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	Simulating Metabolic Flexibility in Low Energy Expenditure Conditions Using Genome-Scale Metabolic Models. Metabolites, 2021, 11, 695.	2.9	1
2	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
3	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
4	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
5	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
6	Multivalency in a Dendritic Hostâ€“Guest System. Macromolecules, 2019, 52, 2778-2788.	4.8	4
7	Computational modelling of energy balance in individuals with Metabolic Syndrome. BMC Systems Biology, 2019, 13, 24.	3.0	6
8	Visible Blue Light Therapy: Molecular Mechanisms and Therapeutic Opportunities. Current Medicinal Chemistry, 2019, 25, 5564-5577.	2.4	50
9	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
10	In Silico Analysis Identifies Intestinal Transit as a Key Determinant of Systemic Bile Acid Metabolism. Frontiers in Physiology, 2018, 9, 631.	2.8	18
11	In vivo and in silico dynamics of the development of Metabolic Syndrome. PLoS Computational Biology, 2018, 14, e1006145.	3.2	12
12	A Dynamic Model for Prediction of Psoriasis Management by Blue Light Irradiation. Frontiers in Physiology, 2017, 8, 28.	2.8	3
13	Coarse-grained simulations of poly(propylene imine) dendrimers in solution. Journal of Chemical Physics, 2016, 144, 074903.	3.0	17
14	Fragmentation and Coagulation in Supramolecular (Co)polymerization Kinetics. ACS Central Science, 2016, 2, 232-241.	11.3	35
15	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
16	Model-Based Quantification of the Systemic Interplay between Glucose and Fatty Acids in the Postprandial State. PLoS ONE, 2015, 10, e0135665.	2.5	15
17	A Physiology-Based Model Describing Heterogeneity in Glucose Metabolism. Journal of Diabetes Science and Technology, 2015, 9, 282-292.	2.2	15
18	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

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19	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
20	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
21	Molecular Simulation of Protein Encapsulation in Vesicle Formation. Journal of Physical Chemistry B, 2014, 118, 3346-3354.	2.6	16
22	Optimal experiment design for model selection in biochemical networks. BMC Systems Biology, 2014, 8, 20.	3.0	31
23	Parameter uncertainty in biochemical models described by ordinary differential equations. Mathematical Biosciences, 2013, 246, 305-314.	1.9	153
24	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
25	Evaporative self-assembly of single-chain, polymeric nanoparticles. Chemical Communications, 2013, 49, 3122.	4.1	16
26	Monomer Formation Model versus Chain Growth Model of the Fischerâ€“Tropsch Reaction. Journal of Physical Chemistry C, 2013, 117, 4488-4504.	3.1	55
27	Parameter Trajectory Analysis to Identify Treatment Effects of Pharmacological Interventions. PLoS Computational Biology, 2013, 9, e1003166.	3.2	27
28	Applications of analysis of dynamic adaptations in parameter trajectories. Interface Focus, 2013, 3, 20120084.	3.0	6
29	An integrated strategy for prediction uncertainty analysis. Bioinformatics, 2012, 28, 1130-1135.	4.1	59
30	A Bayesian approach to targeted experiment design. Bioinformatics, 2012, 28, 1136-1142.	4.1	79
31	Directional interactions in semiflexible single-chain polymer folding. Soft Matter, 2012, 8, 7610.	2.7	16
32	On Protein Crowding and Bilayer Bulging in Spontaneous Vesicle Formation. Journal of Physical Chemistry B, 2012, 116, 12677-12683.	2.6	12
33	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
34	An Equilibrium Model for Chiral Amplification in Supramolecular Polymers. Journal of Physical Chemistry B, 2012, 116, 5291-5301.	2.6	175
35	Protonation and the Matrix Effect of Oleate Vesicles, a Coarse Grained Molecular Dynamics Study. Biophysical Journal, 2012, 102, 397a.	0.5	0
36	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

