€“Shell Composite Hydrogels for Controlled Nanocrystal Formation and Release of Hydrophobic Active Pharmaceutical Ingredients. Advanced Healthcare Materials, 2016, 5, 1960-1968.	3.9	45
39	Enhancing the performance of the T-peel test for thin and flexible adhered laminates. Review of Scientific Instruments, 2016, 87, 085111.	0.6	21
40	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, 2926-2939.	1.1	6
41	Molecular Investigation of the Mechanism of Non-Enzymatic Hydrolysis of Proteins and the Predictive Algorithm for Susceptibility. Biochemistry, 2016, 55, 3315-3328.	1.2	6
42	Novel Technique for Filtration Avoidance in Continuous Crystallization. Crystal Growth and Design, 2016, 16, 285-296.	1.4	25
43	Quantitative determination of the surfactant-induced split ratio of influenza virus by fluorescence spectroscopy. Human Vaccines and Immunotherapeutics, 2016, 12, 1-9.	1.4	8
44	Advancing Product Quality: a Summary of the Second FDA/PQRI Conference. AAPS Journal, 2016, 18, 528-543.	2.2	17
45	Multistage Continuous Mixed-Suspension, Mixed-Product Removal (MSMPR) Crystallization with Solids Recycle. Organic Process Research and Development, 2016, 20, 510-516.	1.3	64
46	Rational design of therapeutic mAbs against aggregation through protein engineering and incorporation of glycosylation motifs applied to bevacizumab. MAbs, 2016, 8, 99-112.	2.6	76
47	Computational tool for the early screening of monoclonal antibodies for their viscosities. MAbs, 2016, 8, 43-48.	2.6	85
48	A general method for molecular modeling of nucleation from the melt. Journal of Chemical Physics, 2015, 143, 174109.	1.2	19
49	On the connection between nonmonotonic taste behavior and molecular conformation in solution: The case of rebaudioside-A. Journal of Chemical Physics, 2015, 143, 244301.	1.2	10
50	Achieving Continuous Manufacturing for Final Dosage Formation: Challenges and How to Meet Them May 20â€“21 2014 Continuous Manufacturing Symposium. Journal of Pharmaceutical Sciences, 2015, 104, 792-802.	1.6	117
51	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.	1.3	19
52	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, 1443-1455.	2.3	35
53	Effect of Pore Size and Interactions on Paracetamol Aggregation in Porous Polyethylene Glycol Diacrylate Polymers. Journal of Physical Chemistry B, 2015, 119, 8135-8145.	1.2	9
54	Control of Polymorphism in Continuous Crystallization via Mixed Suspension Mixed Product Removal Systems Cascade Design. Crystal Growth and Design, 2015, 15, 3374-3382.	1.4	87

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55	Control of Heterogeneous Nucleation via Rationally Designed Biocompatible Polymer Surfaces with Nanoscale Features. Crystal Growth and Design, 2015, 15, 2176-2186.	1.4	34
56	Rational Design of Biobetters with Enhanced Stability. Journal of Pharmaceutical Sciences, 2015, 104, 2433-2440.	1.6	34
57	BÃ©zier curve string method for the study of rare events in complex chemical systems. Journal of Chemical Physics, 2014, 141, 074110.	1.2	9
58	Properties of reactive oxygen species by quantum Monte Carlo. Journal of Chemical Physics, 2014, 141, 014305.	1.2	14
59	A computational tool to predict the evolutionarily conserved proteinâ€“protein interaction hotâ€spot residues from the structure of the unbound protein. FEBS Letters, 2014, 588, 326-333.	1.3	22
60	Composite Hydrogels Laden with Crystalline Active Pharmaceutical Ingredients of Controlled Size and Loading. Chemistry of Materials, 2014, 26, 6213-6220.	3.2	41
61	Continuous Crystallization and Polymorph Dynamics in the <scp>l</scp>-Glutamic Acid System. Organic Process Research and Development, 2014, 18, 1382-1390.	1.3	68
62	Regulating Nucleation Kinetics through Molecular Interactions at the Polymerâ€“Solute Interface. Crystal Growth and Design, 2014, 14, 678-686.	1.4	49
63	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.	1.4	88
64	Application of Continuous Crystallization in an Integrated Continuous Pharmaceutical Pilot Plant. Crystal Growth and Design, 2014, 14, 2148-2157.	1.4	64
65	Geometric Design of Heterogeneous Nucleation Sites on Biocompatible Surfaces. Crystal Growth and Design, 2013, 13, 3835-3841.	1.4	33
66	Endâ€toâ€End Continuous Manufacturing of Pharmaceuticals: Integrated Synthesis, Purification, and Final Dosage Formation. Angewandte Chemie - International Edition, 2013, 52, 12359-12363.	7.2	505
