Christopher Roland

List of Publications by Year
in descending order

91 papers	3,244 citations	136740 32 h-index	155451 55 g-index
92 all docs	92 docs citations	92 times ranked	2912 citing authors

#	Article	IF	Citations
1	Novel eGZ-motif formed by regularly extruded guanine bases in a left-handed Z-DNA helix as a major motif behind CGG trinucleotide repeats. Nucleic Acids Research, 2022, 50, 4860-4876.	6.5	10
2	The F19W mutation reduces the binding affinity of the transmembrane AÎ²11â€“40 trimer to the membrane bilayer. RSC Advances, 2021, 11, 2664-2676.	1.7	2
3	Molecular conformations and dynamics of nucleotide repeats associated with neurodegenerative diseases: double helices and CAG hairpin loops. Computational and Structural Biotechnology Journal, 2021, 19, 2819-2832.	1.9	11
4	Construction of DNA/RNA Triplex Helices Based on GAA/TTC Trinucleotide Repeats. Bio-protocol, 2021, 11, e4155.	0.2	2
5	Atypical structures of GAA/TTC trinucleotide repeats underlying Friedreichâ€™s ataxia: DNA triplexes and RNA/DNA hybrids. Nucleic Acids Research, 2020, 48, 9899-9917.	6.5	25
6	Dynamics of strand slippage in DNA hairpins formed by CAG repeats: roles of sequence parity and trinucleotide interrupts. Nucleic Acids Research, 2020, 48, 2232-2245.	6.5	39
7	Structure and Dynamics of DNA and RNA Double Helices Obtained from the CCG and GGC Trinucleotide Repeats. Journal of Physical Chemistry B, 2018, 122, 4491-4512.	1.2	16
8	Structural and Dynamical Characterization of DNA and RNA Quadruplexes Obtained from the GGGGCC and GGGCCT Hexanucleotide Repeats Associated with C9FTD/ALS and SCA36 Diseases. ACS Chemical Neuroscience, 2018, 9, 1104-1117.	1.7	22
9	E-motif formed by extrahelical cytosine bases in DNA homoduplexes of trinucleotide and hexanucleotide repeats. Nucleic Acids Research, 2018, 46, 942-955.	6.5	19
10	Structure and Dynamics of DNA and RNA Double Helices Obtained from the GGGGCC and CCCCGG Hexanucleotide Repeats That Are the Hallmark of C9FTD/ALS Diseases. ACS Chemical Neuroscience, 2017, 8, 578-591.	1.7	31
11	Structure and Dynamics of DNA and RNA Double Helices of CAG and GAC Trinucleotide Repeats. Biophysical Journal, 2017, 113, 19-36.	0.2	19
12	Comparative melting and healing of B-DNA and Z-DNA by an infrared laser pulse. Journal of Chemical Physics, 2016, 144, 145101.	1.2	6
13	Picosecond infrared laser-induced all-atom nonequilibrium molecular dynamics simulation of dissociation of viruses. Physical Chemistry Chemical Physics, 2016, 18, 11951-11958.	1.3	9
14	Amyloid Properties of Asparagine and Glutamine in Prion-like Proteins. ACS Chemical Neuroscience, 2016, 7, 576-587.	1.7	30
15	Picosecond dissociation of amyloid fibrils with infrared laser: A nonequilibrium simulation study. Journal of Chemical Physics, 2015, 143, 155101.	1.2	41
16	Calculating transition and reaction rates with nonequilibrium work measurements. Journal of Physics: Conference Series, 2015, 640, 012014.	0.3	0
17	The Adaptively Biased Molecular Dynamics method revisited: New capabilities and an application. Journal of Physics: Conference Series, 2015, 640, 012020.	0.3	12
18	Structural Determinants of Polyglutamine Protofibrils and Crystallites. ACS Chemical Neuroscience, 2015, 6, 632-645.	1.7	12

