John W Brady

List of Publications by Year
in descending order

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67 papers	7,059 citations	186265 28 h-index	106344 65 g-index
67 all docs	67 docs citations	67 times ranked	8078 citing authors

#	Article	IF	Citations
1	Biomass Recalcitrance: Engineering Plants and Enzymes for Biofuels Production. Science, 2007, 315, 804-807.	12.6	3,749
2	Additive empirical force field for hexopyranose monosaccharides. Journal of Computational Chemistry, 2008, 29, 2543-2564.	3.3	483
3	Computer simulation studies of microcrystalline cellulose Iî². Carbohydrate Research, 2006, 341, 138-152.	2.3	357
4	A revised potential-energy surface for molecular mechanics studies of carbohydrates. Carbohydrate Research, 1988, 180, 207-221.	2.3	294
5	The Structure of Aqueous Guanidinium Chloride Solutions. Journal of the American Chemical Society, 2004, 126, 11462-11470.	13.7	245
6	Simulation studies of the insolubility of cellulose. Carbohydrate Research, 2010, 345, 2060-2066.	2.3	166
7	High-Temperature Behavior of Cellulose I. Journal of Physical Chemistry B, 2011, 115, 2155-2166.	2.6	121
8	Comparison of Cellulose Iî² Simulations with Three Carbohydrate Force Fields. Journal of Chemical Theory and Computation, 2012, 8, 735-748.	5.3	113
9	The O-Glycosylated Linker from the Trichoderma reesei Family 7 Cellulase Is a Flexible, Disordered Protein. Biophysical Journal, 2010, 99, 3773-3781.	0.5	96
10	The Interaction of Guanidinium Ions with a Model Peptide. Biophysical Journal, 2007, 93, L04-L06.	0.5	86
11	Molecular modeling suggests induced fit of Family I carbohydrate-binding modules with a broken-chain cellulose surface. Protein Engineering, Design and Selection, 2007, 20, 179-187.	2.1	79
12	Molecular Dynamics Simulation Studies of Caffeine Aggregation in Aqueous Solution. Journal of Physical Chemistry B, 2011, 115, 10957-10966.	2.6	79
13	Preferential Interactions of Guanidinum Ions with Aromatic Groups over Aliphatic Groups. Journal of the American Chemical Society, 2009, 131, 16689-16696.	13.7	70
14	Specificity of Ionâ^'Protein Interactions: Complementary and Competitive Effects of Tetrapropylammonium, Guanidinium, Sulfate, and Chloride Ions. Journal of Physical Chemistry B, 2009, 113, 3227-3234.	2.6	66
15	Molecular Dynamics Simulations of the Ionic Liquid 1-n-Butyl-3-Methylimidazolium Chloride and Its Binary Mixtures with Ethanol. Journal of Chemical Theory and Computation, 2014, 10, 4465-4479.	5.3	50
16	Configuration entropy of the alanine dipeptide in vacuum and in solution: a molecular dynamics study. Journal of the American Chemical Society, 1985, 107, 6103-6105.	13.7	49
17	Computational simulations of the Trichoderma reesei cellobiohydrolase I acting on microcrystalline cellulose Iî²: the enzymeâ€“substrate complex. Carbohydrate Research, 2009, 344, 1984-1992.	2.3	49
18	Classical dynamics study of intramolecular energy flow in benzene. Journal of Chemical Physics, 1986, 85, 1848-1853.	3.0	48

