Peter V Coveney

List of Publications by Year
in descending order

128 papers	4,754 citations	87888 38 h-index	123424 61 g-index
133 all docs	133 docs citations	133 times ranked	5459 citing authors

#	Article	IF	Citations
1	Thermodynamic and structural insights into the repurposing of drugs that bind to SARS-CoV-2 main protease. Molecular Systems Design and Engineering, 2022, 7, 123-131.	3.4	5
2	Hybrid parallelization of molecular dynamics simulations to reduce load imbalance. Journal of Supercomputing, 2022, 78, 9184-9215.	3.6	3
3	Large Scale Study of Ligandâ€“Protein Relative Binding Free Energy Calculations: Actionable Predictions from Statistically Robust Protocols. Journal of Chemical Theory and Computation, 2022, 18, 2687-2702.	5.3	14
4	Ensemble Simulations and Experimental Free Energy Distributions: Evaluation and Characterization of Isoxazole Amides as SMYD3 Inhibitors. Journal of Chemical Information and Modeling, 2022, 62, 2561-2570.	5.4	6
5	Alchemical Free Energy Estimators and Molecular Dynamics Engines: Accuracy, Precision, and Reproducibility. Journal of Chemical Theory and Computation, 2022, 18, 3972-3987.	5.3	12
6	The performance of ensemble-based free energy protocols in computing binding affinities to ROS1 kinase. Scientific Reports, 2022, 12, .	3.3	2
7	Accelerating Heterogeneous Multiscale Simulations of Advanced Materials Properties with Graphâ€Based Clustering. Advanced Theory and Simulations, 2021, 4, 2000234.	2.8	1
8	The influence of external electric fields on proton transfer tautomerism in the guanineâ€“cytosine base pair. Physical Chemistry Chemical Physics, 2021, 23, 6252-6265.	2.8	10
9	Pharmaceutical Industryâ€”Academia Cooperation. , 2021, , 307-322.		0
10	The impact of uncertainty on predictions of the CovidSim epidemiological code. Nature Computational Science, 2021, 1, 128-135.	8.0	45
11	When we can trust computers (and when we can't). Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200067.	3.4	12
12	Reliability and reproducibility in computational science: implementing validation, verification and uncertainty quantification in silico. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200409.	3.4	9
13	Uncertainty quantification in classical molecular dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200082.	3.4	44
14	The effect of protein mutations on drug binding suggests ensuing personalised drug selection. Scientific Reports, 2021, 11, 13452.	3.3	11
15	Scalable HPC & AI infrastructure for COVID-19 therapeutics. , 2021, , .		12
16	Ensembles Are Required to Handle Aleatoric and Parametric Uncertainty in Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2021, 17, 5187-5197.	5.3	18
17	Tutorial applications for Verification, Validation and Uncertainty Quantification using VECMA toolkit. Journal of Computational Science, 2021, 53, 101402.	2.9	4
18	Implementation of measurement reduction for the variational quantum eigensolver. Physical Review Research, 2021, 3, .	3.6	10