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37	Pathway complexity in supramolecular polymerization. Nature, 2012, 481, 492-496.	27.8	812
38	Kinetics of the Fischerâ€“Tropsch Reaction. Angewandte Chemie - International Edition, 2012, 51, 9015-9019.	13.8	55
39	Unchanged muscle fiber conduction velocity relates to mild acidosis during exhaustive bicycling. European Journal of Applied Physiology, 2012, 112, 1593-1602.	2.5	26
40	The CUMULUS Coarse Graining Method: Transferable Potentials for Water and Solutes. Journal of Physical Chemistry B, 2011, 115, 10001-10012.	2.6	20
41	A novel Method for Coarse Graining of Atomistic Simulations Using Boltzmann Inversion. Biophysical Journal, 2011, 100, 309a.	0.5	2
42	Simulations of trabecular remodeling and fatigue: Is remodeling helpful or harmful?. Bone, 2011, 48, 1210-1215.	2.9	26
43	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
44	Theoretical models of nonlinear effects in two-component cooperative supramolecular copolymerizations. Nature Communications, 2011, 2, 509.	12.8	184
45	A sclerostin-based theory for strain-induced bone formation. Biomechanics and Modeling in Mechanobiology, 2011, 10, 663-670.	2.8	22
46	Parameter adaptations during phenotype transitions in progressive diseases. BMC Systems Biology, 2011, 5, 174.	3.0	22
47	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
48	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
49	An MRâ€compatible bicycle ergometer for inâ€magnet wholeâ€body human exercise testing. Magnetic Resonance in Medicine, 2010, 63, 257-261.	3.0	37
50	Silencing of glycolysis in muscle: experimental observation and numerical analysis. Experimental Physiology, 2010, 95, 380-397.	2.0	25
51	The role of collagen in bone apatite formation in the presence of hydroxyapatite nucleation inhibitors. Nature Materials, 2010, 9, 1004-1009.	27.5	960
52	Quantifying the Composition of Human Skin for Glucose Sensor Development. Journal of Diabetes Science and Technology, 2010, 4, 1032-1040.	2.2	52
53	Computing the Stochastic Dynamics of Phosphorylation Networks. Journal of Computational Biology, 2010, 17, 189-199.	1.6	2
54	Coarse Grained Molecular Dynamics Simulations of Transmembrane Protein-Lipid Systems. International Journal of Molecular Sciences, 2010, 11, 2393-2420.	4.1	25

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55	Self-Reproduction of Fatty Acid Vesicles: A Combined Experimental andÂSimulation Study. Biophysical Journal, 2010, 99, 1520-1528.	0.5	50
56	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
57	Computation of accommodation coefficients and the use of velocity correlation profiles in molecular dynamics simulations. Physical Review E, 2010, 81, 011203.	2.1	72
58	Single-variable reaction systems: Deterministic and stochastic models. Mathematical Biosciences, 2010, 227, 105-116.	1.9	2
59	Evaporative Microchannel Cooling: An Atomistic Approach. , 2010, , .		2
60	Speckle-initialized dynamic segmentation of the prostate. , 2009, 2009, 6352-5.		1
61	Large Scale Analysis of Small Repeats via Mining of the Human Genome. , 2009, , .		1
62	Adaptive Ensemble Models of Extreme Learning Machines for Time Series Prediction. Lecture Notes in Computer Science, 2009, , 305-314.	1.3	63
63	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
64	Computing Algebraic Functions with Biochemical Reaction Networks. Artificial Life, 2009, 15, 5-19.	1.3	46
65	Magnitude and control of mitochondrial sensitivity to ADP. American Journal of Physiology - Endocrinology and Metabolism, 2009, 297, E774-E784.	3.5	41
66	Vesicle Deformation by Draining: Geometrical and Topological Shape Changes. Journal of Physical Chemistry B, 2009, 113, 8731-8737.	2.6	41
67	Mining Maximal Frequent Subgraphs in KEGG Reaction Networks. , 2009, , .		1
68	Mechanoelectric Feedback as a Trigger Mechanism for Cardiac Electrical Remodeling: A Model Study. Annals of Biomedical Engineering, 2008, 36, 1816-1835.	2.5	13
69	A unified theory for osteonal and hemi-osteonal remodeling. Bone, 2008, 42, 250-259.	2.9	152
70	Relating osteon diameter to strain. Bone, 2008, 43, 476-482.	2.9	103
71	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
72	Modeling Glucose and Water Dynamics in Human Skin. Diabetes Technology and Therapeutics, 2008, 10, 283-293.	4.4	30

