Peter A J Hilbers

List of Publications by Year
in descending order

126 papers	7,116 citations	71102 41 h-index	58581 82 g-index
129 all docs	129 docs citations	129 times ranked	8532 citing authors

#	Article	IF	Citations
1	The role of collagen in bone apatite formation in the presence of hydroxyapatite nucleation inhibitors. Nature Materials, 2010, 9, 1004-1009.	27.5	960
2	Pathway complexity in supramolecular polymerization. Nature, 2012, 481, 492-496.	27.8	812
3	Computer simulations of a water/oil interface in the presence of micelles. Nature, 1990, 348, 624-625.	27.8	294
4	Simulating the Self-Assembly of Gemini (Dimeric) Surfactants. Science, 1994, 266, 254-256.	12.6	283
5	Structure of a water/oil interface in the presence of micelles: a computer simulation study. The Journal of Physical Chemistry, 1991, 95, 6361-6368.	2.9	208
6	Efficient Monte Carlo methods for the simulation of catalytic surface reactions. Physical Review E, 1998, 58, 2598-2610.	2.1	198
7	Monte Carlo simulations of a simple model for the electrocatalytic CO oxidation on platinum. Journal of Chemical Physics, 1998, 109, 6051-6062.	3.0	189
8	Theoretical models of nonlinear effects in two-component cooperative supramolecular copolymerizations. Nature Communications, 2011, 2, 509.	12.8	184
9	An Equilibrium Model for Chiral Amplification in Supramolecular Polymers. Journal of Physical Chemistry B, 2012, 116, 5291-5301.	2.6	175
10	Computer simulations of surfactant self-assembly. Langmuir, 1993, 9, 9-11.	3.5	164
11	Parameter uncertainty in biochemical models described by ordinary differential equations. Mathematical Biosciences, 2013, 246, 305-314.	1.9	153
12	A unified theory for osteonal and hemi-osteonal remodeling. Bone, 2008, 42, 250-259.	2.9	152
13	The twisted cube. Lecture Notes in Computer Science, 1987, , 152-159.	1.3	132
14	Programmable chemical reaction networks: emulating regulatory functions in living cells using a bottom-up approach. Chemical Society Reviews, 2015, 44, 7465-7483.	38.1	123
15	Understanding Cooperativity in Hydrogen-Bond-Induced Supramolecular Polymerization: A Density Functional Theory Study. Journal of Physical Chemistry B, 2010, 114, 13667-13674.	2.6	119
16	Molecular dynamics simulations of oil solubilization in surfactant solutions. Langmuir, 1993, 9, 1175-1178.	3.5	112
17	A Detailed Look at Vesicle Fusion. Journal of Physical Chemistry B, 2006, 110, 13212-13219.	2.6	103
18	Relating osteon diameter to strain. Bone, 2008, 43, 476-482.	2.9	103

