Steven J Stuart

List of Publications by Year
in descending order

45 papers	8,989 citations	331259 21 h-index	315357 38 g-index
45 all docs	45 docs citations	45 times ranked	6948 citing authors

#	Article	IF	Citations
1	A reactive potential for hydrocarbons with intermolecular interactions. Journal of Chemical Physics, 2000, 112, 6472-6486.	1.2	3,589
2	A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons. Journal of Physics Condensed Matter, 2002, 14, 783-802.	0.7	2,826
3	Dynamical fluctuating charge force fields: Application to liquid water. Journal of Chemical Physics, 1994, 101, 6141-6156.	1.2	1,133
4	Molecular Dynamics Simulations on the Effects of Diameter and Chirality on Hydrogen Adsorption in Single Walled Carbon Nanotubes. Journal of Physical Chemistry B, 2005, 109, 3780-3786.	1.2	135
5	Molecular Simulation To Characterize the Adsorption Behavior of a Fibrinogen Î³-Chain Fragment. Langmuir, 2005, 21, 1103-1117.	1.6	135
6	Molecular dynamics with multiple time scales: The selection of efficient reference system propagators. Journal of Chemical Physics, 1996, 105, 1426-1436.	1.2	121
7	Surface Curvature Effects in the Aqueous Ionic Solvation of the Chloride Ion. Journal of Physical Chemistry A, 1999, 103, 10300-10307.	1.1	117
8	Molecular Dynamics Simulations of Peptideâ^'Surface Interactions. Langmuir, 2005, 21, 1629-1639.	1.6	115
9	Role of Defects in Compression and Friction of Anchored Hydrocarbon Chains on Diamond. Langmuir, 2000, 16, 291-296.	1.6	89
10	Indentation Analysis of Linear-Chain Hydrocarbon Monolayers Anchored to Diamond. Journal of Physical Chemistry B, 1999, 103, 11357-11365.	1.2	79
11	Potentials and Algorithms for Incorporating Polarizability in Computer Simulations. , 0, , 89-146.		67
12	Assessment of the Transferability of a Protein Force Field for the Simulation of Peptide-Surface Interactions. Langmuir, 2010, 26, 7396-7404.	1.6	63
13	Comparison Between Empirical Protein Force Fields for the Simulation of the Adsorption Behavior of Structured LK Peptides on Functionalized Surfaces. Biointerphases, 2012, 7, 24.	0.6	45
14	Calculation of adsorption free energy for solute-surface interactions using biased replica-exchange molecular dynamics. Biointerphases, 2008, 3, 9-18.	0.6	44
15	TIGER2: An improved algorithm for temperature intervals with global exchange of replicas. Journal of Chemical Physics, 2009, 130, 174106.	1.2	42
16	Parallel replica dynamics for driven systems: Derivation and application to strained nanotubes. Physical Review B, 2007, 75, .	1.1	34
17	Cluster analysis of molecular simulation trajectories for systems where both conformation and orientation of the sampled states are important. Journal of Computational Chemistry, 2016, 37, 1973-1982.	1.5	31
18	An improved replica-exchange sampling method: Temperature intervals with global energy reassignment. Journal of Chemical Physics, 2007, 127, 164116.	1.2	29