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73	Heat Transfer on Walls in Molecular Dynamics Simulations: Modelling With Vibrating Reflective Walls. , 2008, , .		1
74	Velocity Correlations Between Impinging and Reflecting Particles Using MD Simulations and Different Wall Models. , 2008, , .		1
75	Velocity Correlations and Accommodation Coefficients for Gas-Wall Interactions in Nanochannels. , 2008, , .		5
76	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
77	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
78	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
79	New Derivation of a Particle Wall Boundary Condition in Molecular Dynamics. , 2007, , 767.		0
80	Stepwise Noncovalent Synthesis Leading to Dendrimer-Based Assemblies in Water. Journal of the American Chemical Society, 2007, 129, 15631-15638.	13.7	49
81	Lipid-Based Mechanisms for Vesicle Fission. Journal of Physical Chemistry B, 2007, 111, 5719-5725.	2.6	54
82	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
83	Heat Transfer Predictions for Micro/Nano-Channels at Atomistic Level Using Combined Molecular Dynamics and Monte Carlo Techniques. , 2007, , .		2
84	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
85	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
86	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
87	Vesicle Shapes from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 22780-22785.	2.6	62
88	A Detailed Look at Vesicle Fusion. Journal of Physical Chemistry B, 2006, 110, 13212-13219.	2.6	103
89	Novel Hybrid Simulations for Heat Transfer at Atomistic Level. , 2006, , 1315.		1
90	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

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91	Quantification of atherosclerotic plaque components using in vivo MRI and supervised classifiers. Magnetic Resonance in Medicine, 2006, 55, 790-799.	3.0	47
92	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
93	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
94	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
95	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
96	Computer simulations of successful defibrillation in decoupled and non-uniform cardiac tissue. Europace, 2005, 7, S166-S177.	1.7	17
97	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
98	Molecular dynamics study of the influence of wall-gas interactions on heat flow in nanochannels. Physical Review E, 2005, 71, 066702.	2.1	82
99	The Bilayerâ^'Vesicle Transition Is Entropy Driven. Journal of Physical Chemistry B, 2005, 109, 22649-22654.	2.6	80
100	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
101	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
102	Infinitely fast diffusion in single-file systems. Physical Review E, 2003, 67, 046707.	2.1	11
103	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
104	Laterally coupled jellium-like two-dimensional quantum dots. Journal of Physics Condensed Matter, 2003, 15, 6977-6984.	1.8	3
105	Steady-state properties of single-file systems with conversion. Physical Review E, 2002, 65, 066701.	2.1	25
106	Transient behavior in single-file systems. Physical Review E, 2002, 66, 066705.	2.1	9
107	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
108	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

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109	Efficient Monte Carlo methods for the simulation of catalytic surface reactions. Physical Review E, 1998, 58, 2598-2610.	2.1	198
110	Dynamic Monte Carlo Simulations of Oscillatory Reactions. Israel Journal of Chemistry, 1998, 38, 415-428.	2.3	5
111	Simulation of small-angle scattering from large assemblies of multi-type scatterer particles. Journal of Molecular Structure, 1996, 383, 303-308.	3.6	24
112	16. Parallel Molecular Dynamics on a Torus Network. , 1996, , 177-186.		0
113	Simulating Complex Fluids. Molecular Simulation, 1995, 14, 259-274.	2.0	14
114	Volume fraction dependence and reorganization in clusterâ€“cluster aggregation processes. Journal of Chemical Physics, 1995, 102, 480-495.	3.0	30
115	Simulating surfactant self-assembly. Journal of Physics Condensed Matter, 1994, 6, A351-A356.	1.8	10
116	Molecular dynamics study of nucleation and melting ofnâ€alkanes. Journal of Chemical Physics, 1994, 101, 9033-9041.	3.0	94
117	Simulating the Self-Assembly of Gemini (Dimeric) Surfactants. Science, 1994, 266, 254-256.	12.6	283
118	Parallel Computing and Molecular Dynamics Simulations. , 1993, , 473-495.		6
119	Computer simulations of surfactant self-assembly. Langmuir, 1993, 9, 9-11.	3.5	164
120	Molecular dynamics simulations of oil solubilization in surfactant solutions. Langmuir, 1993, 9, 1175-1178.	3.5	112
121	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
122	Computer simulations of surfactants at a liquid/liquid interface. , 1992, , 519-533.		3
123	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
124	Computer simulations of a water/oil interface in the presence of micelles. Nature, 1990, 348, 624-625.	27.8	294
125	Deadlock-free message routing in multicomputer networks. Distributed Computing, 1989, 3, 178-186.	0.8	9
126	The twisted cube. Lecture Notes in Computer Science, 1987, , 152-159.	1.3	132