67	Mathematical modeling and design of layer crystallization in a concentric annulus with and without recirculation. AICHE Journal, 2013, 59, 1308-1321.	1.8	24
68	Protein-Associated Cation Clusters in Aqueous Arginine Solutions and Their Effects on Protein Stability and Size. ACS Chemical Biology, 2013, 8, 416-422.	1.6	62
69	Electrospun Formulations Containing Crystalline Active Pharmaceutical Ingredients. Pharmaceutical Research, 2013, 30, 238-246.	1.7	43
70	Understanding the Role of Arginine and Citrate as Eluents in Affinity Chromatography. ACS Symposium Series, 2013, , 67-86.	0.5	1
71	Templated Nucleation of Acetaminophen on Spherical Excipient Agglomerates. Langmuir, 2013, 29, 3292-3300.	1.6	30
72	Free Surface Electrospinning of Fibers Containing Microparticles. Langmuir, 2012, 28, 9714-9721.	1.6	55

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73	Continuous Crystallization of Aliskiren Hemifumarate. Crystal Growth and Design, 2012, 12, 3036-3044.	1.4	122
74	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.	1.4	112
75	Nucleation under Soft Confinement: Role of Polymerâ€“Solute Interactions. Crystal Growth and Design, 2012, 12, 508-517.	1.4	51
76	Gel-Induced Selective Crystallization of Polymorphs. Journal of the American Chemical Society, 2012, 134, 673-684.	6.6	129
77	Toward the Rational Design of Crystalline Surfaces for Heteroepitaxy: Role of Molecular Functionality. Crystal Growth and Design, 2012, 12, 1159-1166.	1.4	61
78	Computational Methods to Predict Therapeutic Protein Aggregation. Methods in Molecular Biology, 2012, 899, 425-451.	0.4	53
79	Developability Index: A Rapid In Silico Tool for the Screening of Antibody Aggregation Propensity. Journal of Pharmaceutical Sciences, 2012, 101, 102-115.	1.6	161
80	Production and Characterization of Carbamazepine Nanocrystals by Electrospraying for Continuous Pharmaceutical Manufacturing. Journal of Pharmaceutical Sciences, 2012, 101, 1178-1188.	1.6	77
81	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, 127-132.	1.8	16
82	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, 12381-12395.	1.6	6
83	Computer Simulations of Homogeneous Nucleation of Benzene from the Melt. Journal of Physical Chemistry B, 2011, 115, 10400-10412.	1.2	37
84	Arginine and the Hofmeister Series: The Role of Ionâ€“Ion Interactions in Protein Aggregation Suppression. Journal of Physical Chemistry B, 2011, 115, 7447-7458.	1.2	125
85	Understanding the Synergistic Effect of Arginine and Glutamic Acid Mixtures on Protein Solubility. Journal of Physical Chemistry B, 2011, 115, 11831-11839.	1.2	66
86	Economic Analysis of Integrated Continuous and Batch Pharmaceutical Manufacturing: A Case Study. Industrial & Engineering Chemistry Research, 2011, 50, 10083-10092.	1.8	389
87	Conformational stability and aggregation of therapeutic monoclonal antibodies studied with ANS and Thioflavin T binding. MAbs, 2011, 3, 408-411.	2.6	49
88	Surface Design for Controlled Crystallization: The Role of Surface Chemistry and Nanoscale Pores in Heterogeneous Nucleation. Langmuir, 2011, 27, 5324-5334.	1.6	186
89	Preferential Interaction Coefficients of Proteins in Aqueous Arginine Solutions and Their Molecular Origins. Journal of Physical Chemistry B, 2011, 115, 1243-1253.	1.2	53
90	Complex Interactions between Molecular Ions in Solution and Their Effect on Protein Stability. Journal of the American Chemical Society, 2011, 133, 18713-18718.	6.6	37

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91	Effects of PAMAM Dendrimer Salt Solutions on Protein Stability. Journal of Physical Chemistry Letters, 2011, 2, 1782-1788.	2.1	19
92	Understanding the Role of Arginine as an Eluent in Affinity Chromatography via Molecular Computations. Journal of Physical Chemistry B, 2011, 115, 2645-2654.	1.2	40
93	Effects of Solute-Solute Interactions on Protein Stability Studied Using Various Counterions and Dendrimers. PLoS ONE, 2011, 6, e27665.	1.1	18
94	Glycosylation influences on the aggregation propensity of therapeutic monoclonal antibodies. Biotechnology Journal, 2011, 6, 38-44.	1.8	135
95	A general set of order parameters for molecular crystals. Journal of Chemical Physics, 2011, 134, 064109.	1.2	87
