Niels Hansen

List of Publications by Year in Descending Order

63 papers	1,368 citations	19 h-index	36 g-index
66 ext. papers	1,570 ext. citations	4.6 avg, IF	4.92 L-index

#	Paper	IF	Citations
63	Binding free energies for the SAMPL8 CB8 "Drugs of Abuse" challenge from umbrella sampling combined with Hamiltonian replica exchange.. *Journal of Computer-Aided Molecular Design*, **2022**, 36, 1	4.2	0
62	Molecular dynamics simulation or structure refinement of proteins: are solvent molecules required? A case study using hen lysozyme.. *European Biophysics Journal*, **2022**, 1	1.9	0
61	Exploring the Effect of Enhanced Sampling on Protein Stability Prediction.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	1
60	Influence of layer slipping on adsorption of light gases in covalent organic frameworks: A combined experimental and computational study. *Microporous and Mesoporous Materials*, **2022**, 336, 111796	5.3	1
59	Computational Study of Confinement Effects in Molecular Heterogeneous Catalysis **2021**, 101-114		
58	Umbrella sampling and double decoupling data for methanol binding to lipase B. *Data in Brief*, **2021**, 39, 107618	1.2	
57	Confined Ru-catalysts in a Two-phase Heptane/Ionic Liquid Solution: Modeling Aspects. *ChemCatChem*, **2021**, 13, 739-746	5.2	0
56	On the Use of Side-Chain NMR Relaxation Data to Derive Structural and Dynamical Information on Proteins: A Case Study Using Hen Lysozyme. *ChemBioChem*, **2021**, 22, 1049-1064	3.8	4
55	Adsorption of light gases in covalent organic frameworks: comparison of classical density functional theory and grand canonical Monte Carlo simulations. *Microporous and Mesoporous Materials*, **2021**, 324, 111263	5.3	4
54	Confinement Effects for Efficient Macrocyclization Reactions with Supported Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Complexes. *ACS Catalysis*, **2021**, 11, 11570-11578	13.1	4
53	On the use of J-coupling NMR data to derive structural information on proteins. *Journal of Biomolecular NMR*, **2021**, 75, 39-70	3	2
52	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bio-Molecular Systems: Overview and Perspective on Issues. *ChemPhysChem*, **2021**, 22, 264-282	3.2	2
51	Transferable Anisotropic Mie-Potential Force Field for n-Alcohols: Static and Dynamic Fluid Properties of Pure Substances and Binary Mixtures. *Industrial & Engineering Chemistry Research*, **2020**, 59, 919-929	3.9	2
50	Combining Molecular Dynamics and Machine Learning to Predict Self-Solvation Free Energies and Limiting Activity Coefficients. *Journal of Chemical Information and Modeling*, **2020**, 60, 5319-5330	6.1	14
49	Generalized Fickian approach for phase separating fluid mixtures in Smoothed Particle Hydrodynamics. *Computers and Fluids*, **2019**, 179, 78-90	2.8	
48	Rotational barriers of carbamate-protected amine crosslinkers for hydrogels: A combined experimental and computational study. *Journal of Physical Organic Chemistry*, **2019**, 32, e3936	2.1	2
47	Thermophysical properties of glyceline-water mixtures investigated by molecular modelling. *Physical Chemistry Chemical Physics*, **2019**, 21, 6467-6476	3.6	30