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19	Empirical bondâ€order potential for hydrocarbons: Adaptive treatment of van der Waals interactions. Journal of Computational Chemistry, 2008, 29, 601-611.	1.5	27
20	Parallel replica dynamics with a heterogeneous distribution of barriers: Application ton-hexadecane pyrolysis. Journal of Chemical Physics, 2004, 121, 9808-9819.	1.2	25
21	Bond-order potentials with split-charge equilibration: Application to C-, H-, and O-containing systems. Journal of Chemical Physics, 2012, 136, 164701.	1.2	25
22	Development of molecular simulation methods to accurately represent protein-surface interactions: The effect of pressure and its determination for a system with constrained atoms. Biointerphases, 2010, 5, 85-95.	0.6	23
23	Simulation of multiphase systems utilizing independent force fields to control intraphase and interphase behavior. Journal of Computational Chemistry, 2012, 33, 1458-1466.	1.5	21
24	Molecular dynamics investigation on liquidâ€“liquid phase change in carbon with empirical bond-order potentials. Journal of Chemical Physics, 2003, 119, 6053-6056.	1.2	20
25	Simulated annealing with adaptive cooling rates. Journal of Chemical Physics, 2020, 153, 114103.	1.2	19
26	Development of a Tuned Interfacial Force Field Parameter Set for the Simulation of Protein Adsorption to Silica Glass. Biointerphases, 2012, 7, 56.	0.6	17
27	Molecular dynamics simulations on hydrogen adsorption in finite single walled carbon nanotube bundles. Journal of Molecular Modeling, 2008, 14, 343-351.	0.8	15
28	Development of molecular simulation methods to accurately represent protein-surface interactions: Method assessment for the calculation of electrostatic effects. Biointerphases, 2009, 4, 57-64.	0.6	15
29	Physical Adsorption Strength in Open Systems. Journal of Physical Chemistry B, 2006, 110, 22957-22960.	1.2	12
30	Application of advanced sampling and analysis methods to predict the structure of adsorbed protein on a material surface. Biointerphases, 2017, 12, 02D409.	0.6	12
31	Parameterization of an interfacial force field for accurate representation of peptide adsorption free energy on high-density polyethylene. Biointerphases, 2015, 10, 021002.	0.6	11
32	Reactive Bond-Order Simulations Using Both Spatial and Temporal Approaches to Parallelism. Structural Chemistry, 2004, 15, 479-486.	1.0	10
33	TIGER2 with solvent energy averaging (TIGER2A): An accelerated sampling method for large molecular systems with explicit representation of solvent. Journal of Chemical Physics, 2015, 143, 144105.	1.2	10
34	Polarizable Molecular Dynamics Simulations of Aqueous Dipeptides. Journal of Physical Chemistry B, 2012, 116, 8733-8740.	1.2	8
35	An Iterative Variable-timestep Algorithm for Molecular Dynamics Simulations. Molecular Simulation, 2003, 29, 177-186.	0.9	6
36	Molecular dynamics for nonequilibrium systems in which there are a small number of very hot particles in a cold bath: Reference system propagator methods. Journal of Chemical Physics, 1996, 105, 235-239.	1.2	4

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37	Raman intensity and vibrational modes of armchair CNTs. Chemical Physics Letters, 2017, 679, 45-51.	1.2	4
38	A New, Reactive Potential Energy Function to Study the Indentation and Friction of n-Alkane C13 Monolayers. ACS Symposium Series, 2000, , 216-229.	0.5	3
39	Automated, Parallel Optimization Algorithms for Stochastic Functions. , 2011, , .		3
40	Simulation of carbon nanotube welding through Ar bombardment. Journal of Molecular Modeling, 2017, 23, 148.	0.8	3
41	Automated, Parallel Optimization of Stochastic Functions Using a Modified Simplex Algorithm. , 2010, , .		2
42	Hydrocarbon Reactions in Carbon Nanotubes: Pyrolysis. Materials Research Society Symposia Proceedings, 2000, 651, 1.	0.1	0
43	A Molecular Dynamics Simulation Study Towards Understanding the Effects of Diameter and Chirality on Hydrogen Adsorption in Singlewalled Carbon Nanotubes. Materials Research Society Symposia Proceedings, 2003, 801, 175.	0.1	0
44	Curvature-induced Symmetry Lowering and Anomalous Dispersion of Phonons in Single-Walled Carbon Nanotubes. Materials Research Society Symposia Proceedings, 2011, 1284, 143.	0.1	0
45	Modeling ion permeation in wild-type and mutant human Î±7 nachr ion channels. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850045.	1.8	0