Lars V SchÃ¤fer

List of Publications by Year
in descending order

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85	5,678	126907	85541
papers	citations	33 h-index	71 g-index

87	87	87	6825
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Remotely controllable supramolecular rotor mounted inside a porphyrinic cage. CheM, 2022, 8, 543-556.	11.7	24
2	Accurate evaluation of combustion enthalpy by ab-initio computations. Scientific Reports, 2022, 12, 5834.	3.3	3
3	How Much Entropy Is Contained in NMR Relaxation Parameters?. Journal of Physical Chemistry B, 2022, 126, 54-68.	2.6	17
4	VCD spectroscopy reveals conformational changes of chiral crown ethers upon complexation of potassium and ammonium cations. Physical Chemistry Chemical Physics, 2022, 24, 11721-11728.	2.8	8
5	Spatially Resolved Hydration Thermodynamics in Biomolecular Systems. Journal of Physical Chemistry B, 2022, 126, 3619-3631.	2.6	10
6	Protein flexibility reduces solvent-mediated friction barriers of ligand binding to a hydrophobic surface patch. Physical Chemistry Chemical Physics, 2021, 23, 5665-5672.	2.8	3
7	Atomistic Dynamics of Alternating Access Mechanism of an ABC Transporter. , 2021, , 117-124.		0
8	Spectrally Resolved Estimation of Water Entropy in the Active Site of Human Carbonic Anhydrase II. Journal of Chemical Theory and Computation, 2021, 17, 5409-5418.	5.3	5
9	The CTPase activity of ParB determines the size and dynamics of prokaryotic DNA partition complexes. Molecular Cell, 2021, 81, 3992-4007.e10.	9.7	37
10	Thermodynamic driving forces of guest confinement in a photoswitchable cage. Physical Chemistry Chemical Physics, 2021, 23, 7321-7332.	2.8	15
11	Conformational Preferences of an Intrinsically Disordered Protein Domain: A Case Study for Modern Force Fields. Journal of Physical Chemistry B, 2021, 125, 24-35.	2.6	23
12	Protein Motional Details Revealed by Complementary Structural Biology Techniques. Structure, 2020, 28, 1024-1034.e3.	3.3	11
13	Atomistic Movie of Substrate Transport in an ABC Exporter. Biophysical Journal, 2020, 118, 444a.	0.5	0
14	Atomistic structure and dynamics of the human MHC-I peptide-loading complex. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 20597-20606.	7.1	40
15	The Active Site of a Prototypical â€œRigidâ€•Drug Target is Marked by Extensive Conformational Dynamics. Angewandte Chemie - International Edition, 2020, 59, 22916-22921.	13.8	17
16	The Active Site of a Prototypical â€œRigidâ€•Drug Target is Marked by Extensive Conformational Dynamics. Angewandte Chemie, 2020, 132, 23116-23121.	2.0	2
17	Frontispiz: The Active Site of a Prototypical â€œRigidâ€•Drug Target is Marked by Extensive Conformational Dynamics. Angewandte Chemie, 2020, 132, .	2.0	0
18	Frontispiece: The Active Site of a Prototypical â€œRigidâ€•Drug Target is Marked by Extensive Conformational Dynamics. Angewandte Chemie - International Edition, 2020, 59, .	13.8	0

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19	Capturing the Flexibility of a Proteinâ€“Ligand Complex: Binding Free Energies from Different Enhanced Sampling Techniques. Journal of Chemical Theory and Computation, 2020, 16, 4615-4630.	5.3	15
20	Capturing Substrate Translocation in an ABC Exporter at the Atomic Level. Journal of the American Chemical Society, 2020, 142, 12791-12801.	13.7	22
21	Predicting NMR relaxation of proteins from molecular dynamics simulations with accurate methyl rotation barriers. Journal of Chemical Physics, 2020, 152, 084102.	3.0	22
22	Partial Dissociation of Antigenic Peptides from MHC I or How To Deal with Conflicting Results from Different Enhanced Sampling Methods?. Biophysical Journal, 2020, 118, 519a.	0.5	0
23	Î±-Aminoisobutyric Acid-Stabilized Peptide SAMs with Low Nonspecific Protein Adsorption and Resistance against Marine Biofouling. ACS Sustainable Chemistry and Engineering, 2020, 8, 2665-2671.	6.7	11
24	Fast Microsecond Dynamics of the Proteinâ€“Water Network in the Active Site of Human Carbonic Anhydrase II Studied by Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2019, 141, 19276-19288.	13.7	46
25	The extracellular gate shapes the energy profile of an ABC exporter. Nature Communications, 2019, 10, 2260.	12.8	55
26	On Obtaining Boltzmann-Distributed Configurational Ensembles from Expanded Ensemble Simulations with Fast State Mixing. Journal of Chemical Theory and Computation, 2019, 15, 2774-2779.	5.3	1
27	Atomistic characterization of collective proteinâ€“waterâ€“membrane dynamics. Physical Chemistry Chemical Physics, 2019, 21, 15958-15965.	2.8	9
28	Hydration-mediated stiffening of collective membrane dynamics by cholesterol. Physical Chemistry Chemical Physics, 2019, 21, 10370-10376.	2.8	9
29	Structure of a Therapeutic Full-Length Anti-NPRA IgG4 Antibody: Dissecting Conformational Diversity. Biophysical Journal, 2019, 116, 1637-1649.	0.5	17
30	NMR Relaxation and Molecular Dynamics Simulations of Side Chain Dynamics in Proteins. Biophysical Journal, 2018, 114, 339a.	0.5	0
31	Accurate Methyl Group Dynamics in Protein Simulations with AMBER Force Fields. Journal of Physical Chemistry B, 2018, 122, 5038-5048.	2.6	38
32	Atomistic Mechanism of Large-Scale Conformational Transition in a Heterodimeric ABC Exporter. Journal of the American Chemical Society, 2018, 140, 4543-4551.	13.7	39
33	Structural and functional insights into the interaction and targeting hub TMD0 of the polypeptide transporter TAPL. Scientific Reports, 2018, 8, 15662.	3.3	7
34	Mechanism of Large-Scale Alternating Access Conformational Transition in the ABC Exporter TM287/288. Biophysical Journal, 2018, 114, 148a.	0.5	0
35	Molecular Mechanism of ATP Hydrolysis in an ABC Transporter. ACS Central Science, 2018, 4, 1334-1343.	11.3	65
36	Narrowing the gap between experimental and computational determination of methyl group dynamics in proteins. Physical Chemistry Chemical Physics, 2018, 20, 24577-24590.	2.8	36