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19	Principles of Small-Molecule Transport through Synthetic Nanopores. ACS Nano, 2021, 15, 16194-16206.	14.6	14
20	TIES 20: Relative Binding Free Energy with a Flexible Superimposition Algorithm and Partial Ring Morphing. Journal of Chemical Theory and Computation, 2021, 17, 1250-1265.	5.3	14
21	IMPECCABLE: Integrated Modeling PipelinE for COVID Cure by Assessing Better LEads. , 2021, , .		13
22	Pandemic drugs at pandemic speed: infrastructure for accelerating COVID-19 drug discovery with hybrid machine learning- and physics-based simulations on high-performance computers. Interface Focus, 2021, 11, 20210018.	3.0	23
23	Computational biomedicine. Part II: organs and systems. Interface Focus, 2021, 11, 20200082.	3.0	3
24	Towards blood flow in the virtual human: efficient self-coupling of HemeLB. Interface Focus, 2021, 11, 20190119.	3.0	10
25	Principles governing control of aggregation and dispersion of aqueous graphene oxide. Scientific Reports, 2021, 11, 22460.	3.3	17
26	Toward High Fidelity Materials Property Prediction from Multiscale Modeling and Simulation. Advanced Theory and Simulations, 2020, 3, 1900122.	2.8	12
27	Accuracy and Precision of Alchemical Relative Free Energy Predictions with and without Replicaâ€Exchange. Advanced Theory and Simulations, 2020, 3, 1900195.	2.8	30
28	Building Confidence in Simulation: Applications of EasyVVUQ. Advanced Theory and Simulations, 2020, 3, 1900246.	2.8	21
29	Principles Governing Control of Aggregation and Dispersion of Graphene and Graphene Oxide in Polymer Melts. Advanced Materials, 2020, 32, e2003213.	21.0	97
30	Hit-to-lead and lead optimization binding free energy calculations for G protein-coupled receptors. Interface Focus, 2020, 10, 20190128.	3.0	11
31	Large-scale binding affinity calculations on commodity compute clouds. Interface Focus, 2020, 10, 20190133.	3.0	3
32	Rapid, accurate, precise and reproducible ligandâ€“protein binding free energy prediction. Interface Focus, 2020, 10, 20200007.	3.0	77
33	Computational biomedicine. Part 1: molecular medicine. Interface Focus, 2020, 10, 20200047.	3.0	3
34	The influence of base pair tautomerism on single point mutations in aqueous DNA. Interface Focus, 2020, 10, 20190120.	3.0	29
35	From digital hype to analogue reality: Universal simulation beyond the quantum and exascale eras. Journal of Computational Science, 2020, 46, 101093.	2.9	5
36	Application of the ESMACS Binding Free Energy Protocol to a Multiâ€Binding Site Lactate Dehydogenase A Ligand Dataset. Advanced Theory and Simulations, 2020, 3, 1900194.	2.8	9

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37	EasyVVUQ: A Library for Verification, Validation and Uncertainty Quantification in High Performance Computing. Journal of Open Research Software, 2020, 8, 11.	5.9	34
38	Introducing VECMAtk - Verification, Validation and Uncertainty Quantification for Multiscale and HPC Simulations. Lecture Notes in Computer Science, 2019, , 479-492.	1.3	14
39	A New Pathology in the Simulation of Chaotic Dynamical Systems on Digital Computers. Advanced Theory and Simulations, 2019, 2, 1900125.	2.8	22
40	The Role of Graphene in Enhancing the Material Properties of Thermosetting Polymers. Advanced Theory and Simulations, 2019, 2, 1800168.	2.8	13
41	Modeling Nanostructure in Graphene Oxide: Inhomogeneity and the Percolation Threshold. Journal of Chemical Information and Modeling, 2019, 59, 2741-2745.	5.4	48
42	Ensemble-Based Steered Molecular Dynamics Predicts Relative Residence Time of A_{2A} Receptor Binders. Journal of Chemical Theory and Computation, 2019, 15, 3316-3330.	5.3	39
43	Big data: the end of the scientific method?. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180145.	3.4	68
44	Multiscale modelling, simulation and computing: from the desktop to the exascale. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180355.	3.4	12
45	Multiscale computing for science and engineering in the era of exascale performance. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180144.	3.4	18
46	Application of ESMACS binding free energy protocols to diverse datasets: Bromodomain-containing protein 4. Scientific Reports, 2019, 9, 6017.	3.3	18
47	The heterogeneous multiscale method applied to inelastic polymer mechanics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180150.	3.4	12
48	Micromechanical exfoliation of graphene on the atomistic scale. Physical Chemistry Chemical Physics, 2019, 21, 5716-5722.	2.8	84
49	Ordering of Trotterization: Impact on Errors in Quantum Simulation of Electronic Structure. Entropy, 2019, 21, 1218.	2.2	33
50	Ensemble-Based Replica Exchange Alchemical Free Energy Methods: The Effect of Protein Mutations on Inhibitor Binding. Journal of Chemical Theory and Computation, 2019, 15, 1265-1277.	5.3	28
51	Uncertainty Quantification in Alchemical Free Energy Methods. Journal of Chemical Theory and Computation, 2018, 14, 2867-2880.	5.3	54
52	Grapheneâ€“Graphene Interactions: Friction, Superlubricity, and Exfoliation. Advanced Materials, 2018, 30, e1705791.	21.0	105
53	Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations. , 2018, , .		7
54	High-throughput binding affinity calculations at extreme scales. BMC Bioinformatics, 2018, 19, 482.	2.6	14