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19	Picosecond melting of peptide nanotubes using an infrared laser: a nonequilibrium simulation study. Physical Chemistry Chemical Physics, 2015, 17, 27275-27280.	1.3	14
20	Investigating rare events with nonequilibrium work measurements. II. Transition and reaction rates. Journal of Chemical Physics, 2014, 140, 034115.	1.2	13
21	Investigating rare events with nonequilibrium work measurements. I. Nonequilibrium transition path probabilities. Journal of Chemical Physics, 2014, 140, 034114.	1.2	14
22	Ion distributions around left- and right-handed DNA and RNA duplexes: a comparative study. Nucleic Acids Research, 2014, 42, 13981-13996.	6.5	53
23	Recipes for Free Energy Calculations in Biomolecular Systems. Methods in Molecular Biology, 2013, 924, 313-337.	0.4	6
24	Reaction path ensemble of the Bâ€“Z-DNA transition: a comprehensive atomistic study. Nucleic Acids Research, 2013, 41, 33-43.	6.5	48
25	Are Long-Range Structural Correlations Behind the Aggregration Phenomena of Polyglutamine Diseases?. PLoS Computational Biology, 2012, 8, e1002501.	1.5	18
26	A Statistical Analysis of the PPII Propensity of Amino Acid Guests in Proline-Rich Peptides. Biophysical Journal, 2011, 100, 1083-1093.	0.2	24
27	PPII Propensity of Multiple-Guest Amino Acids in a Proline-Rich Environment. Journal of Physical Chemistry B, 2011, 115, 8645-8656.	1.2	17
28	Calculating relative transition rates with driven nonequilibrium simulations. Chemical Physics Letters, 2011, 518, 109-113.	1.2	18
29	The Î±â€sheet: A missingâ€inâ€action secondary structure?. Proteins: Structure, Function and Bioinformatics, 2011, 79, 937-946.	1.5	19
30	Free energy and structure of polyproline peptides: An ab initio and classical molecular dynamics investigation. International Journal of Quantum Chemistry, 2010, 110, 2865-2879.	1.0	16
31	Dimerization free energy of vancomycinâ€group antibiotics and the cooperative effect: A density functional approach. International Journal of Quantum Chemistry, 2010, 110, 2894-2902.	1.0	2
32	A classical molecular dynamics investigation of the free energy and structure of short polyproline conformers. Journal of Chemical Physics, 2010, 133, 125104.	1.2	32
33	Conformations and free energy landscapes of polyproline peptides. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20746-20751.	3.3	92
34	Adaptively biased molecular dynamics: An umbrella sampling method with a timeâ€dependent potential. International Journal of Quantum Chemistry, 2009, 109, 3666-3678.	1.0	35
35	Structural determination of large molecules through the reassembly of optimized fragments. Journal of Molecular Graphics and Modelling, 2008, 27, 364-375.	1.3	4
36	Amino Acid Adsorption on the Si(100) Surface:â€‰ The Case of Glycine. Journal of Physical Chemistry C, 2008, 112, 2640-2648.	1.5	11

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37	Adaptively biased molecular dynamics for free energy calculations. Journal of Chemical Physics, 2008, 128, 134101.	1.2	168
38	Ab initiosimulations of H2in Li-doped carbon nanotube systems. Journal of Physics Condensed Matter, 2007, 19, 086226.	0.7	8
39	Chapter 7 Nonequilibrium Green's function modeling of the quantum transport of molecular electronic devices. Theoretical and Computational Chemistry, 2007, , 187-204.	0.2	2
40	Deprotonation of Solvated Formic Acid:Â Carâ"Parrinello and Metadynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 2325-2331.	1.2	51
41	The free energy landscape of small peptides as obtained from metadynamics with umbrella sampling corrections. Journal of Chemical Physics, 2006, 125, 204909.	1.2	74
42	New Distributed Multipole Metdhods for Accurate Electrostatics in Large-Scale Biomolecular Simulations. , 2006, , 297-312.		1
43	Quantum Chemistry Simulations of Glycopeptide Antibiotics. , 2006, , 343-351.		2
44	Self-assembled patterns and strain-induced instabilities for modulated systems. Physical Review E, 2005, 72, 021504.	0.8	9
45	New and Exotic Self-Organized Patterns for Modulated Nanoscale Systems. Nano Letters, 2005, 5, 389-395.	4.5	5
46	Quantum Simulations of the Structure and Binding of Glycopeptide Antibiotic Aglycons to Cell Wall Analogues. Journal of Physical Chemistry B, 2005, 109, 20588-20596.	1.2	10
47	Capacitance, induced charges, and bound states of biased carbon nanotube systems. Physical Review B, 2004, 69, .	1.1	30
48	Ab initio calculation of electrostatic multipoles with Wannier functions for large-scale biomolecular simulations. Journal of Chemical Physics, 2004, 120, 4530-4544.	1.2	31
49	First Principles Investigation of Vancomycin and Teicoplanin Binding to Bacterial Cell Wall Termini. Journal of the American Chemical Society, 2004, 126, 8384-8385.	6.6	25
50	First-principles investigation of carbon nanotube capacitance. Physical Review B, 2003, 67, .	1.1	17
51	Charge transport through small silicon clusters. Physical Review B, 2002, 66, .	1.1	55
52	Field Emission Properties of BN/C and BN@C Hybrid Nanotubes. Materials Research Society Symposia Proceedings, 2002, 739, 571.	0.1	0
53	Electronic and field emission properties of boron nitride/carbon nanotube superlattices. Applied Physics Letters, 2002, 81, 46-48.	1.5	118
54	Ab InitioInvestigations of Lithium Diffusion in Carbon Nanotube Systems. Physical Review Letters, 2002, 88, 075506.	2.9	254