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37	Is ATP Hydrolysis the Power Stroke in ABC Transporters?. Biophysical Journal, 2018, 114, 148a.	0.5	0
38	Donorâ€Siteâ€Directed Rational Assembly of Heteroleptic cisâ€[Pd₂L₂Lâ€²₂] Coordination Cages from Picolyl Ligands. Chemistry - A European Journal, 2018, 24, 12976-12982.	3.3	64
39	A refined polarizable water model for the coarse-grained MARTINI force field with long-range electrostatic interactions. Journal of Chemical Physics, 2017, 146, 054501.	3.0	69
40	Systematic evaluation of CS-Rosetta for membrane protein structure prediction with sparse NOE restraints. Proteins: Structure, Function and Bioinformatics, 2017, 85, 812-826.	2.6	8
41	Improved Solution-State Properties of Monoclonal Antibodies by Targeted Mutations. Journal of Physical Chemistry B, 2017, 121, 10818-10827.	2.6	25
42	High-concentration protein formulations: How high is high?. European Journal of Pharmaceutics and Biopharmaceutics, 2017, 119, 353-360.	4.3	126
43	Partial Dissociation of Truncated Peptides Influences the Structural Dynamics of the MHCI Binding Groove. Frontiers in Immunology, 2017, 8, 408.	4.8	24
44	Solvent effects on ligand binding to a serine protease. Physical Chemistry Chemical Physics, 2017, 19, 10753-10766.	2.8	30
45	Molecular mechanism of peptide editing in the tapasinâ€“MHC I complex. Scientific Reports, 2016, 6, 19085.	3.3	51
46	Systematic Evaluation of the CS-Rosetta De Novo Structure Prediction Method for Membrane Proteins. Biophysical Journal, 2016, 110, 39a.	0.5	0
47	Protein Complexes from MD Simulations: The Rope-Pulling Game of Tapasin and Histocompatibility Molecules. Biophysical Journal, 2016, 110, 529a.	0.5	0
48	Hydration Dynamics of a Peripheral Membrane Protein. Journal of the American Chemical Society, 2016, 138, 11526-11535.	13.7	57
49	Release of Entropic Spring Reveals Conformational Coupling Mechanism in the ABC Transporter BtuCD-F. Biophysical Journal, 2016, 110, 2407-2418.	0.5	9
50	Assembly of the MHC I peptide-loading complex determined by a conserved ionic lock-switch. Scientific Reports, 2015, 5, 17341.	3.3	19
51	Structure and Dynamics of Phospholipid Nanodiscs from All-Atom and Coarse-Grained Simulations. Journal of Physical Chemistry B, 2015, 119, 6991-7002.	2.6	41
52	On Using Atomistic Solvent Layers in Hybrid All-Atom/Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 4460-4472.	5.3	16
53	Systematic evaluation of bundled SPC water for biomolecular simulations. Physical Chemistry Chemical Physics, 2015, 17, 8393-8406.	2.8	26
54	Mechanistic Basis for Epitope Proofreading in the Peptide-Loading Complex. Journal of Immunology, 2015, 195, 4503-4513.	0.8	43