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55	A Comparison of the Bravyiâ€“Kitaev and Jordanâ€“Wigner Transformations for the Quantum Simulation of Quantum Chemistry. Journal of Chemical Theory and Computation, 2018, 14, 5617-5630.	5.3	75
56	Validation of Patient-Specific Cerebral Blood Flow Simulation Using Transcranial Doppler Measurements. Frontiers in Physiology, 2018, 9, 721.	2.8	22
57	A Mechanistic Model for Predicting Cell Surface Presentation of Competing Peptides by MHC Class I Molecules. Frontiers in Immunology, 2018, 9, 1538.	4.8	35
58	PolNet: A Tool to Quantify Network-Level Cell Polarity and Blood Flow in Vascular Remodeling. Biophysical Journal, 2018, 114, 2052-2058.	0.5	29
59	Enabling Trade-offs Between Accuracy and Computational Cost: Adaptive Algorithms to Reduce Time to Clinical Insight. , 2018, , .		5
60	Chemically Specific Multiscale Modeling of the Shear-Induced Exfoliation of Clayâ€“Polymer Nanocomposites. ACS Omega, 2018, 3, 6439-6445.	3.5	8
61	An Ensemble-Based Protocol for the Computational Prediction of Helixâ€“Helix Interactions in G Protein-Coupled Receptors using Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 2254-2270.	5.3	27
62	Evaluation and Characterization of Trk Kinase Inhibitors for the Treatment of Pain: Reliable Binding Affinity Predictions from Theory and Computation. Journal of Chemical Information and Modeling, 2017, 57, 897-909.	5.4	30
63	Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study. Journal of Chemical Theory and Computation, 2017, 13, 784-795.	5.3	59
64	Rapid, Accurate, Precise, and Reliable Relative Free Energy Prediction Using Ensemble Based Thermodynamic Integration. Journal of Chemical Theory and Computation, 2017, 13, 210-222.	5.3	101
65	Multiscale computing in the exascale era. Journal of Computational Science, 2017, 22, 15-25.	2.9	54
66	Host genotype and time dependent antigen presentation of viral peptides: predictions from theory. Scientific Reports, 2017, 7, 14367.	3.3	14
67	The Role of Multiscale Protein Dynamics in Antigen Presentation and T Lymphocyte Recognition. Frontiers in Immunology, 2017, 8, 797.	4.8	17
68	On the calculation of equilibrium thermodynamic properties from molecular dynamics. Physical Chemistry Chemical Physics, 2016, 18, 30236-30240.	2.8	80
69	Big data need big theory too. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160153.	3.4	139
70	Bridging the gaps at the physicsâ€“chemistryâ€“biology interface. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160335.	3.4	35
71	FabSim: Facilitating computational research through automation on large-scale and distributed e-infrastructures. Computer Physics Communications, 2016, 207, 375-385.	7.5	32
72	Non-canonical Wnt signalling modulates the endothelial shear stress flow sensor in vascular remodelling. ELife, 2016, 5, e07727.	6.0	125

