

Thomas E Ouldrige

List of Publications by Year in descending order

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65
papers

3,967
citations

172386

29
h-index

133188

59
g-index

72
all docs

72
docs citations

72
times ranked

2684
citing authors

#	ARTICLE	IF	CITATIONS
1	On the biophysics and kinetics of toehold-mediated DNA strand displacement. <i>Nucleic Acids Research</i> , 2013, 41, 10641-10658.	6.5	423
2	Structural, mechanical, and thermodynamic properties of a coarse-grained DNA model. <i>Journal of Chemical Physics</i> , 2011, 134, 085101.	1.2	379
3	Introducing improved structural properties and salt dependence into a coarse-grained model of DNA. <i>Journal of Chemical Physics</i> , 2015, 142, 234901.	1.2	267
4	Sequence-dependent thermodynamics of a coarse-grained DNA model. <i>Journal of Chemical Physics</i> , 2012, 137, 135101.	1.2	265
5	DNA hybridization kinetics: zippering, internal displacement and sequence dependence. <i>Nucleic Acids Research</i> , 2013, 41, 8886-8895.	6.5	203
6	Coarse-graining DNA for simulations of DNA nanotechnology. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20395.	1.3	173
7	Programmable energy landscapes for kinetic control of DNA strand displacement. <i>Nature Communications</i> , 2014, 5, 5324.	5.8	172
8	DNA Nanotweezers Studied with a Coarse-Grained Model of DNA. <i>Physical Review Letters</i> , 2010, 104, 178101.	2.9	162
9	Guiding the folding pathway of DNA origami. <i>Nature</i> , 2015, 525, 82-86.	13.7	146
10	A nucleotide-level coarse-grained model of RNA. <i>Journal of Chemical Physics</i> , 2014, 140, 235102.	1.2	117
11	Optimizing DNA Nanotechnology through Coarse-Grained Modeling: A Two-Footed DNA Walker. <i>ACS Nano</i> , 2013, 7, 2479-2490.	7.3	88
12	Force-Induced Rupture of a DNA Duplex: From Fundamentals to Force Sensors. <i>ACS Nano</i> , 2015, 9, 11993-12003.	7.3	86
13	Direct Simulation of the Self-Assembly of a Small DNA Origami. <i>ACS Nano</i> , 2016, 10, 1724-1737.	7.3	86
14	Plectoneme tip bubbles: Coupled denaturation and writhing in supercoiled DNA. <i>Scientific Reports</i> , 2015, 5, 7655.	1.6	84
15	Fundamental Limits to Cellular Sensing. <i>Journal of Statistical Physics</i> , 2016, 162, 1395-1424.	0.5	74
16	Modeling DNA-Strand Displacement Reactions in the Presence of Base-Pair Mismatches. <i>Journal of the American Chemical Society</i> , 2020, 142, 11451-11463.	6.6	70
17	Coarse-grained simulations of DNA overstretching. <i>Journal of Chemical Physics</i> , 2013, 138, 085101.	1.2	66
18	Design of hidden thermodynamic driving for non-equilibrium systems via mismatch elimination during DNA strand displacement. <i>Nature Communications</i> , 2020, 11, 2562.	5.8	66

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19	DNA hairpins destabilize duplexes primarily by promoting melting rather than by inhibiting hybridization. <i>Nucleic Acids Research</i> , 2015, 43, 6181-6190.	6.5	54
20	Modelling Toehold-Mediated RNA Strand Displacement. <i>Biophysical Journal</i> , 2015, 108, 1238-1247.	0.2	54
21	Extracting bulk properties of self-assembling systems from small simulations. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 104102.	0.7	47
22	Biochemical Machines for the Interconversion of Mutual Information and Work. <i>Physical Review Letters</i> , 2017, 118, 028101.	2.9	46
23	Coarse-grained simulation of DNA using LAMMPS. <i>European Physical Journal E</i> , 2018, 41, 57.	0.7	46
24	Thermodynamics of Computational Copying in Biochemical Systems. <i>Physical Review X</i> , 2017, 7, .	2.8	44
25	New Langevin and gradient thermostats for rigid body dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 144114.	1.2	37
26	The self-assembly of DNA Holliday junctions studied with a minimal model. <i>Journal of Chemical Physics</i> , 2009, 130, 065101.	1.2	36
27	DNA Cruciform Arms Nucleate through a Correlated but Asynchronous Cooperative Mechanism. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11616-11625.	1.2	36
28	DNA nanotechnology: understanding and optimisation through simulation. <i>Molecular Physics</i> , 2015, 113, 1-15.	0.8	34
29	Kinetics of RNA and RNA:DNA Hybrid Strand Displacement. <i>ACS Synthetic Biology</i> , 2021, 10, 3066-3073.	1.9	34
30	DNA bipedal motor walking dynamics: an experimental and theoretical study of the dependency on step size. <i>Nucleic Acids Research</i> , 2018, 46, 1553-1561.	6.5	33
31	Fundamental Costs in the Production and Destruction of Persistent Polymer Copies. <i>Physical Review Letters</i> , 2017, 118, 158103.	2.9	31
32	Simulating a burnt-bridges DNA motor with a coarse-grained DNA model. <i>Natural Computing</i> , 2014, 13, 535-547.	1.8	30
33	Coarse-Grained Modelling of DNA and DNA Self-Assembly. <i>Springer Theses</i> , 2012, , .	0.0	29
34	Self-Limiting Polymerization of DNA Origami Subunits with Strain Accumulation. <i>ACS Nano</i> , 2020, 14, 17428-17441.	7.3	29
35	A Primer on the oxDNA Model of DNA: When to Use it, How to Simulate it and How to Interpret the Results. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 693710.	1.6	29
36	The effect of topology on the structure and free energy landscape of DNA kissing complexes. <i>Journal of Chemical Physics</i> , 2012, 136, 215102.	1.2	28