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55	Ab Intio Simulations of Quatum Transport: Si Clusters and Fullerene Chains. Materials Research Society Symposia Proceedings, 2002, 727, 1.	0.1	1
56	CONDUCTANCE OF CARBON NANOTUBES ACTING AS QUANTUM DOTS. , 2002, , .		0
57	Carbon nanotubes in the Coulomb blockade regime. Physical Review B, 2001, 63, .	1.1	13
58	Li Uptake in Carbon Nanotube Systems: A First Principles Investigation. Materials Research Society Symposia Proceedings, 2001, 706, 1.	0.1	0
59	Liquid-crystal phases of capped carbon nanotubes. Physical Review B, 2001, 63, .	1.1	55
60	Carbon nanotube parametric electron pump: A molecular device. Physical Review B, 2001, 64, .	1.1	36
61	Resonant transmission through finite-sized carbon nanotubes. Physical Review B, 2001, 63, .	1.1	80
62	Resonant Andreev reflections in superconductorâ€“carbon-nanotube devices. Physical Review B, 2001, 63, .	1.1	38
63	Ab initiolâ^'Vcharacteristics of shortC20chains. Physical Review B, 2001, 65, .	1.1	36
64	Quantum Transport Properties of Carbon Nanotubes in the Coulomb Blockade Regime. Materials Research Society Symposia Proceedings, 2000, 633, 1461.	0.1	0
65	Two- and three-dimensional simulations of the phase separation of elastically coherent binary alloys subject to external stresses. Physical Review B, 2000, 62, 3160-3168.	1.1	19
66	Carbon Nanotube Based Magnetic Tunnel Junctions. Physical Review Letters, 2000, 84, 2682-2685.	2.9	153
67	Dynamic Conductance of Carbon Nanotubes. Physical Review Letters, 2000, 84, 2921-2924.	2.9	67
68	Theoretical STM signatures and transport properties of native defects in carbon nanotubes. Physical Review B, 2000, 61, 14194-14203.	1.1	96
69	Large-scale simulations of phase separation of elastically coherent binary alloy systems. Physical Review B, 1999, 59, 8646-8659.	1.1	52
70	Ad-dimers on Strained Carbon Nanotubes: A New Route for Quantum Dot Formation?. Physical Review Letters, 1999, 83, 4132-4135.	2.9	104
71	Phase Separation and Elastic Fields: Three Dimensional Simulations of a Phase Field Model. Materials Research Society Symposia Proceedings, 1999, 580, 21.	0.1	0
72	Thin film deposition: fundamentals and modeling. Computational Materials Science, 1998, 12, 354-380.	1.4	112

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73	Three-dimensional simulations of Ostwald ripening with elastic effects. Physical Review E, 1998, 58, R4092-R4095.	0.8	27
74	Nanotubes. Current Opinion in Solid State and Materials Science, 1997, 2, 706-715.	5.6	61
75	Applications of molecular dynamics simulations to crystal growth: step energies and low temperature growth. Computational Materials Science, 1996, 6, 135-139.	1.4	2
76	PHASE SEPARATION OF TWO-DIMENSIONAL FLUID MIXTURES IN THE DISSIPATIVE REGIME. Modern Physics Letters B, 1996, 10, 577-598.	1.0	0
77	Kinetics of nucleation-dominated step flow. Physical Review B, 1996, 54, 2931-2936.	1.1	11
78	Low-temperature growth and ion-assisted deposition. Physical Review B, 1995, 51, 5061-5064.	1.1	40
79	Simulations of crystal growth: Effects of atomic beam energy. Applied Physics Letters, 1994, 65, 824-826.	1.5	59
80	Growth of germanium films on Si(001) substrates. Physical Review B, 1993, 47, 16286-16298.	1.1	67
81	Epitaxy on surfaces vicinal to Si(001). II. Growth properties of Si(001) steps. Physical Review B, 1992, 46, 13437-13451.	1.1	39
82	Interfacial dynamics with long-range screening. Physical Review A, 1992, 45, 3903-3912.	1.0	26
83	Epitaxy on surfaces vicinal to Si(001). I. Diffusion of silicon adatoms over the terraces. Physical Review B, 1992, 46, 13428-13436.	1.1	88
84	Growth Properties of the Si(100) Steps: A Molecular Dynamics Study. Materials Research Society Symposia Proceedings, 1991, 237, 217.	0.1	0
85	Binding sites and diffusion barriers of single-height Si(001) steps. Physical Review Letters, 1991, 67, 3188-3191.	2.9	59
86	Interface growth with a shadow instability. Physical Review Letters, 1991, 66, 2104-2107.	2.9	46
87	Monte Carlo renormalization-group study of domain growth in the Potts model on a triangular lattice. Physical Review B, 1990, 41, 4663-4668.	1.1	15
88	Kinetics of quenched systems with long-range repulsive interactions. Physical Review B, 1990, 42, 6658-6669.	1.1	74
89	Monte Carlo renormalization-group study of spinodal decomposition: Scaling and growth. Physical Review B, 1989, 39, 11971-11981.	1.1	74
90	Lack of self-averaging, multiscaling, and 1/fnoise in the kinetics of domain growth. Physical Review Letters, 1989, 63, 551-554.	2.9	28

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91	Monte Carlo Renormalization-Group Study of the Late-Stage Dynamics of Spinodal Decomposition. Physical Review Letters, 1988, 60, 2657-2660.	2.9	64