Lars V Schfer

List of Publications by Year in Descending Order

71 papers	4,298 citations	30 h-index	65 g-index
87 ext. papers	5,065 ext. citations	6.1 avg, IF	5.48 L-index

#	Paper	IF	Citations
71	Remotely controllable supramolecular rotor mounted inside a porphyrinic cage. *CheM*, **2022**, 8, 543-556	16.2	2
70	Accurate evaluation of combustion enthalpy by ab-intio computations.. *Scientific Reports*, **2022**, 12, 5834	4.9	1
69	VCD spectroscopy reveals conformational changes of chiral crown ethers upon complexation of potassium and ammonium cations.. *Physical Chemistry Chemical Physics*, **2022**, 24, 11721-11728	3.6	0
68	Conformational Preferences of an Intrinsically Disordered Protein Domain: A Case Study for Modern Force Fields. *Journal of Physical Chemistry B*, **2021**, 125, 24-35	3.4	3
67	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	6.4	1
66	Protein flexibility reduces solvent-mediated friction barriers of ligand binding to a hydrophobic surface patch. *Physical Chemistry Chemical Physics*, **2021**, 23, 5665-5672	3.6	1
65	Atomistic Dynamics of Alternating Access Mechanism of an ABC Transporter **2021**, 117-124		
64	The CTPase activity of ParB determines the size and dynamics of prokaryotic DNA partition complexes. *Molecular Cell*, **2021**, 81, 3992-4007.e10	17.6	6
63	Thermodynamic driving forces of guest confinement in a photoswitchable cage. *Physical Chemistry Chemical Physics*, **2021**, 23, 7321-7332	3.6	4
62	Capturing the Flexibility of a Protein-Ligand Complex: Binding Free Energies from Different Enhanced Sampling Techniques. *Journal of Chemical Theory and Computation*, **2020**, 16, 4615-4630	6.4	4
61	Capturing Substrate Translocation in an ABC Exporter at the Atomic Level. *Journal of the American Chemical Society*, **2020**, 142, 12791-12801	16.4	5
60	Predicting NMR relaxation of proteins from molecular dynamics simulations with accurate methyl rotation barriers. *Journal of Chemical Physics*, **2020**, 152, 084102	3.9	10
59	Aminoisobutyric Acid-Stabilized Peptide SAMs with Low Nonspecific Protein Adsorption and Resistance against Marine Biofouling. *ACS Sustainable Chemistry and Engineering*, **2020**, 8, 2665-2671	8.3	6
58	Protein Motional Details Revealed by Complementary Structural Biology Techniques. *Structure*, **2020**, 28, 1024-1034.e3	5.2	1
57	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	11.5	19
56	The Active Site of a Prototypical "Rigid" Drug Target is Marked by Extensive Conformational Dynamics. *Angewandte Chemie - International Edition*, **2020**, 59, 22916-22921	16.4	6
55	The Active Site of a Prototypical Rigid Drug Target is Marked by Extensive Conformational Dynamics. *Angewandte Chemie*, **2020**, 132, 23116-23121	3.6	

54	The extracellular gate shapes the energy profile of an ABC exporter. *Nature Communications*, **2019**, 10, 2260	17.4	39
53	On Obtaining Boltzmann-Distributed Configurational Ensembles from Expanded Ensemble Simulations with Fast State Mixing. *Journal of Chemical Theory and Computation*, **2019**, 15, 2774-2779	6.4	1
52	Atomistic characterization of collective protein-water-membrane dynamics. *Physical Chemistry Chemical Physics*, **2019**, 21, 15958-15965	3.6	7
51	Hydration-mediated stiffening of collective membrane dynamics by cholesterol. *Physical Chemistry Chemical Physics*, **2019**, 21, 10370-10376	3.6	7
50	Structure of a Therapeutic Full-Length Anti-NPRA IgG4 Antibody: Dissecting Conformational Diversity. *Biophysical Journal*, **2019**, 116, 1637-1649	2.9	7
49	Fast Microsecond Dynamics of the Protein-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	16.4	22
48	Accurate Methyl Group Dynamics in Protein Simulations with AMBER Force Fields. *Journal of Physical Chemistry B*, **2018**, 122, 5038-5048	3.4	22
47	Atomistic Mechanism of Large-Scale Conformational Transition in a Heterodimeric ABC Exporter. *Journal of the American Chemical Society*, **2018**, 140, 4543-4551	16.4	28
46	Structural and functional insights into the interaction and targeting hub TMD0 of the polypeptide transporter TAPL. *Scientific Reports*, **2018**, 8, 15662	4.9	6
45	Molecular Mechanism of ATP Hydrolysis in an ABC Transporter. *ACS Central Science*, **2018**, 4, 1334-1343	16.8	38
44	Narrowing the gap between experimental and computational determination of methyl group dynamics in proteins. *Physical Chemistry Chemical Physics*, **2018**, 20, 24577-24590	3.6	21
43	Donor-Site-Directed Rational Assembly of Heteroleptic cis-[Pd L L'] Coordination Cages from Picolyl Ligands. *Chemistry - A European Journal*, **2018**, 24, 12976-12982	4.8	39
42	A refined polarizable water model for the coarse-grained MARTINI force field with long-range electrostatic interactions. *Journal of Chemical Physics*, **2017**, 146, 054501	3.9	47
41	Systematic evaluation of CS-Rosetta for membrane protein structure prediction with sparse NOE restraints. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 812-826	4.2	4
40	Improved Solution-State Properties of Monoclonal Antibodies by Targeted Mutations. *Journal of Physical Chemistry B*, **2017**, 121, 10818-10827	3.4	15
39	High-concentration protein formulations: How high is high?. *European Journal of Pharmaceutics and Biopharmaceutics*, **2017**, 119, 353-360	5.7	79
38	Partial Dissociation of Truncated Peptides Influences the Structural Dynamics of the MHCI Binding Groove. *Frontiers in Immunology*, **2017**, 8, 408	8.4	17
37	Solvent effects on ligand binding to a serine protease. *Physical Chemistry Chemical Physics*, **2017**, 19, 10753-10766	3.6	18

