Karteek K Bejagam

List of Publications by Year
in descending order

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30 papers	1,050 citations	394421 19 h-index	434195 31 g-index
31 all docs	31 docs citations	31 times ranked	1314 citing authors

#	Article	IF	Citations
1	Durable and highly selective ion transport of a sulfonated Diels Alder Poly(phenylene) for vanadium redox flow batteries. Journal of Power Sources, 2022, 520, 230805.	7.8	9
2	Predicting the Mechanical Response of Polyhydroxyalkanoate Biopolymers Using Molecular Dynamics Simulations. Polymers, 2022, 14, 345.	4.5	7
3	Machine Learning for Melting Temperature Predictions and Design in Polyhydroxyalkanoate-Based Biopolymers. Journal of Physical Chemistry B, 2022, 126, 934-945.	2.6	15
4	Composition and Configuration Dependence of Glass-Transition Temperature in Binary Copolymers and Blends of Polyhydroxyalkanoate Biopolymers. Macromolecules, 2021, 54, 5618-5628.	4.8	11
5	Dehydration of polymer chains initiates graphene folding in water. Carbon, 2021, 180, 244-253.	10.3	5
6	Molecular dynamics simulations for glass transition temperature predictions of polyhydroxyalkanoate biopolymers. Physical Chemistry Chemical Physics, 2020, 22, 17880-17889.	2.8	19
7	Development of transferable coarse-grained models of amino acids. Molecular Systems Design and Engineering, 2020, 5, 675-685.	3.4	16
8	Solvation dynamics of N-substituted acrylamide polymers and the importance for phase transition behavior. Soft Matter, 2020, 16, 1582-1593.	2.7	20
9	Development of an Accurate Coarse-Grained Model of Poly(acrylic acid) in Explicit Solvents. Macromolecules, 2019, 52, 4875-4887.	4.8	21
10	Machine-Learning Based Stacked Ensemble Model for Accurate Analysis of Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2019, 123, 5190-5198.	2.5	26
11	Development of non-bonded interaction parameters between hexagonal boron-nitride and water. Computational Materials Science, 2019, 161, 339-345.	3.0	10
12	Unraveling the Conformations of Backbone and Side Chains in Thermosensitive Bottlebrush Polymers. Macromolecules, 2019, 52, 9398-9408.	4.8	28
13	Development of Transferable Nonbonded Interactions between Coarse-Grained Hydrocarbon and Water Models. Journal of Physical Chemistry B, 2019, 123, 909-921.	2.6	12
14	Biomimetic temporal self-assembly via fuel-driven controlled supramolecular polymerization. Nature Communications, 2018, 9, 1295.	12.8	148
15	PSO-Assisted Development of New Transferable Coarse-Grained Water Models. Journal of Physical Chemistry B, 2018, 122, 1958-1971.	2.6	39
16	Development of nonâ€bonded interaction parameters between graphene and water using particle swarm optimization. Journal of Computational Chemistry, 2018, 39, 721-734.	3.3	18
17	Nanoparticle activated and directed assembly of graphene into a nanoscroll. Carbon, 2018, 134, 43-52.	10.3	29
18	Machine-Learning Enabled New Insights into the Coil-to-Globule Transition of Thermosensitive Polymers Using a Coarse-Grained Model. Journal of Physical Chemistry Letters, 2018, 9, 6480-6488.	4.6	34

#	Article	IF	Citations
19	Machine-Learned Coarse-Grained Models. Journal of Physical Chemistry Letters, 2018, 9, 4667-4672.	4.6	48
20	Development of New Transferable Coarse-Grained Models of Hydrocarbons. Journal of Physical Chemistry B, 2018, 122, 7143-7153.	2.6	28
21	Solvent Clathrate Driven Dynamic Stereomutation of a Supramolecular Polymer with Molecular Pockets. Journal of the American Chemical Society, 2017, 139, 13867-13875.	13.7	86
22	Supramolecular Polymerization of N,Nâ€²,Nâ€³,Nâ€´-tetra-(Tetradecyl)-1,3,6,8-pyrenetetracarboxamide: A Computational Study. Journal of Physical Chemistry B, 2017, 121, 11492-11503.	2.6	10
23	Understanding the self-assembly of amino ester-based benzene-1,3,5-tricarboxamides using molecular dynamics simulations. Physical Chemistry Chemical Physics, 2017, 19, 258-266.	2.8	11
24	Hostâ€“Guest [2+2] Cycloaddition Reaction: Postsynthetic Modulation of CO₂ Selectivity and Magnetic Properties in a Bimodal Metalâ€“Organic Framework. Chemistry - A European Journal, 2016, 22, 7792-7799.	3.3	30
25	Autoresolution of Segregated and Mixed pâ€n Stacks by Stereoselective Supramolecular Polymerization in Solution. Angewandte Chemie - International Edition, 2015, 54, 13053-13057.	13.8	61
26	Dissolution of Cellulose in Room Temperature Ionic Liquids: Anion Dependence. Journal of Physical Chemistry B, 2015, 119, 1654-1659.	2.6	44
27	Supramolecular Polymerization: A Coarse Grained Molecular Dynamics Study. Journal of Physical Chemistry B, 2015, 119, 5738-5746.	2.6	38
28	Dipole-Moment-Driven Cooperative Supramolecular Polymerization. Journal of the American Chemical Society, 2015, 137, 3924-3932.	13.7	115
29	External electric field reverses helical handedness of a supramolecular columnar stack. Chemical Communications, 2015, 51, 16049-16052.	4.1	22
30	Supramolecular Polymerization of Benzene-1,3,5-tricarboxamide: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 5218-5228.	2.6	61