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19	Molecular dynamics study of nucleation and melting ofnâ€alkanes. Journal of Chemical Physics, 1994, 101, 9033-9041.	3.0	94
20	Monte Carlo simulations of a surface reaction model showing spatio-temporal pattern formations and oscillations. Journal of Chemical Physics, 1998, 108, 5921-5934.	3.0	86
21	Molecular dynamics study of the influence of wall-gas interactions on heat flow in nanochannels. Physical Review E, 2005, 71, 066702.	2.1	82
22	The Bilayerâ^'Vesicle Transition Is Entropy Driven. Journal of Physical Chemistry B, 2005, 109, 22649-22654.	2.6	80
23	A Bayesian approach to targeted experiment design. Bioinformatics, 2012, 28, 1136-1142.	4.1	79
24	Computation of accommodation coefficients and the use of velocity correlation profiles in molecular dynamics simulations. Physical Review E, 2010, 81, 011203.	2.1	72
25	Mechanoelectric feedback leads to conduction slowing and block in acutely dilated atria: a modeling study of cardiac electromechanics. American Journal of Physiology - Heart and Circulatory Physiology, 2007, 292, H2832-H2853.	3.2	69
26	A genomeâ€scale metabolic network reconstruction of tomato (Solanum lycopersicum L.) and its application to photorespiratory metabolism. Plant Journal, 2016, 85, 289-304.	5.7	66
27	Switching fromS- toR-Selectivity in theCandidaantarcticaLipase B-Catalyzed Ring-Opening of Ï‰-Methylated Lactones:Â Tuning Polymerizations by Ring Size. Journal of the American Chemical Society, 2007, 129, 7393-7398.	13.7	65
28	Adaptive Ensemble Models of Extreme Learning Machines for Time Series Prediction. Lecture Notes in Computer Science, 2009, , 305-314.	1.3	63
29	Vesicle Shapes from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 22780-22785.	2.6	62
30	An integrated strategy for prediction uncertainty analysis. Bioinformatics, 2012, 28, 1130-1135.	4.1	59
31	Kinetics of the Fischerâ€“Tropsch Reaction. Angewandte Chemie - International Edition, 2012, 51, 9015-9019.	13.8	55
32	Monomer Formation Model versus Chain Growth Model of the Fischerâ€“Tropsch Reaction. Journal of Physical Chemistry C, 2013, 117, 4488-4504.	3.1	55
33	Lipid-Based Mechanisms for Vesicle Fission. Journal of Physical Chemistry B, 2007, 111, 5719-5725.	2.6	54
34	Quantifying the Composition of Human Skin for Glucose Sensor Development. Journal of Diabetes Science and Technology, 2010, 4, 1032-1040.	2.2	52
35	Construction of 3D models of the CYP11B family as a tool to predict ligand binding characteristics. Journal of Computer-Aided Molecular Design, 2007, 21, 455-471.	2.9	51
36	Self-Reproduction of Fatty Acid Vesicles: A Combined Experimental andÂSimulation Study. Biophysical Journal, 2010, 99, 1520-1528.	0.5	50

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37	Visible Blue Light Therapy: Molecular Mechanisms and Therapeutic Opportunities. Current Medicinal Chemistry, 2019, 25, 5564-5577.	2.4	50
38	Stepwise Noncovalent Synthesis Leading to Dendrimer-Based Assemblies in Water. Journal of the American Chemical Society, 2007, 129, 15631-15638.	13.7	49
39	Quantification of atherosclerotic plaque components using in vivo MRI and supervised classifiers. Magnetic Resonance in Medicine, 2006, 55, 790-799.	3.0	47
40	Computing Algebraic Functions with Biochemical Reaction Networks. Artificial Life, 2009, 15, 5-19.	1.3	46
41	Quantification of lateral repulsion between coadsorbed CO and N on Rh(100) using temperature-programmed desorption, low-energy electron diffraction, and Monte Carlo simulations. Journal of Chemical Physics, 2003, 119, 524-532.	3.0	43
42	Dynamic behavior of fully solvated beta2-adrenergic receptor, embedded in the membrane with bound agonist or antagonist. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 4882-4887.	7.1	43
43	Hybrid method coupling molecular dynamics and Monte Carlo simulations to study the properties of gases in microchannels and nanochannels. Physical Review E, 2005, 72, 016705.	2.1	41
44	Magnitude and control of mitochondrial sensitivity to ADP. American Journal of Physiology - Endocrinology and Metabolism, 2009, 297, E774-E784.	3.5	41
45	Vesicle Deformation by Draining: Geometrical and Topological Shape Changes. Journal of Physical Chemistry B, 2009, 113, 8731-8737.	2.6	41
46	Synthesis, Biological Evaluation, and Molecular Modeling of 1-Benzyl-1H-imidazoles as Selective Inhibitors of Aldosterone Synthase (CYP11B2). Journal of Medicinal Chemistry, 2010, 53, 1712-1725.	6.4	38
47	An MRâ€compatible bicycle ergometer for inâ€magnet wholeâ€body human exercise testing. Magnetic Resonance in Medicine, 2010, 63, 257-261.	3.0	37
48	Fragmentation and Coagulation in Supramolecular (Co)polymerization Kinetics. ACS Central Science, 2016, 2, 232-241.	11.3	35
49	Coarse-Grained Transmembrane Proteins:â€‰ Hydrophobic Matching, Aggregation, and Their Effect on Fusion. Journal of Physical Chemistry B, 2006, 110, 13614-13623.	2.6	32
50	Optimal experiment design for model selection in biochemical networks. BMC Systems Biology, 2014, 8, 20.	3.0	31
51	Volume fraction dependence and reorganization in clusterâ€“cluster aggregation processes. Journal of Chemical Physics, 1995, 102, 480-495.	3.0	30
52	Quantifying lateral adsorbate interactions by kinetic Monte-Carlo simulations and density-functional theory: NO dissociation on Rh(100). Physical Chemistry Chemical Physics, 2004, 6, 1830.	2.8	30
53	Modeling Glucose and Water Dynamics in Human Skin. Diabetes Technology and Therapeutics, 2008, 10, 283-293.	4.4	30
54	Parameter Trajectory Analysis to Identify Treatment Effects of Pharmacological Interventions. PLoS Computational Biology, 2013, 9, e1003166.	3.2	27