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73	The <scp>B</scp>ravyiâ€“<scp>K</scp>itaev transformation: Properties and applications. International Journal of Quantum Chemistry, 2015, 115, 1431-1441.	2.0	93
74	Rapid, Precise, and Reproducible Prediction of Peptideâ€“MHC Binding Affinities from Molecular Dynamics That Correlate Well with Experiment. Journal of Chemical Theory and Computation, 2015, 11, 3346-3356.	5.3	122
75	Mechanism of Exfoliation and Prediction of Materials Properties of Clayâ€“Polymer Nanocomposites from Multiscale Modeling. Nano Letters, 2015, 15, 8108-8113.	9.1	45
76	The Effect of Mutations on Drug Sensitivity and Kinase Activity of Fibroblast Growth Factor Receptors: A Combined Experimental and Theoretical Study. EBioMedicine, 2015, 2, 194-204.	6.1	60
77	Mutation V111I in HIV-2 Reverse Transcriptase Increases the Fitness of the Nucleoside Analogue-Resistant K65R and Q151M Viruses. Journal of Virology, 2015, 89, 833-843.	3.4	15
78	An automated multiscale ensemble simulation approach for vascular blood flow. Journal of Computational Science, 2015, 9, 150-155.	2.9	14
79	Chemically Specific Multiscale Modeling of Clayâ€“Polymer Nanocomposites Reveals Intercalation Dynamics, Tactoid Selfâ€Assembly and Emergent Materials Properties. Advanced Materials, 2015, 27, 966-984.	21.0	98
80	Computing the Role of Near Attack Conformations in an Enzyme-Catalyzed Nucleophilic Bimolecular Reaction. Journal of Chemical Theory and Computation, 2015, 11, 316-324.	5.3	35
81	Comparative analysis of nucleotide translocation through protein nanopores using steered molecular dynamics and an adaptive biasing force. Journal of Computational Chemistry, 2014, 35, 692-702.	3.3	23
82	Detachment energies of spheroidal particles from fluid-fluid interfaces. Journal of Chemical Physics, 2014, 141, 154902.	3.0	46
83	Survey of Multiscale and Multiphysics Applications and Communities. Computing in Science and Engineering, 2014, 16, 34-43.	1.2	56
84	Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2014, 10, 1228-1241.	5.3	123
85	Choice of boundary condition for lattice-Boltzmann simulation of moderate-Reynolds-number flow in complex domains. Physical Review E, 2014, 89, 023303.	2.1	48
86	Deformability-based red blood cell separation in deterministic lateral displacement devicesâ€”A simulation study. Biomicrofluidics, 2014, 8, 054114.	2.4	116
87	Multiscale modelling and simulation: a position paper. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130377.	3.4	64
88	Computer simulations reveal complex distribution of haemodynamic forces in a mouse retina model of angiogenesis. Journal of the Royal Society Interface, 2014, 11, 20140543.	3.4	87
89	Multiscale modelling: approaches and challenges. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130390.	3.4	31
90	Integrative approaches to computational biomedicine. Interface Focus, 2013, 3, 20130003.	3.0	10

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91	Impact of blood rheology on wall shear stress in a model of the middle cerebral artery. Interface Focus, 2013, 3, 20120094.	3.0	41
92	Disentangling Steric and Electrostatic Factors in Nanoscale Transport Through Confined Space. Nano Letters, 2013, 13, 3890-3896.	9.1	19
93	Navigating legal constraints in clinical data warehousing: a case study in personalized medicine. Interface Focus, 2013, 3, 20120088.	3.0	2
94	Mechanism of Drug Efficacy Within the EGF Receptor Revealed by Microsecond Molecular Dynamics Simulation. Molecular Cancer Therapeutics, 2012, 11, 2394-2400.	4.1	13
95	From base pair to bedside: molecular simulation and the translation of genomics to personalized medicine. Wiley Interdisciplinary Reviews: Systems Biology and Medicine, 2012, 4, 585-598.	6.6	11
96	Theory, modelling and simulation in origins of life studies. Chemical Society Reviews, 2012, 41, 5430.	38.1	65
97	IMENSE: An e-infrastructure environment for patient specific multiscale data integration, modelling and clinical treatment. Journal of Computational Science, 2012, 3, 314-327.	2.9	13
98	Global Conformational Dynamics of HIV-1 Reverse Transcriptase Bound to Non-Nucleoside Inhibitors. Biology, 2012, 1, 222-244.	2.8	6
99	Quantized Water Access to the HIV-1 Protease Active Site as a Proposed Mechanism for Cooperative Mutations in Drug Affinity. Biochemistry, 2012, 51, 6487-6489.	2.5	3
100	Resolution of Discordant HIV-1 Protease Resistance Rankings Using Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2011, 51, 2636-2649.	5.4	10
101	Rapid and accurate ranking of binding affinities of epidermal growth factor receptor sequences with selected lung cancer drugs. Journal of the Royal Society Interface, 2011, 8, 1114-1127.	3.4	33
102	T-cell epitope prediction and immune complex simulation using molecular dynamics: state of the art and persisting challenges. Immunome Research, 2010, 6, S4.	0.1	25
103	Accurate Ensemble Molecular Dynamics Binding Free Energy Ranking of Multidrug-Resistant HIV-1 Proteases. Journal of Chemical Information and Modeling, 2010, 50, 890-905.	5.4	82
104	Computer simulation study of the materials properties of intercalated and exfoliated poly(ethylene)glycol clay nanocomposites. Soft Matter, 2009, 5, 2239.	2.7	57
105	Determination of Free Energy Profiles for the Translocation of Polynucleotides through Î±-Hemolysin Nanopores using Non-Equilibrium Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2009, 5, 2135-2148.	5.3	33
106	Materials properties of clay nanocomposites: onset of negative Poisson ratio in large-scale molecular dynamics simulation. Soft Matter, 2009, 5, 3896.	2.7	15
107	Determining materials properties of natural composites using molecular simulation. Journal of Materials Chemistry, 2009, 19, 7251.	6.7	21
108	Recent advances in large-scale atomistic and coarse-grained molecular dynamics simulation of clay minerals. Journal of Materials Chemistry, 2009, 19, 2482.	6.7	74