96	Molecular level insight into intra-solvent interaction effects on protein stability and aggregation. Advanced Drug Delivery Reviews, 2011, 63, 1074-1085.	6.6	83
97	Tryptophan-Tryptophan Energy Transfer and Classification of Tryptophan Residues in Proteins Using a Therapeutic Monoclonal Antibody as a Model. Journal of Fluorescence, 2011, 21, 275-288.	1.3	16
98	Prediction of protein binding regions. Proteins: Structure, Function and Bioinformatics, 2011, 79, 888-897.	1.5	16
99	Evaluation of a Non-Arrhenius Model for Therapeutic Monoclonal Antibody Aggregation. Journal of Pharmaceutical Sciences, 2011, 100, 2526-2542.	1.6	96
100	Aggregation in Protein-Based Biotherapeutics: Computational Studies and Tools to Identify Aggregation-Prone Regions. Journal of Pharmaceutical Sciences, 2011, 100, 5081-5095.	1.6	125
101	The role of nanopore shape in surface-induced crystallization. Nature Materials, 2011, 10, 867-871.	13.3	159
102	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.	1.4	70
103	Design and Application of Antibody Cysteine Variants. Bioconjugate Chemistry, 2010, 21, 385-392.	1.8	37
104	Interaction of Arginine with Proteins and the Mechanism by Which It Inhibits Aggregation. Journal of Physical Chemistry B, 2010, 114, 13426-13438.	1.2	183
105	Prediction of Aggregation Prone Regions of Therapeutic Proteins. Journal of Physical Chemistry B, 2010, 114, 6614-6624.	1.2	187
106	Design of therapeutic proteins with enhanced stability. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11937-11942.	3.3	498
107	Predictive tools for stabilization of therapeutic proteins. MAbs, 2009, 1, 580-582.	2.6	63
108	Mechanisms of Protein Stabilization and Prevention of Protein Aggregation by Glycerol. Biochemistry, 2009, 48, 11084-11096.	1.2	377

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109	Molecular Computations of Preferential Interaction Coefficients of Proteins. Journal of Physical Chemistry B, 2009, 113, 12546-12554.	1.2	79
110	Aggregation-Prone Motifs in Human Immunoglobulin G. Journal of Molecular Biology, 2009, 391, 404-413.	2.0	155
111	Investigation of Cosoluteâ^'Protein Preferential Interaction Coefficients: New Insight into the Mechanism by Which Arginine Inhibits Aggregation. Journal of Physical Chemistry B, 2009, 113, 2050-2058.	1.2	100
112	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, 11743-11753.	1.2	43
113	Dynamic Fluctuations of Protein-Carbohydrate Interactions Promote Protein Aggregation. PLoS ONE, 2009, 4, e8425.	1.1	38
114	Path Sampling Calculation of Methane Diffusivity in Natural Gas Hydrates from a Water-Vacancy Assisted Mechanism. Journal of the American Chemical Society, 2008, 130, 17342-17350.	6.6	124
115	Why Philosophical History is Essential to Teaching the Second Law of Thermodynamics. , 2008, , .		0
116	New Insights on the Nanoparticle Growth Mechanism in the Citrate Reduction of Gold(III) Salt:â€‰ Formation of the Au Nanowire Intermediate and Its Nonlinear Optical Properties. Journal of Physical Chemistry C, 2007, 111, 6281-6287.	1.5	263
117	Interaction of Hydrogen Chloride with Ice Surfaces:â€‰ The Effects of Grain Size, Surface Roughness, and Surface Disorder. Journal of Physical Chemistry A, 2007, 111, 6274-6284.	1.1	53
118	Comparative Oxidation Studies of Methionine Residues Reflect a Structural Effect on Chemical Kinetics in rhG-CSFâ€. Biochemistry, 2006, 45, 15430-15443.	1.2	46
119	Hydrogen chloride-induced surface disordering on ice. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 9422-9427.	3.3	88
120	Effects of Excipients on the Hydrogen Peroxide-Induced Oxidation of Methionine Residues in Granulocyte Colony-Stimulating Factor. Pharmaceutical Research, 2005, 22, 141-147.	1.7	35
121	Role of Arginine in the Stabilization of Proteins against Aggregationâ€. Biochemistry, 2005, 44, 4919-4925.	1.2	223
122	Order Parameter Approach to Understanding and Quantifying the Physico-Chemical Behavior of Complex Systems. , 2005, , 1613-1626.		6
123	Properties of Inhibitors of Methane Hydrate Formation via Molecular Dynamics Simulations. Journal of the American Chemical Society, 2005, 127, 17852-17862.	6.6	244
124	Application of the Cell Potential Method To Predict Phase Equilibria of Multicomponent Gas Hydrate Systems. Journal of Physical Chemistry B, 2005, 109, 8153-8163.	1.2	53