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55	Simulations of trabecular remodeling and fatigue: Is remodeling helpful or harmful?. Bone, 2011, 48, 1210-1215.	2.9	26
56	Prediction of Muscle Energy States at Low Metabolic Rates Requires Feedback Control of Mitochondrial Respiratory Chain Activity by Inorganic Phosphate. PLoS ONE, 2012, 7, e34118.	2.5	26
57	Unchanged muscle fiber conduction velocity relates to mild acidosis during exhaustive bicycling. European Journal of Applied Physiology, 2012, 112, 1593-1602.	2.5	26
58	Steady-state properties of single-file systems with conversion. Physical Review E, 2002, 65, 066701.	2.1	25
59	Silencing of glycolysis in muscle: experimental observation and numerical analysis. Experimental Physiology, 2010, 95, 380-397.	2.0	25
60	Coarse Grained Molecular Dynamics Simulations of Transmembrane Protein-Lipid Systems. International Journal of Molecular Sciences, 2010, 11, 2393-2420.	4.1	25
61	Simulation of small-angle scattering from large assemblies of multi-type scatterer particles. Journal of Molecular Structure, 1996, 383, 303-308.	3.6	24
62	A sclerostin-based theory for strain-induced bone formation. Biomechanics and Modeling in Mechanobiology, 2011, 10, 663-670.	2.8	22
63	Parameter adaptations during phenotype transitions in progressive diseases. BMC Systems Biology, 2011, 5, 174.	3.0	22
64	The CUMULUS Coarse Graining Method: Transferable Potentials for Water and Solutes. Journal of Physical Chemistry B, 2011, 115, 10001-10012.	2.6	20
65	Combined in vivo and in silico investigations of activation of glycolysis in contracting skeletal muscle. American Journal of Physiology - Cell Physiology, 2013, 304, C180-C193.	4.6	20
66	Structural Elucidation of Dendritic Hostâ€“Guest Complexes by Xâ€ray Crystallography and Molecular Dynamics Simulations. Chemistry - A European Journal, 2007, 13, 7883-7889.	3.3	19
67	Fadrozole Reverses Cardiac Fibrosis in Spontaneously Hypertensive Heart Failure Rats: Discordant Enantioselectivity Versus Reduction of Plasma Aldosterone. Endocrinology, 2008, 149, 28-31.	2.8	19
68	Proteomic Analysis in Type 2 Diabetes Patients before and after a Very Low Calorie Diet Reveals Potential Disease State and Intervention Specific Biomarkers. PLoS ONE, 2014, 9, e112835.	2.5	19
69	Characterization of disease-specific cellular abundance profiles of chronic inflammatory skin conditions from deconvolution of biopsy samples. BMC Medical Genomics, 2019, 12, 121.	1.5	19
70	In Silico Analysis Identifies Intestinal Transit as a Key Determinant of Systemic Bile Acid Metabolism. Frontiers in Physiology, 2018, 9, 631.	2.8	18
71	Computer simulations of successful defibrillation in decoupled and non-uniform cardiac tissue. Europace, 2005, 7, S166-S177.	1.7	17
72	Coarse-grained simulations of poly(propylene imine) dendrimers in solution. Journal of Chemical Physics, 2016, 144, 074903.	3.0	17