#	Article	IF	Citations
19	Intramolecular vibrational relaxation of CH stretch overtones in benzene. Journal of Chemical Physics, 1987, 86, 4411-4417.	3.0	46
20	Interactions of the complete cellobiohydrolase I from Trichodera reesei with microcrystalline cellulose Iˆ2. Cellulose, 2008, 15, 261-273.	4.9	46
21	Caffeine and Sugars Interact in Aqueous Solutions: A Simulation and NMR Study. Journal of Physical Chemistry B, 2012, 116, 11701-11711.	2.6	46
22	Concentration enrichment of urea at cellulose surfaces: results from molecular dynamics simulations and NMR spectroscopy. Cellulose, 2012, 19, 1-12.	4.9	38
23	Molecular Dynamics and Neutron Scattering Study of Glucose Solutions Confined in MCM-41. Journal of Physical Chemistry B, 2011, 115, 910-918.	2.6	37
24	Cel48A from Thermobifida fusca: Structure and site directed mutagenesis of key residues. Biotechnology and Bioengineering, 2014, 111, 664-673.	3.3	35
25	Neutron diffraction and simulation studies of the exocyclic hydroxymethyl conformation of glucose. Journal of Chemical Physics, 2006, 125, 224505.	3.0	34
26	Water Confined in Cylindrical Pores: A Molecular Dynamics Study. Food Biophysics, 2011, 6, 233-240.	3.0	33
27	Neutron Diffraction and Simulation Studies of CsNO3and Cs2CO3Solutions. Journal of the American Chemical Society, 2006, 128, 15136-15144.	13.7	30
28	Ligand binding to G-quadruplex DNA: new insights from ultraviolet resonance Raman spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 8128-8140.	2.8	29
29	Water Structuring over the Hydrophobic Surface of Cellulose. Journal of Agricultural and Food Chemistry, 2014, 62, 11017-11023.	5.2	28
30	Glucose interactions with a model peptide. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2224-2232.	2.6	25
31	Free energy surfaces for the interaction of D-glucose with planar aromatic groups in aqueous solution. Journal of Chemical Physics, 2010, 133, 155103.	3.0	24
32	Sugar-binding sites on the surface of the carbohydrate-binding module of CBH I from Trichoderma reesei. Carbohydrate Research, 2011, 346, 839-846.	2.3	24
33	Binding of an antifreeze polypeptide to an ice/water interface via computer simulation. AICHE Journal, 1995, 41, 959-973.	3.6	23
34	Molecular Dynamics Simulation and NMR Study of Aqueous Neocarrabiose 4-Sulfate, a Building Block of Îº-Carrageenan. Journal of Physical Chemistry B, 2001, 105, 8629-8638.	2.6	22
35	Observation of Pyridine Aggregation in Aqueous Solution Using Neutron Scattering Experiments and MD Simulations. Journal of Physical Chemistry B, 2010, 114, 5412-5419.	2.6	22
36	Molecular dynamics simulations of a winter flounder ?antifreeze? polypeptide in aqueous solution. Biopolymers, 1993, 33, 1481-1503.	2.4	20

