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	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
2	Multiscale simulations of protein and membrane systems. Current Opinion in Structural Biology, 2022, 72, 203-208.	5.7	5
3	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
4	Deciphering molecular details of the RACâ€“ribosome interaction by EPR spectroscopy. Scientific Reports, 2021, 11, 8681.	3.3	5
5	Coarse grained simulation of the aggregation and structure control of polyethylene nanocrystals. Journal of Physics Condensed Matter, 2021, 33, 264001.	1.8	2
6	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
7	Guanidine-II aptamer conformations and ligand binding modes through the lens of molecular simulation. Nucleic Acids Research, 2021, 49, 7954-7965.	14.5	6
8	Titin kinase ubiquitination aligns autophagy receptors with mechanical signals in the sarcomere. EMBO Reports, 2021, 22, e48018.	4.5	22
9	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
10	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
11	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
12	Editorial overview: Theory and simulation: Progress, yes; revolutions, no. Current Opinion in Structural Biology, 2020, 61, iii-v.	5.7	0
13	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
14	Anisotropic Extended-Chain Polymer Nanocrystals. Macromolecules, 2019, 52, 6142-6148.	4.8	4
15	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
16	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
17	Simulating and analysing configurational landscapes of proteinâ€“protein contact formation. Interface Focus, 2019, 9, 20180062.	3.0	17
18	Conformational and functional characterization of artificially conjugated non-canonical ubiquitin dimers. Scientific Reports, 2019, 9, 19991.	3.3	7

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19	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
20	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
21	EncoderMap: Dimensionality Reduction and Generation of Molecule Conformations. Journal of Chemical Theory and Computation, 2019, 15, 1209-1215.	5.3	72
22	Relative Resolution: A multipole approximation at appropriate distances. Physical Review Research, 2019, 1, .	3.6	2
23	Towards a molecular basis of ubiquitin signaling: A dual-scale simulation study of ubiquitin dimers. PLoS Computational Biology, 2018, 14, e1006589.	3.2	26
24	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
25	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
26	The structure of the ubiquitin-like modifier FAT10 reveals an alternative targeting mechanism for proteasomal degradation. Nature Communications, 2018, 9, 3321.	12.8	25
27	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
28	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
29	Combining Experimental and Simulation Techniques to Understand Morphology Control in Pentapeptide Nanostructures. Journal of Physical Chemistry B, 2017, 121, 8155-8161.	2.6	6
30	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
31	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
32	Multivalent contacts of the Hsp70 Ssb contribute to its architecture on ribosomes and nascent chain interaction. Nature Communications, 2016, 7, 13695.	12.8	25
33	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
34	Representing environment-induced helix-coil transitions in a coarse grained peptide model. European Physical Journal: Special Topics, 2016, 225, 1463-1481.	2.6	7
35	EPR Distance Measurements in Native Proteins with Genetically Encoded Spin Labels. ACS Chemical Biology, 2015, 10, 2764-2771.	3.4	39
36	Relative resolution: A hybrid formalism for fluid mixtures. Journal of Chemical Physics, 2015, 143, 243107.	3.0	9

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37	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
38	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
39	Molecular Dynamics Simulations of Peptides at the Airâ€“Water Interface: Influencing Factors on Peptide-Templated Mineralization. Langmuir, 2014, 30, 15486-15495.	3.5	17
40	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
41	Computer Simulations of Soft Matter: Linking the Scales. Entropy, 2014, 16, 4199-4245.	2.2	89
42	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
43	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
44	Optimization of an Elastic Network Augmented Coarse Grained Model to Study CCMV Capsid Deformation. PLoS ONE, 2013, 8, e60582.	2.5	45
45	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
46	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
47	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
48	A Challenge for Peptide Coarse Graining: Transferability of Fragmentâ€Based Models. Macromolecular Theory and Simulations, 2011, 20, 451-465.	1.4	27
49	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
50	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
51	Self-assembling dipeptides: conformational sampling in solvent-free coarse-grained simulation. Physical Chemistry Chemical Physics, 2009, 11, 2077.	2.8	79