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37	Modelling DNA origami self-assembly at the domain level. <i>Journal of Chemical Physics</i> , 2015, 143, 165102.	1.2	28
38	Multiscale simulations of anisotropic particles combining molecular dynamics and Green's function reaction dynamics. <i>Journal of Chemical Physics</i> , 2017, 146, 114106.	1.2	28
39	The importance of thermodynamics for molecular systems, and the importance of molecular systems for thermodynamics. <i>Natural Computing</i> , 2018, 17, 3-29.	1.8	28
40	The Role of Loop Stacking in the Dynamics of DNA Hairpin Formation. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14326-14335.	1.2	27
41	Identifying Physical Causes of Apparent Enhanced Cyclization of Short DNA Molecules with a Coarse-Grained Model. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4660-4672.	2.3	22
42	Handhold-Mediated Strand Displacement: A Nucleic Acid Based Mechanism for Generating Far-from-Equilibrium Assemblies through Templated Reactions. <i>ACS Nano</i> , 2021, 15, 3272-3283.	7.3	22
43	Chemical Boltzmann Machines. <i>Lecture Notes in Computer Science</i> , 2017, , 210-231.	1.0	21
44	Inferring bulk self-assembly properties from simulations of small systems with multiple constituent species and small systems in the grand canonical ensemble. <i>Journal of Chemical Physics</i> , 2012, 137, 144105.	1.2	19
45	Multi-scale coarse-graining for the study of assembly pathways in DNA-brick self-assembly. <i>Journal of Chemical Physics</i> , 2018, 148, 134910.	1.2	18
46	Synthetic biology and bioelectrochemical tools for electrogenetic system engineering. <i>Science Advances</i> , 2022, 8, eabm5091.	4.7	17
47	Characterizing the bending and flexibility induced by bulges in DNA duplexes. <i>Journal of Chemical Physics</i> , 2015, 142, 165101.	1.2	16
48	What we learn from the learning rate. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2017, 2017, 063502.	0.9	15
49	The Robustness of Proofreading to Crowding-Induced Pseudo-Processivity in the MAPK Pathway. <i>Biophysical Journal</i> , 2014, 107, 2425-2435.	0.2	14
50	Nonequilibrium correlations in minimal dynamical models of polymer copying. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 1946-1951.	3.3	14
51	Biochemical Szilard engines for memory-limited inference. <i>New Journal of Physics</i> , 2019, 21, 063022.	1.2	11
52	<i>In situ</i> Generation of RNA Complexes for Synthetic Molecular Strand-Displacement Circuits in Autonomous Systems. <i>Nano Letters</i> , 2021, 21, 265-271.	4.5	11
53	Physical limitations of work extraction from temporal correlations. <i>Physical Review E</i> , 2019, 99, 042115.	0.8	7
54	Designing the optimal bit: balancing energetic cost, speed and reliability. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2017, 473, 20170117.	1.0	6

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55	Geometric integrator for Langevin systems with quaternion-based rotational degrees of freedom and hydrodynamic interactions. <i>Journal of Chemical Physics</i> , 2017, 147, 224103.	1.2	6
56	Quasi-robust control of biochemical reaction networks via stochastic morphing. <i>Journal of the Royal Society Interface</i> , 2021, 18, 20200985.	1.5	6
57	Edge-effects dominate copying thermodynamics for finite-length molecular oligomers. <i>New Journal of Physics</i> , 2021, 23, 063061.	1.2	4
58	Building an RNA-Based Toggle Switch Using Inhibitory RNA Aptamers. <i>ACS Synthetic Biology</i> , 2022, 11, 562-569.	1.9	4
59	High rates of fuel consumption are not required by insulating motifs to suppress retroactivity in biochemical circuits. <i>Engineering Biology</i> , 2017, 1, 86-99.	0.8	3
60	Minimal mechanism for cyclic templating of length-controlled copolymers under isothermal conditions. <i>Journal of Chemical Physics</i> , 2022, 156, 074103.	1.2	3
61	Optimizing enzymatic catalysts for rapid turnover of substrates with low enzyme sequestration. <i>Biological Cybernetics</i> , 2020, 114, 653-668.	0.6	2
62	Modelling DNA Tweezers. <i>Springer Theses</i> , 2012, , 93-100.	0.0	0
63	Thermodynamic Properties of Model DNA. <i>Springer Theses</i> , 2012, , 71-92.	0.0	0
64	Students go through the gears at the iGEM competition for engineering biology. <i>Biochemist</i> , 2019, 41, 58-61.	0.2	0
65	Free energy landscapes of DNA and its assemblies: perspectives from coarse-grained modelling. <i>Frontiers of Nanoscience</i> , 2022, , 195-210.	0.3	0