36	Hydration Dynamics of a Peripheral Membrane Protein. *Journal of the American Chemical Society*, **2016**, 138, 11526-35	16.4	40
35	Release of Entropic Spring Reveals Conformational Coupling Mechanism in the ABC Transporter BtuCD-F. *Biophysical Journal*, **2016**, 110, 2407-2418	2.9	8
34	Molecular mechanism of peptide editing in the tapasin-MHC I complex. *Scientific Reports*, **2016**, 6, 19085	4.9	39
33	On Using Atomistic Solvent Layers in Hybrid All-Atom/Coarse-Grained Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 4460-72	6.4	15
32	Systematic evaluation of bundled SPC water for biomolecular simulations. *Physical Chemistry Chemical Physics*, **2015**, 17, 8393-406	3.6	19
31	Mechanistic Basis for Epitope Proofreading in the Peptide-Loading Complex. *Journal of Immunology* , **2015**, 195, 4503-13	5.3	30
30	Assembly of the MHC I peptide-loading complex determined by a conserved ionic lock-switch. *Scientific Reports*, **2015**, 5, 17341	4.9	17
29	Structure and Dynamics of Phospholipid Nanodiscs from All-Atom and Coarse-Grained Simulations. *Journal of Physical Chemistry B*, **2015**, 119, 6991-7002	3.4	30
28	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, 33098-108	5.4	25
27	In vivo trp scanning of the small multidrug resistance protein EmrE confirms 3D structure models'. *Journal of Molecular Biology*, **2013**, 425, 4642-51	6.5	14
26	Improved Parameters for the Martini Coarse-Grained Protein Force Field. *Journal of Chemical Theory and Computation*, **2013**, 9, 687-97	6.4	782
25	Substrate-induced conformational changes in the S-component ThiT from an energy coupling factor transporter. *Structure*, **2013**, 21, 861-7	5.2	28
24	Mixing MARTINI: electrostatic coupling in hybrid atomistic-coarse-grained biomolecular simulations. *Journal of Physical Chemistry B*, **2013**, 117, 3516-30	3.4	117
23	Transmembrane helices can induce domain formation in crowded model membranes. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 984-94	3.8	102
22	Determining equilibrium constants for dimerization reactions from molecular dynamics simulations. *Journal of Computational Chemistry*, **2011**, 32, 1919-28	3.5	45
21	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, 2189-99	6.4	115
20	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, 1343-8	11.5	193
19	Polarizable water model for the coarse-grained MARTINI force field. *PLoS Computational Biology*, **2010**, 6, e1000810	5	587

18	Computer Simulations of Photobiological Processes: The Effect of the Protein Environment. *Advances in Quantum Chemistry*, **2010**, 181-212	1.4	12
17	Influence of hydrophobic mismatch and amino acid composition on the lateral diffusion of transmembrane peptides. *Biophysical Journal*, **2010**, 99, 1447-54	2.9	72
16	Partitioning of lipids at domain boundaries in model membranes. *Biophysical Journal*, **2010**, 99, L91-3	2.9	72
15	Cholesterol in bilayers with PUFA chains: doping with DMPC or POPC results in sterol reorientation and membrane-domain formation. *Biochemistry*, **2010**, 49, 7485-93	3.2	90
14	Understanding the dynamics behind the photoisomerization of a light-driven fluorene molecular rotary motor. *Journal of Physical Chemistry A*, **2010**, 114, 5058-67	2.8	83
13	Reconstruction of atomistic details from coarse-grained structures. *Journal of Computational Chemistry*, **2010**, 31, 1333-43	3.5	127
12	Arginine52 controls the photoisomerization process in photoactive yellow protein. *Journal of the American Chemical Society*, **2008**, 130, 3250-1	16.4	77
11	Mechanoenzymatics of titin kinase. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 13385-90	11.5	280
10	Chromophore protonation state controls photoswitching of the fluoroprotein asFP595. *PLoS Computational Biology*, **2008**, 4, e1000034	5	89
9	Ultrafast deactivation of an excited cytosine-guanine base pair in DNA. *Journal of the American Chemical Society*, **2007**, 129, 6812-9	16.4	154
8	Photoswitching of the fluorescent protein asFP595: mechanism, proton pathways, and absorption spectra. *Angewandte Chemie - International Edition*, **2007**, 46, 530-6	16.4	89
7	Elastic properties of photoswitchable azobenzene polymers from molecular dynamics simulations. *Angewandte Chemie - International Edition*, **2007**, 46, 2232-7	16.4	46
6	Ultrafast deactivation channel for thymine dimerization. *Journal of the American Chemical Society*, **2007**, 129, 10996-7	16.4	115
5	Flooding in GROMACS: accelerated barrier crossings in molecular dynamics. *Journal of Computational Chemistry*, **2006**, 27, 1693-702	3.5	53
4	Photodissociation dynamics of SOCl2. *Physical Chemistry Chemical Physics*, **2005**, 7, 301-9	3.6	18
3	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, 13070-4	11.5	222
2	Recoil velocity-dependent spinorbit state distribution of chlorine photofragments. *Chemical Physics*, **2004**, 301, 213-224	2.3	5
1	The extracellular gate shapes the energy profile of an ABC exporter		1