Celeste Sagui

List of Publications by Year
in descending order

80 papers	3,585 citations	159525 30 h-index	138417 58 g-index
85 all docs	85 docs citations	85 times ranked	3426 citing authors

#	Article	IF	Citations
1	MOLECULAR DYNAMICS SIMULATIONS OF BIOMOLECULES: Long-Range Electrostatic Effects. Annual Review of Biophysics and Biomolecular Structure, 1999, 28, 155-179.	18.3	552
2	Efficient particle-mesh Ewald based approach to fixed and induced dipolar interactions. Journal of Chemical Physics, 2000, 113, 10913-10927.	1.2	394
3	Classical Electrostatics for Biomolecular Simulations. Chemical Reviews, 2014, 114, 779-814.	23.0	229
4	Towards an accurate representation of electrostatics in classical force fields: Efficient implementation of multipolar interactions in biomolecular simulations. Journal of Chemical Physics, 2004, 120, 73-87.	1.2	207
5	Adaptively biased molecular dynamics for free energy calculations. Journal of Chemical Physics, 2008, 128, 134101.	1.2	168
6	Multigrid methods for classical molecular dynamics simulations of biomolecules. Journal of Chemical Physics, 2001, 114, 6578-6591.	1.2	119
7	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
8	Kinetics of phase separation in two-dimensional systems with competing interactions. Physical Review E, 1994, 49, 2225-2244.	0.8	80
9	Surface solvation for an ion in a water cluster. Journal of Chemical Physics, 2005, 122, 024513.	1.2	78
10	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
11	Spinodal decomposition in an order-disorder phase transition with elastic fields. Physical Review E, 1994, 50, 4865-4879.	0.8	73
12	Molecular Dynamics Simulations of DNA with Polarizable Force Fields:Â Convergence of an Ideal B-DNA Structure to the Crystallographic Structure. Journal of Physical Chemistry B, 2006, 110, 11571-11581.	1.2	65
13	Chapter 2 Electrostatics in Biomolecular Simulations: Where Are We Now and Where Are We Heading?. Current Topics in Membranes, 2008, 60, 49-89.	0.5	62
14	Liquid-crystal phases of capped carbon nanotubes. Physical Review B, 2001, 63, .	1.1	55
15	Theory of nucleation and growth during phase separation. Physical Review E, 1999, 59, 4175-4187.	0.8	53
16	Ion distributions around left- and right-handed DNA and RNA duplexes: a comparative study. Nucleic Acids Research, 2014, 42, 13981-13996.	6.5	53
17	Large-scale simulations of phase separation of elastically coherent binary alloy systems. Physical Review B, 1999, 59, 8646-8659.	1.1	52
18	Deprotonation of Solvated Formic Acid:Â Carâ€'Parrinello and Metadynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 2325-2331.	1.2	51

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19	Conformational free energies of methyl-Î±-L-iduronic and methyl-Î²-D-glucuronic acids in water. Journal of Chemical Physics, 2010, 132, 104108.	1.2	49
20	Ostwald Ripening in Systems with Competing Interactions. Physical Review Letters, 1995, 74, 1119-1122.	2.9	48
21	Reaction path ensemble of the Bâ€“Z-DNA transition: a comprehensive atomistic study. Nucleic Acids Research, 2013, 41, 33-43.	6.5	48
22	Kinetics of topological defects in systems with competing interactions. Physical Review Letters, 1993, 71, 3995-3998.	2.9	46
23	Picosecond dissociation of amyloid fibrils with infrared laser: A nonequilibrium simulation study. Journal of Chemical Physics, 2015, 143, 155101.	1.2	41
24	Secondary structure assignment for conformationally irregular peptides: Comparison between DSSP, STRIDE and KAKSI. Journal of Molecular Graphics and Modelling, 2015, 55, 72-84.	1.3	40
25	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
26	Molecular dynamics simulations of the d(CCAACGTTGG)2 decamer in crystal environment: Comparison of atomic point-charge, extra-point, and polarizable force fields. Journal of Chemical Physics, 2004, 121, 6998-7008.	1.2	36
27	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
28	Late-stage kinetics of systems with competing interactions quenched into the hexagonal phase. Physical Review E, 1995, 52, 2807-2821.	0.8	34
29	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
30	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
31	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
32	Amyloid Properties of Asparagine and Glutamine in Prion-like Proteins. ACS Chemical Neuroscience, 2016, 7, 576-587.	1.7	30
33	Three-dimensional simulations of Ostwald ripening with elastic effects. Physical Review E, 1998, 58, R4092-R4095.	0.8	27
34	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
35	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
36	Effects of long-range repulsive interactions on Ostwald ripening. Physical Review E, 1995, 52, 2822-2840.	0.8	24

