

Brian R Novak

List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	Complexation of Lignin Dimers with β -Cyclodextrin and Binding Stability Analysis by ESI-MS, Isothermal Titration Calorimetry, and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1655-1667.	1.2	2
2	Unraveling the Role of Charge Patterning in the Micellar Structure of Sequence-Defined Amphiphilic Peptoid Oligomers by Molecular Dynamics Simulations. <i>Macromolecules</i> , 2022, 55, 5197-5212.	2.2	8
3	Single Nucleotides Moving through Nanoslits Composed of Self-Assembled Monolayers via Equilibrium and Nonequilibrium Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1259-1270.	1.2	2
4	Molecular dynamics simulation study of the positioning and dynamics of α -tocopherol in phospholipid bilayers. <i>European Biophysics Journal</i> , 2021, 50, 889-903.	1.2	5
5	Quantitative prediction of rapid solidification by integrated atomistic and phase-field modeling. <i>Acta Materialia</i> , 2021, 211, 116885.	3.8	10
6	Interaction of lignin dimers with model cell membranes: A quartz crystal microbalance and molecular dynamics simulation study. <i>Biointerphases</i> , 2021, 16, 041003.	0.6	3
7	Modified embedded-atom method potential for high-temperature crystal-melt properties of Ti-Ni alloys and its application to phase field simulation of solidification. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2020, 28, 015006.	0.8	24
8	Interface kinetics of rapid solidification of binary alloys by atomistic simulations: Application to Ti-Ni alloys. <i>Computational Materials Science</i> , 2020, 184, 109854.	1.4	24
9	Rapid microwave-assisted biomass delignification and lignin depolymerization in deep eutectic solvents. <i>Energy Conversion and Management</i> , 2019, 196, 1080-1088.	4.4	117
10	Experimental and Molecular Dynamics Simulation Study of the Effects of Lignin Dimers on the Gel-to-Fluid Phase Transition in DPPC Bilayers. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8247-8260.	1.2	13
11	Combined molecular dynamics and phase field simulation investigations of crystal-melt interfacial properties and dendritic solidification of highly undercooled titanium. <i>Computational Materials Science</i> , 2019, 163, 218-229.	1.4	32
12	Identifying structural changes with unsupervised machine learning methods. <i>Physical Review E</i> , 2018, 98, .	0.8	12
13	The role of the asymmetric bolaamphiphilic character of VECAR on the kinetic and structural aspects of its self-assembly: A molecular dynamics simulation study. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2017, 523, 9-18.	2.3	3
14	Electrophoretic Transport of Single DNA Nucleotides through Nanoslits: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11443-11458.	1.2	10
15	Distinguishing Single DNA Nucleotides Based on Their Times of Flight Through Nanoslits: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3271-3279.	1.2	13
16	Multi-species Fluid Flow Simulations Using a Hybrid Computational Fluid Dynamics - Molecular Dynamics Approach. , 2012, , .		1
17	Molecular Dynamics Simulation Study of the Effect of DMSO on Structural and Permeation Properties of DMPC Lipid Bilayers. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1299-1308.	1.2	27
18	Behavior of the ATP grasp domain of biotin carboxylase monomers and dimers studied using molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 622-632.	1.5	5

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19	Umbrella Sampling Simulations of Biotin Carboxylase: Is a Structure with an Open ATP Grasp Domain Stable in Solution?. Journal of Physical Chemistry B, 2009, 113, 10097-10103.	1.2	6
20	An Atomistic Simulation Study of the Role of Asperities and Indentations on Heterogeneous Bubble Nucleation. Journal of Heat Transfer, 2008, 130, .	1.2	25
21	Comparison of heterogeneous and homogeneous bubble nucleation using molecular simulations. Physical Review B, 2007, 75, .	1.1	58
22	Title is missing!. Journal of Sol-Gel Science and Technology, 2002, 23, 215-220.	1.1	14
23	Electrochemiluminescence of Ruthenium(II) Tris(bipyridine) Encapsulated in Solâˆ“Gel Glasses. Analytical Chemistry, 2000, 72, 2914-2918.	3.2	116