46	On the use of transport properties to discriminate Mie-type molecular models for 1-propanol optimized against VLE data. *European Physical Journal: Special Topics*, **2019**, 227, 1529-1545	2.3	3
45	Olefin Metathesis in Confined Geometries: A Biomimetic Approach toward Selective Macrocyclization. *Journal of the American Chemical Society*, **2019**, 141, 19014-19022	16.4	28
44	Lessons Learned from the Calculation of One-Dimensional Potentials of Mean Force [Article v1.0]. *Living Journal of Computational Molecular Science*, **2019**, 1,	10.1	7
43	Thermodynamic Characterization of the Dimerization of an Anionic Perylene Bisimide Dye Using Molecular Simulation. *Journal of Physical Chemistry C*, **2019**, 123, 8027-8036	3.8	2
42	Interpretation of cytochrome P450 monooxygenase kinetics by modeling of thermodynamic activity. *Journal of Inorganic Biochemistry*, **2018**, 183, 172-178	4.2	6
41	Validation and Comparison of Force Fields for Native Cyclodextrins in Aqueous Solution. *Journal of Physical Chemistry B*, **2018**, 122, 1608-1626	3.4	25
40	Validierung von molekularen Simulationen: eine Übersicht verschiedener Aspekte. *Angewandte Chemie*, **2018**, 130, 894-915	3.6	3
39	Validation of Molecular Simulation: An Overview of Issues. *Angewandte Chemie - International Edition*, **2018**, 57, 884-902	16.4	74
38	Comparison of free-energy methods using a tripeptide-water model system. *Journal of Computational Chemistry*, **2018**, 39, 2226-2242	3.5	8
37	Insights into Noncovalent Binding Obtained from Molecular Dynamics Simulations. *Chemie-Ingenieur-Technik*, **2018**, 90, 1864-1875	0.8	8
36	Overcoming Convergence Issues in Free-Energy Calculations of Amide-to-Ester Mutations in the Pin1-WW Domain. *Journal of Chemical Information and Modeling*, **2018**, 58, 2305-2318	6.1	2
35	Evolutionary Analysis As a Powerful Complement to Energy Calculations for Protein Stabilization. *ACS Catalysis*, **2018**, 8, 9420-9428	13.1	11
34	Interpretation of Seemingly Contradictory Data: Low NMR S Order Parameters Observed in Helices and High NMR S Order Parameters in Disordered Loops of the Protein hGH at Low pH. *Chemistry - A European Journal*, **2017**, 23, 9585-9591	4.8	2
33	Using Complementary NMR Data Sets To Detect Inconsistencies and Model Flaws in the Structure Determination of Human Interleukin-4. *Journal of Physical Chemistry B*, **2017**, 121, 7055-7063	3.4	2
32	Validation of Trimethylamine-N-oxide (TMAO) Force Fields Based on Thermophysical Properties of Aqueous TMAO Solutions. *Journal of Physical Chemistry B*, **2017**, 121, 10674-10688	3.4	22
31	Molecular Simulations of Thermodynamic Properties for the System β-Cyclodextrin/Alcohol in Aqueous Solution. *Chemie-Ingenieur-Technik*, **2017**, 89, 1306-1314	0.8	8
30	Bestimmung von Strukturinformation aus experimentellen Messdaten für Biomoleküle. *Angewandte Chemie*, **2016**, 128, 16222-16244	3.6	7
29	On the use of time-averaging restraints when deriving biomolecular structure from J-coupling values obtained from NMR experiments. *Journal of Biomolecular NMR*, **2016**, 66, 69-83	3	1

