Christine Peter

List of Publications by Year
in descending order

51 papers	1,621 citations	331670 21 h-index	302126 39 g-index
54 all docs	54 docs citations	54 times ranked	1825 citing authors

#	Article	IF	Citations
1	Multiscale simulation of soft matter systems â€“ from the atomistic to the coarse-grained level and back. Soft Matter, 2009, 5, 4357.	2.7	397
2	Machine Learning Force Fields and Coarse-Grained Variables in Molecular Dynamics: Application to Materials and Biological Systems. Journal of Chemical Theory and Computation, 2020, 16, 4757-4775.	5.3	120
3	Computer Simulations of Soft Matter: Linking the Scales. Entropy, 2014, 16, 4199-4245.	2.2	89
4	Self-assembling dipeptides: conformational sampling in solvent-free coarse-grained simulation. Physical Chemistry Chemical Physics, 2009, 11, 2077.	2.8	79
5	EncoderMap: Dimensionality Reduction and Generation of Molecule Conformations. Journal of Chemical Theory and Computation, 2019, 15, 1209-1215.	5.3	72
6	Transferability of Nonbonded Interaction Potentials for Coarse-Grained Simulations: Benzene in Water. Journal of Chemical Theory and Computation, 2010, 6, 2434-2444.	5.3	66
7	Derivation of Coarse Grained Models for Multiscale Simulation of Liquid Crystalline Phase Transitions. Journal of Physical Chemistry B, 2012, 116, 8474-8484.	2.6	63
8	Optimization of an Elastic Network Augmented Coarse Grained Model to Study CCMV Capsid Deformation. PLoS ONE, 2013, 8, e60582.	2.5	45
9	Interaction of Charged Amino-Acid Side Chains with Ions: An Optimization Strategy for Classical Force Fields. Journal of Physical Chemistry B, 2014, 118, 3960-3972.	2.6	41
10	EPR Distance Measurements in Native Proteins with Genetically Encoded Spin Labels. ACS Chemical Biology, 2015, 10, 2764-2771.	3.4	39
11	Neural Network Based Prediction of Conformational Free Energies - A New Route toward Coarse-Grained Simulation Models. Journal of Chemical Theory and Computation, 2017, 13, 6213-6221.	5.3	36
12	Evaluation and Optimization of Interface Force Fields for Water on Gold Surfaces. Journal of Chemical Theory and Computation, 2017, 13, 5610-5623.	5.3	34
13	Tipping the Scale from Disorder to Alpha-helix: Folding of Amphiphilic Peptides in the Presence of Macroscopic and Molecular Interfaces. PLoS Computational Biology, 2015, 11, e1004328.	3.2	33
14	Using Dimensionality Reduction to Systematically Expand Conformational Sampling of Intrinsically Disordered Peptides. Journal of Chemical Theory and Computation, 2016, 12, 4726-4734.	5.3	32
15	A transferable coarse-grained model for diphenylalanine: How to represent an environment driven conformational transition. Journal of Chemical Physics, 2013, 139, 234115.	3.0	30
16	Multiscale simulation of small peptides: Consistent conformational sampling in atomistic and coarseâ€grained models. Journal of Computational Chemistry, 2012, 33, 937-949.	3.3	28
17	A Challenge for Peptide Coarse Graining: Transferability of Fragmentâ€Based Models. Macromolecular Theory and Simulations, 2011, 20, 451-465.	1.4	27
18	Towards a molecular basis of ubiquitin signaling: A dual-scale simulation study of ubiquitin dimers. PLoS Computational Biology, 2018, 14, e1006589.	3.2	26