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73	Heat Transfer Predictions for Micro-/Nanochannels at the Atomistic Level Using Combined Molecular Dynamics and Monte Carlo Techniques. Journal of Heat Transfer, 2009, 131, .	2.1	16
74	Directional interactions in semiflexible single-chain polymer folding. Soft Matter, 2012, 8, 7610.	2.7	16
75	Evaporative self-assembly of single-chain, polymeric nanoparticles. Chemical Communications, 2013, 49, 3122.	4.1	16
76	Molecular Simulation of Protein Encapsulation in Vesicle Formation. Journal of Physical Chemistry B, 2014, 118, 3346-3354.	2.6	16
77	The Role of the Hyperpolarization-Activated Inward Current<tex>$I_rm f$</tex>in Arrhythmogenesis: A Computer Model Study. IEEE Transactions on Biomedical Engineering, 2006, 53, 1499-1511.	4.2	15
78	A Computational Model for the Analysis of Lipoprotein Distributions in the Mouse: Translating FPLC Profiles to Lipoprotein Metabolism. PLoS Computational Biology, 2014, 10, e1003579.	3.2	15
79	Model-Based Quantification of the Systemic Interplay between Glucose and Fatty Acids in the Postprandial State. PLoS ONE, 2015, 10, e0135665.	2.5	15
80	A Physiology-Based Model Describing Heterogeneity in Glucose Metabolism. Journal of Diabetes Science and Technology, 2015, 9, 282-292.	2.2	15
81	Simulating Complex Fluids. Molecular Simulation, 1995, 14, 259-274.	2.0	14
82	Mechanoelectric Feedback as a Trigger Mechanism for Cardiac Electrical Remodeling: A Model Study. Annals of Biomedical Engineering, 2008, 36, 1816-1835.	2.5	13
83	Computational model of excitable cell indicates ATP free energy dynamics in response to calcium oscillations are undampened by cytosolic ATP buffers. IET Systems Biology, 2006, 153, 405.	2.0	12
84	On Protein Crowding and Bilayer Bulging in Spontaneous Vesicle Formation. Journal of Physical Chemistry B, 2012, 116, 12677-12683.	2.6	12
85	In vivo and in silico dynamics of the development of Metabolic Syndrome. PLoS Computational Biology, 2018, 14, e1006145.	3.2	12
86	Infinitely fast diffusion in single-file systems. Physical Review E, 2003, 67, 046707.	2.1	11
87	Computer Simulations of Simple Oil/Water/Surfactants Systems / Computer Simulations of Simple Oil/Water/Surfactants Systems. Tenside, Surfactants, Detergents, 1993, 30, 287-293.	1.2	11
88	Simulating surfactant self-assembly. Journal of Physics Condensed Matter, 1994, 6, A351-A356.	1.8	10
89	Implicit particle wall boundary condition in molecular dynamics. Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, 2008, 222, 855-864.	2.1	10
90	A Distance-Based Framework for the Characterization of Metabolic Heterogeneity in Large Sets of Genome-Scale Metabolic Models. Patterns, 2020, 1, 100080.	5.9	10