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55	An Annular Lipid Belt Is Essential for Allosteric Coupling and Viral Inhibition of the Antigen Translocation Complex TAP (Transporter Associated with Antigen Processing). Journal of Biological Chemistry, 2014, 289, 33098-33108.	3.4	27
56	In Vivo Trp Scanning of the Small Multidrug Resistance Protein EmrE Confirms 3D Structure Models'. Journal of Molecular Biology, 2013, 425, 4642-4651.	4.2	15
57	Improved Parameters for the Martini Coarse-Grained Protein Force Field. Journal of Chemical Theory and Computation, 2013, 9, 687-697.	5.3	1,181
58	Substrate-Induced Conformational Changes in the S-Component ThiT from an Energy Coupling Factor Transporter. Structure, 2013, 21, 861-867.	3.3	29
59	Mixing MARTINI: Electrostatic Coupling in Hybrid Atomisticâ€“Coarse-Grained Biomolecular Simulations. Journal of Physical Chemistry B, 2013, 117, 3516-3530.	2.6	145
60	Mixing Martinis: Atomistic Simulations of MscL in a Coarse Grained Environment. Biophysical Journal, 2012, 102, 241a.	0.5	0
61	Transmembrane helices can induce domain formation in crowded model membranes. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 984-994.	2.6	113
62	Surface Hopping Excited-State Dynamics Study of the Photoisomerization of a Light-Driven Fluorene Molecular Rotary Motor. Journal of Chemical Theory and Computation, 2011, 7, 2189-2199.	5.3	134
63	Determining equilibrium constants for dimerization reactions from molecular dynamics simulations. Journal of Computational Chemistry, 2011, 32, 1919-1928.	3.3	69
64	Lipid packing drives the segregation of transmembrane helices into disordered lipid domains in model membranes. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 1343-1348.	7.1	220
65	Reconstruction of atomistic details from coarseâ€grained structures. Journal of Computational Chemistry, 2010, 31, 1333-1343.	3.3	149
66	Polarizable Water Model for the Coarse-Grained MARTINI Force Field. PLoS Computational Biology, 2010, 6, e1000810.	3.2	726
67	Computer Simulations of Photobiological Processes: The Effect of the Protein Environment. Advances in Quantum Chemistry, 2010, , 181-212.	0.8	12
68	Sorting and Clustering of Transmembrane Helices in Coexisting Fluid Domains in Model Membranes. Biophysical Journal, 2010, 98, 59a-60a.	0.5	0
69	Influence of Hydrophobic Mismatch and Amino Acid Composition on the Lateral Diffusion of Transmembrane Peptides. Biophysical Journal, 2010, 99, 1447-1454.	0.5	84
70	Partitioning of Lipids at Domain Boundaries in Model Membranes. Biophysical Journal, 2010, 99, L91-L93.	0.5	88
71	Cholesterol in Bilayers with PUFA Chains: Doping with DMPC or POPC Results in Sterol Reorientation and Membrane-Domain Formation. Biochemistry, 2010, 49, 7485-7493.	2.5	109
72	Understanding the Dynamics Behind the Photoisomerization of a Light-Driven Fluorene Molecular Rotary Motor. Journal of Physical Chemistry A, 2010, 114, 5058-5067.	2.5	96

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73	From fast light-activated processes in biomolecules to large-scale aggregation of membrane proteins: molecular dynamics simulations at different time and length scales. Chemistry Central Journal, 2009, 3, .	2.6	0
74	Single-Molecule Force Spectroscopy Reveals the Function of Titin Kinase as Force Sensor. Biophysical Journal, 2009, 96, 643a.	0.5	0
75	Arginine52 Controls the Photoisomerization Process in Photoactive Yellow Protein. Journal of the American Chemical Society, 2008, 130, 3250-3251.	13.7	80
76	Mechanoenzymatics of titin kinase. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 13385-13390.	7.1	311
77	Chromophore Protonation State Controls Photoswitching of the Fluoroprotein asFP595. PLoS Computational Biology, 2008, 4, e1000034.	3.2	98
78	Ultrafast Deactivation Channel for Thymine Dimerization. Journal of the American Chemical Society, 2007, 129, 10996-10997.	13.7	125
79	Ultrafast Deactivation of an Excited Cytosineâ"Guanine Base Pair in DNA. Journal of the American Chemical Society, 2007, 129, 6812-6819.	13.7	164
80	Photoswitching of the Fluorescent Protein asFP595: Mechanism, Proton Pathways, and Absorption Spectra. Angewandte Chemie - International Edition, 2007, 46, 530-536.	13.8	95
81	Elastic Properties of Photoswitchable Azobenzene Polymers from Molecular Dynamics Simulations. Angewandte Chemie - International Edition, 2007, 46, 2232-2237.	13.8	46
82	Flooding inGROMACS: Accelerated barrier crossings in molecular dynamics. Journal of Computational Chemistry, 2006, 27, 1693-1702.	3.3	63
83	Structure and mechanism of the reversible photoswitch of a fluorescent protein. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13070-13074.	7.1	253
84	Photodissociation dynamics of SOCl2. Physical Chemistry Chemical Physics, 2005, 7, 301-309.	2.8	22
85	Recoil velocity-dependent spinâ€"orbit state distribution of chlorine photofragments. Chemical Physics, 2004, 301, 213-224.	1.9	7