125	Order Parameter Approach to Understanding and Quantifying the Physico-Chemical Behavior of Complex Systems. , 2005, , 1613-1626.		0
126	Lateral interactions between oxygen atoms adsorbed on platinum (111) by first principles. Molecular Physics, 2004, 102, 273-279.	0.8	33

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127	Phase diagram of oxygen adsorbed on platinum (111) by first-principles investigation. Physical Review B, 2004, 70, .	1.1	103
128	Density-functional theory characterization of acid sites in chabazite. Journal of Catalysis, 2004, 227, 77-89.	3.1	68
129	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, 2377-2383.	1.7	39
130	A comprehensive picture of nonâ€site specific oxidation of methionine residues by peroxides in protein pharmaceuticals. Journal of Pharmaceutical Sciences, 2004, 93, 3096-3102.	1.6	54
131	A Structural and Mechanistic Study of the Oxidation of Methionine Residues in hPTH(1â^'34) via Experiments and Simulationsâ€. Biochemistry, 2004, 43, 14139-14148.	1.2	25
132	Molecular Dynamics Simulations and Oxidation Rates of Methionine Residues of Granulocyte Colony-Stimulating Factor at Different pH Values. Biochemistry, 2004, 43, 1019-1029.	1.2	51
133	On the Mechanisms of Oxidation of Organic Sulfides by H2O2in Aqueous Solutions. Journal of the American Chemical Society, 2004, 126, 900-908.	6.6	98
134	Methanol coupling in the zeolite chabazite studied via Carâ€"Parrinello molecular dynamics. Molecular Physics, 2004, 102, 281-288.	0.8	25
135	Chemistry of Sulfur Oxides on Transition Metals. III. Oxidation of SO2and Self-Diffusion of O, SO2, and SO3on Pt(111). Journal of Physical Chemistry B, 2004, 108, 13329-13340.	1.2	40
136	Accurate Potentials for Argonâ^'Water and Methaneâ^'Water Interactions via ab Initio Methods and Their Application to Clathrate Hydrates. Journal of Physical Chemistry B, 2004, 108, 18705-18715.	1.2	76
137	Rational Design of Solution Additives for the Prevention of Protein Aggregation. Biophysical Journal, 2004, 87, 1631-1639.	0.2	99
138	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.	4.4	20
139	Nucleation of Crystalline Phases of Water in Homogeneous and Inhomogeneous Environments. Physical Review Letters, 2003, 90, 158301.	2.9	50
140	Proteins in Mixed Solvents:â€‰ A Molecular-Level Perspective. Journal of Physical Chemistry B, 2003, 107, 14058-14067.	1.2	143
141	Computations of diffusivities in ice and CO2 clathrate hydrates via molecular dynamics and Monte Carlo simulations. Journal of Chemical Physics, 2002, 116, 702-709.	1.2	99
142	Sensitivity Analysis of Hydrate Thermodynamic Reference Properties Using Experimental Data and ab Initio Methods. Journal of Physical Chemistry B, 2002, 106, 7681-7687.	1.2	19
143	A Theoretical Study of the Interaction of HCl with Crystalline NAT. Journal of Physical Chemistry A, 2002, 106, 6972-6981.	1.1	13
144	A new approach for studying nucleation phenomena using molecular simulations: Application to CO2 hydrate clathrates. Journal of Chemical Physics, 2002, 117, 1786-1796.	1.2	268

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145	Molecular Computations Using Robust Hydrocarbonâ"Water Potentials for Predicting Gas Hydrate Phase Equilibria. Journal of Physical Chemistry B, 2001, 105, 10950-10960.	1.2	75
146	Computation of the methaneâ€"water potential energy hypersurface via ab initio methods. Journal of Chemical Physics, 2001, 115, 2550-2559.	1.2	63
147	First-Principles Theoretical Study of Molecular HCl Adsorption on a Hexagonal Ice (0001) Surface. Journal of Physical Chemistry A, 2001, 105, 7037-7046.	1.1	37
148	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.	1.2	32
149	The interaction of HCl with the (0001) face of hexagonal ice studied theoretically via Carâ€"Parrinello molecular dynamics. Chemical Physics Letters, 2001, 348, 285-292.	1.2	51
150	Thermochemistry of gas phase CF2 reactions: A density functional theory study. Journal of Chemical Physics, 2000, 113, 4103-4108.	1.2	30
151	First-principles molecular-dynamics study of surface disordering of the (0001) face of hexagonal ice. Journal of Chemical Physics, 2000, 113, 10733-10743.	1.2	47
152	Configurational Properties of Water Clathrates:â€‰ Monte Carlo and Multidimensional Integration versus the Lennard-Jones and Devonshire Approximation. Journal of Physical Chemistry B, 1999, 103, 6300-6308.	1.2	51