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91	Deadlock-free message routing in multicomputer networks. Distributed Computing, 1989, 3, 178-186.	0.8	9
92	Transient behavior in single-file systems. Physical Review E, 2002, 66, 066705.	2.1	9
93	Similar mitochondrial activation kinetics in wild-type and creatine kinase-deficient fast-twitch muscle indicate significant Pi control of respiration. American Journal of Physiology - Regulatory Integrative and Comparative Physiology, 2011, 300, R1316-R1325.	1.8	9
94	Computational modelling identifies the impact of subtle anatomical variations between amphibian and mammalian skeletal muscle on spatiotemporal calcium dynamics. IET Systems Biology, 2008, 2, 411-422.	1.5	8
95	Molecular Dynamics and Monte Carlo Simulations for Heat Transfer in Micro- and Nanochannels. International Journal for Multiscale Computational Engineering, 2006, 4, 391-397.	1.2	8
96	Molecular Dynamics and Monte Carlo Simulations for Heat Transfer in Micro and Nano-channels. Lecture Notes in Computer Science, 2004, , 661-666.	1.3	7
97	Metabolic Modeling Combined With Machine Learning Integrates Longitudinal Data and Identifies the Origin of LXR-Induced Hepatic Steatosis. Frontiers in Bioengineering and Biotechnology, 2020, 8, 536957.	4.1	7
98	Parallel Computing and Molecular Dynamics Simulations. , 1993, , 473-495.		6
99	Applications of analysis of dynamic adaptations in parameter trajectories. Interface Focus, 2013, 3, 20120084.	3.0	6
100	Computational modelling of energy balance in individuals with Metabolic Syndrome. BMC Systems Biology, 2019, 13, 24.	3.0	6
101	Dynamic Monte Carlo Simulations of Oscillatory Reactions. Israel Journal of Chemistry, 1998, 38, 415-428.	2.3	5
102	Velocity Correlations and Accommodation Coefficients for Gas-Wall Interactions in Nanochannels. , 2008, , .		5
103	Modeling the interference between shear and longitudinal waves under high intensity focused ultrasound propagation in bone. Physics in Medicine and Biology, 2018, 63, 235024.	3.0	4
104	Multivalency in a Dendritic Hostâ€“Guest System. Macromolecules, 2019, 52, 2778-2788.	4.8	4
105	Laterally coupled jellium-like two-dimensional quantum dots. Journal of Physics Condensed Matter, 2003, 15, 6977-6984.	1.8	3
106	The origin of isotope-induced helical-sense bias in supramolecular polymers of benzene-1,3,5-tricarboxamides. Physical Chemistry Chemical Physics, 2012, 14, 13997.	2.8	3
107	A Dynamic Model for Prediction of Psoriasis Management by Blue Light Irradiation. Frontiers in Physiology, 2017, 8, 28.	2.8	3
108	Computer simulations of surfactants at a liquid/liquid interface. , 1992, , 519-533.		3

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109	Heat Transfer Predictions for Micro/Nano-Channels at Atomistic Level Using Combined Molecular Dynamics and Monte Carlo Techniques. , 2007, , .		2
110	Computing the Stochastic Dynamics of Phosphorylation Networks. Journal of Computational Biology, 2010, 17, 189-199.	1.6	2
111	Single-variable reaction systems: Deterministic and stochastic models. Mathematical Biosciences, 2010, 227, 105-116.	1.9	2
112	A novel Method for Coarse Graining of Atomistic Simulations Using Boltzmann Inversion. Biophysical Journal, 2011, 100, 309a.	0.5	2
113	Application of a ligandâ€based theoretical approach to derive conversion paths and ligand conformations in CYP11B2â€mediated aldosterone formation. Journal of Computational Chemistry, 2011, 32, 2441-2448.	3.3	2
114	Evaporative Microchannel Cooling: An Atomistic Approach. , 2010, , .		2
115	Novel Hybrid Simulations for Heat Transfer at Atomistic Level. , 2006, , 1315.		1
116	Heat Transfer on Walls in Molecular Dynamics Simulations: Modelling With Vibrating Reflective Walls. , 2008, , .		1
117	Velocity Correlations Between Impinging and Reflecting Particles Using MD Simulations and Different Wall Models. , 2008, , .		1
118	Speckle-initialized dynamic segmentation of the prostate. , 2009, 2009, 6352-5.		1
119	Large Scale Analysis of Small Repeats via Mining of the Human Genome. , 2009, , .		1
120	Mining Maximal Frequent Subgraphs in KEGG Reaction Networks. , 2009, , .		1
121	In Silico Clinical Studies on the Efficacy of Blue Light for Treating Psoriasis in Virtual Patients. Systems Medicine (New Rochelle, N Y), 2019, 2, 10-18.	1.1	1
122	Simulating Metabolic Flexibility in Low Energy Expenditure Conditions Using Genome-Scale Metabolic Models. Metabolites, 2021, 11, 695.	2.9	1
123	16. Parallel Molecular Dynamics on a Torus Network. , 1996, , 177-186.		0
124	Hybrid Molecular Dynamics-Monte Carlo Simulations for the properties of a dense and dilute hard-sphere gas in a microchannel. AIP Conference Proceedings, 2005, , .	0.4	0
125	New Derivation of a Particle Wall Boundary Condition in Molecular Dynamics. , 2007, , 767.		0
126	Protonation and the Matrix Effect of Oleate Vesicles, a Coarse Grained Molecular Dynamics Study. Biophysical Journal, 2012, 102, 397a.	0.5	0