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109	A critical appraisal of polymerâ€“clay nanocomposites. Chemical Society Reviews, 2008, 37, 568-594.	38.1	369
110	Automated Molecular Simulation Based Binding Affinity Calculator for Ligand-Bound HIV-1 Proteases. Journal of Chemical Information and Modeling, 2008, 48, 1909-1919.	5.4	52
111	Patient-specific simulation as a basis for clinical decision-making. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2008, 366, 3199-3219.	3.4	37
112	Virtual Physiological Human research initiative: the future for rational HIV treatment design?. Future HIV Therapy, 2008, 2, 419-425.	0.4	1
113	Rapid, Accurate, and Precise Calculation of Relative Binding Affinities for the SH2 Domain Using a Computational Grid. Journal of Chemical Theory and Computation, 2007, 3, 1193-1202.	5.3	16
114	NEKTAR, SPICE and Vortonics: using federated grids for large scale scientific applications. Cluster Computing, 2007, 10, 351-364.	5.0	22
115	On the application of computer simulation techniques to anionic and cationic clays: A materials chemistry perspective. Journal of Materials Chemistry, 2006, 16, 708-723.	6.7	124
116	Intercalation and in situ polymerization of poly(alkylene oxide) derivatives within M+-montmorillonite (M = Li, Na, K). Journal of Materials Chemistry, 2006, 16, 1082.	6.7	45
117	Coarse-graining and renormalization group methods for the elucidation of the kinetics of complex nucleation and growth processes. Molecular Physics, 2006, 104, 177-185.	1.7	7
118	Grid-based steered thermodynamic integration accelerates the calculation of binding free energies. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 1999-2015.	3.4	23
119	WEDS: a Web services-based environment for distributed simulation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 1807-1816.	3.4	7
120	Scientific Grid computing. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 1707-1713.	3.4	27
121	Morphology and elastic modulus of novel poly[oligo(ethylene glycol) diacrylate]-montmorillonite nanocomposites. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 1785-1793.	2.1	9
122	Chiral polymerization and the RNA world. International Journal of Astrobiology, 2005, 4, 63-73.	1.6	5
123	Molecular Basis of Peptide Recognition by the TCR: Affinity Differences Calculated Using Large Scale Computing. Journal of Immunology, 2005, 175, 1715-1723.	0.8	31
124	Peptide recognition by the T cell receptor: comparison of binding free energies from thermodynamic integration, Poissonâ€“Boltzmann and linear interaction energy approximations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 2037-2053.	3.4	32
125	Modelling biological complexity: a physical scientist's perspective. Journal of the Royal Society Interface, 2005, 2, 267-280.	3.4	104
126	Combined experimental and theoretical investigations of clayâ€“polymer nanocomposites: intercalation of single bifunctional organic compounds in Na+-montmorillonite and Na+-hectorite clays for the design of new materials. Journal of Materials Chemistry, 2003, 13, 2540-2550.	6.7	55

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127	Selfâ€“organization and complexity: a new age for theory, computation and experiment. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 1057-1079.	3.4	39
128	The arrow of time. Nature, 1991, 350, 456-456.	27.8	15