#	Article	IF	Citations
19	Multivalent contacts of the Hsp70 Ssb contribute to its architecture on ribosomes and nascent chain interaction. Nature Communications, 2016, 7, 13695.	12.8	25
20	The structure of the ubiquitin-like modifier FAT10 reveals an alternative targeting mechanism for proteasomal degradation. Nature Communications, 2018, 9, 3321.	12.8	25
21	Sticky water surfaces: Helixâ€“coil transitions suppressed in a cell-penetrating peptide at the air-water interface. Journal of Chemical Physics, 2014, 141, 22D517.	3.0	24
22	Snapshots of a modified nucleotide moving through the confines of a DNA polymerase. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9992-9997.	7.1	23
23	Coarse-Grained and Atomistic Simulations of the Salt-Stable Cowpea Chlorotic Mottle Virus (SS-CCMV) Subunit 26â€“49: Î²-Barrel Stability of the Hexamer and Pentamer Geometries. Journal of Chemical Theory and Computation, 2012, 8, 3750-3758.	5.3	22
24	Titin kinase ubiquitination aligns autophagy receptors with mechanical signals in the sarcomere. EMBO Reports, 2021, 22, e48018.	4.5	22
25	Molecular Dynamics Simulations of Peptides at the Airâ€“Water Interface: Influencing Factors on Peptide-Templated Mineralization. Langmuir, 2014, 30, 15486-15495.	3.5	17
26	Simulating and analysing configurational landscapes of proteinâ€“protein contact formation. Interface Focus, 2019, 9, 20180062.	3.0	17
27	Three Reasons Why Aspartic Acid and Glutamic Acid Sequences Have a Surprisingly Different Influence on Mineralization. Journal of Physical Chemistry B, 2021, 125, 10335-10343.	2.6	17
28	Back-mapping based sampling: Coarse grained free energy landscapes as a guideline for atomistic exploration. Journal of Chemical Physics, 2019, 151, 154102.	3.0	14
29	A Ligand Selection Strategy Identifies Chemical Probes Targeting the Proteases of SARSâ€CoVâ€2. Angewandte Chemie - International Edition, 2021, 60, 6799-6806.	13.8	14
30	EncoderMap(II): Visualizing Important Molecular Motions with Improved Generation of Protein Conformations. Journal of Chemical Information and Modeling, 2019, 59, 4550-4560.	5.4	13
31	The Role of Conserved Residues in the DEDDh Motif: the Proton-Transfer Mechanism of HIV-1 RNase H. ACS Catalysis, 2021, 11, 7915-7927.	11.2	11
32	Efficient Sampling and Characterization of Free Energy Landscapes of Ionâ€“Peptide Systems. Journal of Chemical Theory and Computation, 2018, 14, 5476-5488.	5.3	10
33	Coarse-Grained Simulations of Peptide Nanoparticle Formation: Role of Local Structure and Nonbonded Interactions. Journal of Chemical Theory and Computation, 2019, 15, 1453-1462.	5.3	10
34	Relative resolution: A hybrid formalism for fluid mixtures. Journal of Chemical Physics, 2015, 143, 243107.	3.0	9
35	Molecular simulation of oligo-glutamates in a calcium-rich aqueous solution: insights into peptide-induced polymorph selection. CrystEngComm, 2015, 17, 6863-6867.	2.6	9
36	Machine Learning Driven Analysis of Large Scale Simulations Reveals Conformational Characteristics of Ubiquitin Chains. Journal of Chemical Theory and Computation, 2020, 16, 3205-3220.	5.3	9

#	Article	IF	Citations
37	Single molecule translocation in smectics illustrates the challenge for time-mapping in simulations on multiple scales. Journal of Chemical Physics, 2017, 147, 114501.	3.0	8
38	Representing environment-induced helix-coil transitions in a coarse grained peptide model. European Physical Journal: Special Topics, 2016, 225, 1463-1481.	2.6	7
39	Soluble Oligomeric Nucleants: Simulations of Chain Length, Binding Strength, and Volume Fraction Effects. Journal of Physical Chemistry Letters, 2017, 8, 5815-5820.	4.6	7
40	Conformational and functional characterization of artificially conjugated non-canonical ubiquitin dimers. Scientific Reports, 2019, 9, 19991.	3.3	7
41	Coarse-Grained Simulation of CaCO3 Aggregation and Crystallization Made Possible by Nonbonded Three-Body Interactions. Journal of Physical Chemistry C, 2019, 123, 3152-3160.	3.1	7
42	Combining Experimental and Simulation Techniques to Understand Morphology Control in Pentapeptide Nanostructures. Journal of Physical Chemistry B, 2017, 121, 8155-8161.	2.6	6
43	Guanidine-II aptamer conformations and ligand binding modes through the lens of molecular simulation. Nucleic Acids Research, 2021, 49, 7954-7965.	14.5	6
44	Deciphering molecular details of the RACâ€“ribosome interaction by EPR spectroscopy. Scientific Reports, 2021, 11, 8681.	3.3	5
45	Multiscale simulations of protein and membrane systems. Current Opinion in Structural Biology, 2022, 72, 203-208.	5.7	5
46	Anisotropic Extended-Chain Polymer Nanocrystals. Macromolecules, 2019, 52, 6142-6148.	4.8	4
47	Coarse-Grained Simulation of the Adsorption of Water on Au(111) Surfaces Using a Modified Stillingerâ€“Weber Potential. ACS Omega, 2020, 5, 31055-31059.	3.5	3
48	Coarse grained simulation of the aggregation and structure control of polyethylene nanocrystals. Journal of Physics Condensed Matter, 2021, 33, 264001.	1.8	2
49	Relative Resolution: A multipole approximation at appropriate distances. Physical Review Research, 2019, 1, .	3.6	2
50	Solvent-mediated isotope effects strongly influence the early stages of calcium carbonate formation: exploring D₂O vs. H₂O in a combined computational and experimental approach. Faraday Discussions, 2022, 235, 36-55.	3.2	1
51	Editorial overview: Theory and simulation: Progress, yes; revolutions, no. Current Opinion in Structural Biology, 2020, 61, iii-v.	5.7	0