28	Deriving Structural Information from Experimentally Measured Data on Biomolecules. *Angewandte Chemie - International Edition*, **2016**, 55, 15990-16010	16.4	21
27	Calculation of binding affinities for linear alcohols to β-cyclodextrin by twin-system enveloping distribution sampling simulations. *Fluid Phase Equilibria*, **2016**, 422, 1-17	2.5	14
26	Chapter 6:Free Energy Calculation Methods and Rare Event Sampling Techniques for Biomolecular Simulations. *RSC Theoretical and Computational Chemistry Series*, **2016**, 185-214	1.2	2
25	Characterization of the flexible lip regions in bacteriophage lambda lysozyme using MD simulations. *European Biophysics Journal*, **2015**, 44, 235-47	1.9	3
24	The key to predicting the stability of protein mutants lies in an accurate description and proper configurational sampling of the folded and denatured states. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 983-995	4	7
23	Practical Aspects of Free-Energy Calculations: A Review. *Journal of Chemical Theory and Computation*, **2014**, 10, 2632-47	6.4	271
22	On the Use of a Supramolecular Coarse-Grained Model for the Solvent in Simulations of the Folding Equilibrium of an Octa-β-peptide in MeOH and H2O. *Helvetica Chimica Acta*, **2014**, 97, 1591-1605	2	4
21	Time-averaged order parameter restraints in molecular dynamics simulations. *Journal of Biomolecular NMR*, **2014**, 60, 169-87	3	19
20	Relative free enthalpies for point mutations in two proteins with highly similar sequences but different folds. *Biochemistry*, **2013**, 52, 4962-70	3.2	8
19	Efficient Combination of Environment Change and Alchemical Perturbation within the Enveloping Distribution Sampling (EDS) Scheme: Twin-System EDS and Application to the Determination of Octanol-Water Partition Coefficients. *Journal of Chemical Theory and Computation*, **2013**, 9, 1334-46	6.4	14
18	Multiscale Approaches for Modeling Hydrocarbon Conversion Reactions in Zeolites. *Chemie-Ingenieur-Technik*, **2013**, 85, 413-419	0.8	7
17	Assessment of enveloping distribution sampling to calculate relative free enthalpies of binding for eight netropsin-DNA duplex complexes in aqueous solution. *Journal of Computational Chemistry*, **2012**, 33, 640-51	3.5	21
16	Multiscale Modeling of Reaction and Diffusion in Zeolites: From the Molecular Level to the Reactor. *Soft Materials*, **2012**, 10, 179-201	1.7	19
15	Calculation of Derivative Thermodynamic Hydration and Aqueous Partial Molar Properties of Ions Based on Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2012**, 8, 3542-64	6.4	11
14	Combined Density Functional Theory and Monte Carlo Analysis of Monomolecular Cracking of Light Alkanes Over H-ZSM-5. *Journal of Physical Chemistry C*, **2012**, 116, 23408-23417	3.8	50
13	An effective force field for molecular dynamics simulations of dimethyl sulfone. *Molecular Physics*, **2011**, 109, 2593-2605	1.7	3
12	Current computer modeling cannot explain why two highly similar sequences fold into different structures. *Biochemistry*, **2011**, 50, 10965-73	3.2	27
11	Comparison of enveloping distribution sampling and thermodynamic integration to calculate binding free energies of phenylethanolamine N-methyltransferase inhibitors. *Journal of Chemical Physics*, **2011**, 135, 024105	3.9	36

10	Theoretical Simulation of n-Alkane Cracking on Zeolites. *Journal of Physical Chemistry C*, **2010**, 114, 10229-10239	3.8	94
9	Quantum chemical modeling of benzene ethylation over H-ZSM-5 approaching chemical accuracy: a hybrid MP2:DFT study. *Journal of the American Chemical Society*, **2010**, 132, 11525-38	16.4	127
8	Theoretical Investigation of Benzene Alkylation with Ethene over H-ZSM-5. *Journal of Physical Chemistry C*, **2008**, 112, 15402-15411	3.8	73
7	A Reaction Mechanism for the Nitrous Oxide Decomposition on Binuclear Oxygen Bridged Iron Sites in Fe-ZSM-5. *Journal of Physical Chemistry C*, **2007**, 111, 2092-2101	3.8	73
6	New force fields for nitrous oxide and oxygen and their application to phase equilibria simulations. *Fluid Phase Equilibria*, **2007**, 259, 180-188	2.5	40
5	Nitrous oxide decomposition over Fe-ZSM-5 in the presence of nitric oxide: a comprehensive DFT study. *Journal of Physical Chemistry B*, **2006**, 110, 17096-114	3.4	71
4	Molecular simulation of alkene adsorption in zeolites. *Molecular Physics*, **2005**, 103, 471-489	1.7	48
3	Reactive Monte Carlo and grand-canonical Monte Carlo simulations of the propene metathesis reaction system. *Journal of Chemical Physics*, **2005**, 122, 164705	3.9	43
2	PoreMS: a software tool for generating silica pore models with user-defined surface functionalisation and pore dimensions. *Molecular Simulation*,1-11	2	6
1	An atomistic view on the uptake of aromatic compounds by cyclodextrin immobilized on mesoporous silica. *Adsorption*,1	2.6	