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37	Stacking and Branching in Self-Aggregation of Caffeine in Aqueous Solution: From the Supramolecular to Atomic Scale Clustering. Journal of Physical Chemistry B, 2016, 120, 9987-9996.	2.6	20
38	Molecular Mechanics Studies of Cellulases. ACS Symposium Series, 2000, , 112-130.	0.5	18
39	The conformational free-energy map for solvated neocarrabiose. Carbohydrate Research, 2004, 339, 1953-1960.	2.3	18
40	Interâ€residual Hydrogen Bonding in Carbohydrates Unraveled by NMR Spectroscopy and Molecular Dynamics Simulations. ChemBioChem, 2019, 20, 2519-2528.	2.6	18
41	Structures of Plant Cell Wall Celluloses. , 0, , 188-212.		17
42	Weakly hydrated surfaces and the binding interactions of small biological solutes. European Biophysics Journal, 2012, 41, 369-377.	2.2	16
43	Molecular dynamics simulations of the interaction of glucose with imidazole in aqueous solution. Carbohydrate Research, 2012, 349, 73-77.	2.3	16
44	Crowding and conformation interplay on human DNA G-quadruplex by ultraviolet resonant Raman scattering. Physical Chemistry Chemical Physics, 2019, 21, 2093-2101.	2.8	15
45	Neutron Diffraction and Computer Simulation Studies ofd-Xylose. Journal of the American Chemical Society, 2005, 127, 10991-10998.	13.7	14
46	Determination of a Hydroxyl Conformation in Aqueous Xylose Using Neutron Scattering and Molecular Dynamics. Journal of Physical Chemistry B, 2006, 110, 2981-2983.	2.6	13
47	Comparison of the simulations of cellulosic crystals with three carbohydrate force fields. Carbohydrate Research, 2016, 422, 17-23.	2.3	12
48	The polysaccharide extracted from the biofilm of Burkholderia multivorans strain C1576 binds hydrophobic species and exhibits a compact 3D-structure. International Journal of Biological Macromolecules, 2019, 136, 944-950.	7.5	11
49	Burkholderia cenocepacia H111 Produces a Water-Insoluble Exopolysaccharide in Biofilm: Structural Determination and Molecular Modelling. International Journal of Molecular Sciences, 2020, 21, 1702.	4.1	11
50	The Interaction of Sorbitol with Caffeine in Aqueous Solution. Food Biophysics, 2013, 8, 216-222.	3.0	10
51	Strategies to reduce endâ€product inhibition in family 48 glycoside hydrolases. Proteins: Structure, Function and Bioinformatics, 2016, 84, 295-304.	2.6	10
52	Water structuring above solutes with planar hydrophobic surfaces. Physical Chemistry Chemical Physics, 2017, 19, 11851-11863.	2.8	9
53	Simulation and Neutron Diffraction Studies of Small Biomolecules in Water. Food Biophysics, 2011, 6, 210-216.	3.0	7
54	Natural diversity of glycoside hydrolase family 48 exoglucanases: insights from structure. Biotechnology for Biofuels, 2017, 10, 274.	6.2	7

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55	Aromatic residues surrounding the active site tunnel of TfCel48A influence activity, processivity, and synergistic interactions with other cellulases. Biotechnology and Bioengineering, 2019, 116, 2463-2472.	3.3	7
56	Molecular Dynamics and Neutron Scattering Studies of Potassium Chloride in Aqueous Solution. Journal of Physical Chemistry B, 2019, 123, 10807-10813.	2.6	7
57	Myelography Iodinated Contrast Media. I. Unraveling the Atropisomerism Properties in Solution. Molecular Pharmaceutics, 2015, 12, 1939-1950.	4.6	6
58	Free energy landscapes of the Î±-<scp>d</scp>- and Î²-<scp>d</scp>-glucopyranose conformations in both vacuum and aqueous solution. Molecular Simulation, 2012, 38, 1186-1197.	2.0	5
59	Molecular Dynamics and Neutron Scattering Studies of Mixed Solutions of Caffeine and Pyridine in Water. Journal of Physical Chemistry B, 2018, 122, 5308-5315.	2.6	5
60	Ramachandran conformational energy maps for disaccharide linkages found in Burkholderia multivorans biofilm polysaccharides. International Journal of Biological Macromolecules, 2020, 143, 501-509.	7.5	5
61	The biofilm of Burkholderia cenocepacia H111 contains an exopolysaccharide composed of l-rhamnose and l-mannose: Structural characterization and molecular modelling. Carbohydrate Research, 2021, 499, 108231.	2.3	5
62	Overview of Computer Modeling of Cellulose. Methods in Molecular Biology, 2012, 908, 11-22.	0.9	4
63	The Conformation of a Ribose Derivative in Aqueous Solution: A Neutronâ€Scattering and Molecular Dynamics Study. Biopolymers, 2013, 99, 739-745.	2.4	4
64	Physico-chemical properties of aqueous drug solutions: From the basic thermodynamics to the advanced experimental and simulation results. International Journal of Pharmaceutics, 2018, 540, 65-77.	5.2	3
65	Simulation studies of substrate recognition by the exocellulase CelF from Clostridium cellulolyticum. Biotechnology and Bioengineering, 2016, 113, 1433-1440.	3.3	2
66	The Determination of Specific Ion Structure by Neutron Scattering and Computer Simulation. , 2009, , 171-189.		1
67	Frontiers in Water Biophysics: Water Interaction with Biomolecules. Food Biophysics, 2013, 8, 151-152.	3.0	1