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37	A Statistical Analysis of the PPII Propensity of Amino Acid Guests in Proline-Rich Peptides. Biophysical Journal, 2011, 100, 1083-1093.	0.2	24
38	Nucleation and growth: Decay of a metastable state. Physical Review E, 1997, 56, R21-R24.	0.8	22
39	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
40	Calculation of ionic charging free energies in simulation systems with atomic charges, dipoles, and quadrupoles. Journal of Chemical Physics, 2003, 119, 7621-7632.	1.2	20
41	Elastic effects in the foaming of thermoplastics. Physical Review E, 1998, 58, 4654-4657.	0.8	19
42	P3M and PME: A comparison of the two methods. , 1999, , .		19
43	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
44	The Î±â€sheet: A missingâ€inâ€action secondary structure?. Proteins: Structure, Function and Bioinformatics, 2011, 79, 937-946.	1.5	19
45	Structure and Dynamics of DNA and RNA Double Helices of CAG and GAC Trinucleotide Repeats. Biophysical Journal, 2017, 113, 19-36.	0.2	19
46	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
47	Calculating relative transition rates with driven nonequilibrium simulations. Chemical Physics Letters, 2011, 518, 109-113.	1.2	18
48	Are Long-Range Structural Correlations Behind the Aggregration Phenomena of Polyglutamine Diseases?. PLoS Computational Biology, 2012, 8, e1002501.	1.5	18
49	PPII Propensity of Multiple-Guest Amino Acids in a Proline-Rich Environment. Journal of Physical Chemistry B, 2011, 115, 8645-8656.	1.2	17
50	Exploring Intramolecular Reactions in Complex Systems with Metadynamics:Â The Case of the Malonate Anions. Journal of Physical Chemistry A, 2005, 109, 7682-7687.	1.1	16
51	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
52	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
53	Investigating rare events with nonequilibrium work measurements. I. Nonequilibrium transition path probabilities. Journal of Chemical Physics, 2014, 140, 034114.	1.2	14
54	Picosecond melting of peptide nanotubes using an infrared laser: a nonequilibrium simulation study. Physical Chemistry Chemical Physics, 2015, 17, 27275-27280.	1.3	14

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55	Investigating rare events with nonequilibrium work measurements. II. Transition and reaction rates. Journal of Chemical Physics, 2014, 140, 034115.	1.2	13
56	Molecular dynamics simulations of polarizable DNA in crystal environment. International Journal of Quantum Chemistry, 2006, 106, 3260-3269.	1.0	12
57	The Adaptively Biased Molecular Dynamics method revisited: New capabilities and an application. Journal of Physics: Conference Series, 2015, 640, 012020.	0.3	12
58	Structural Determinants of Polyglutamine Protofibrils and Crystallites. ACS Chemical Neuroscience, 2015, 6, 632-645.	1.7	12
59	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
60	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
61	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
62	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
63	Spinodal decomposition in an order-disorder transition: Effect of interfacial properties. Physical Review E, 1996, 53, 5101-5105.	0.8	9
64	Binding Polymorphism in the DNA Bound State of the Pdx1 Homeodomain. PLoS Computational Biology, 2013, 9, e1003160.	1.5	9
65	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
66	The gp41659â€“671HIV-1 Antibody Epitope: A Structurally Challenging Small Peptide. Journal of Physical Chemistry B, 2014, 118, 69-80.	1.2	7
67	Recipes for Free Energy Calculations in Biomolecular Systems. Methods in Molecular Biology, 2013, 924, 313-337.	0.4	6
68	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
69	New and Exotic Self-Organized Patterns for Modulated Nanoscale Systems. Nano Letters, 2005, 5, 389-395.	4.5	5
70	Theoretical Investigation of the Interaction of Glycine with Diamond C(100) and C(111) (2 Ã— 1) Surfaces. Journal of Physical Chemistry C, 2007, 111, 12760-12767.	1.5	2
71	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
72	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

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73	Construction of DNA/RNA Triplex Helices Based on GAA/TTC Trinucleotide Repeats. Bio-protocol, 2021, 11, e4155.	0.2	2
74	Kinetics of phase ordering in systems with competing interactions. Journal of Magnetism and Magnetic Materials, 1995, 149, 87-92.	1.0	1
75	Stability and Ion Distributions Around Left- and Right-Handed DNA and RNA Duplexes: A Comparative Study. Biophysical Journal, 2016, 110, 407a.	0.2	1
76	Kinetics of an order-disorder phase transition with topological defects. Physical Review E, 1996, 54, 4775-4781.	0.8	0
77	Phase Separation and Elastic Fields: Three Dimensional Simulations of a Phase Field Model. Materials Research Society Symposia Proceedings, 1999, 580, 21.	0.1	0
78	Efficient Treatment of Fixed and Induced Dipolar Interactions. Materials Research Society Symposia Proceedings, 2000, 653, .	0.1	0
79	Efficient Treatment of Fixed and Induced Dipolar Interactions. Materials Research Society Symposia Proceedings, 2000, 653, 1.	0.1	0
80	Structure of a pathologic amyloid nucleus determined by rational genetic deconstruction of an intracellular nucleation barrier. FASEB Journal, 2022, 36, .	0.2	0