Alessandro Laio

List of Publications by Year
in descending order

154	21,295	34105 52	9589 142
papers	citations	h-index	g-index

160	160	160	16833
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	When kinetics plays strange tricks. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2122078119.	7.1	0
2	Model Folded Hydrophobic Polymers Reside in Highly Branched Voids. Journal of Physical Chemistry Letters, 2022, 13, 183-189.	4.6	5
3	Computational Evolution Protocol for Peptide Design. Methods in Molecular Biology, 2022, 2405, 335-359.	0.9	3
4	Ranking the information content of distance measures. , 2022, 1, .		13
5	Multiple-Allele MHC Class II Epitope Engineering by a Molecular Dynamics-Based Evolution Protocol. Frontiers in Immunology, 2022, 13, 862851.	4.8	7
6	PARCE: Protocol for Amino acid Refinement through Computational Evolution. Computer Physics Communications, 2021, 260, 107716.	7.5	12
7	Candidate Binding Sites for Allosteric Inhibition of the SARS-CoV-2 Main Protease from the Analysis of Large-Scale Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2021, 12, 65-72.	4.6	18
8	A Rosetta-based protein design protocol converging to natural sequences. Journal of Chemical Physics, 2021, 154, 074114.	3.0	4
9	Density Peak clustering of protein sequences associated to a Pfam clan reveals clear similarities and interesting differences with respect to manual family annotation. BMC Bioinformatics, 2021, 22, 121.	2.6	1
10	Statistically unbiased free energy estimates from biased simulations. Molecular Physics, 2021, 119, .	1.7	4
11	Unsupervised Learning Methods for Molecular Simulation Data. Chemical Reviews, 2021, 121, 9722-9758.	47.7	182
12	Dynamical landscape and multistability of a climate model. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2021, 477, 20210019.	2.1	18
13	Automatic topography of high-dimensional data sets by non-parametric density peak clustering. Information Sciences, 2021, 560, 476-492.	6.9	25
14	Improving acute stroke assessment in non-enhanced CT: Automated tool for early ischemic lesion volume detection. Journal of the Neurological Sciences, 2021, 429, 119611.	0.6	0
15	Explicit Characterization of the Free-Energy Landscape of a Protein in the Space of All Its C_{Î±} Carbons. Journal of Chemical Theory and Computation, 2020, 16, 80-87.	5.3	15
16	Data segmentation based on the local intrinsic dimension. Scientific Reports, 2020, 10, 16449.	3.3	17
17	Automatic classification of single-molecule force spectroscopy traces from heterogeneous samples. Bioinformatics, 2020, 36, 5014-5020.	4.1	7
18	Using metadynamics to explore complex free-energy landscapes. Nature Reviews Physics, 2020, 2, 200-212.	26.6	346

#	Article	IF	Citations
19	Computational Design of Peptides Bound to the Major Histocompatibility Complex Class II. Biophysical Journal, 2020, 118, 359a.	0.5	0
20	Metadynamics: A Unified Framework for Accelerating Rare Events and Sampling Thermodynamics and Kinetics. , 2020, , 565-595.		13
21	Brain network dynamics during spontaneous strategy shifts and incremental task optimization. NeuroImage, 2020, 217, 116854.	4.2	15
22	Predicting the Affinity of Peptides to Major Histocompatibility Complex Class II by Scoring Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2019, 59, 3464-3473.	5.4	34
23	Spontaneously Forming Dendritic Voids in Liquid Water Can Host Small Polymers. Journal of Physical Chemistry Letters, 2019, 10, 5585-5591.	4.6	21
24	The Subtle Trade-Off between Evolutionary and Energetic Constraints in Proteinâ€“Protein Interactions. Journal of Physical Chemistry Letters, 2019, 10, 1489-1497.	4.6	20
25	The intrinsic dimension of protein sequence evolution. PLoS Computational Biology, 2019, 15, e1006767.	3.2	19
26	A common root for coevolution and substitution rate variability in protein sequence evolution. Scientific Reports, 2019, 9, 18032.	3.3	4
27	A consensus protocol for the in silico optimisation of antibody fragments. Chemical Communications, 2019, 55, 14043-14046.	4.1	32
28	Computing the Free Energy without Collective Variables. Journal of Chemical Theory and Computation, 2018, 14, 1206-1215.	5.3	37
29	Vibrational entropy estimation can improve binding affinity prediction for nonâ€obligatory protein complexes. Proteins: Structure, Function and Bioinformatics, 2018, 86, 393-404.	2.6	7
30	Binding affinity prediction of nanobodyâ€“protein complexes by scoring of molecular dynamics trajectories. Physical Chemistry Chemical Physics, 2018, 20, 3438-3444.	2.8	31
31	Peptide biosensors for anticancer drugs: Design in silico to work in denaturizing environment. Biosensors and Bioelectronics, 2018, 100, 298-303.	10.1	20
32	Assessing the capability ofin silicomutation protocols for predicting the finite temperature conformation of amino acids. Physical Chemistry Chemical Physics, 2018, 20, 25901-25909.	2.8	18
33	Metadynamics: A Unified Framework for Accelerating Rare Events and Sampling Thermodynamics and Kinetics. , 2018, , 1-31.		11
34	The permeation mechanism of organic cations through a CNG mimic channel. PLoS Computational Biology, 2018, 14, e1006295.	3.2	1
35	Preface: Special Topic on Enhanced Sampling for Molecular Systems. Journal of Chemical Physics, 2018, 149, 072001.	3.0	4
36	Toward a unified scoring function for native state discrimination and drug-binding pocket recognition. Physical Chemistry Chemical Physics, 2018, 20, 17148-17155.	2.8	5

#	Article	IF	Citations
37	Computational design of cyclic peptides for the customized oriented immobilization of globular proteins. Physical Chemistry Chemical Physics, 2017, 19, 2740-2748.	2.8	20
38	METAGUI 3: A graphical user interface for choosing the collective variables in molecular dynamics simulations. Computer Physics Communications, 2017, 217, 204-209.	7.5	34
39	A Markov state modeling analysis of sliding dynamics of a 2D model. Journal of Chemical Physics, 2017, 147, 152721.	3.0	1
40	Estimating the intrinsic dimension of datasets by a minimal neighborhood information. Scientific Reports, 2017, 7, 12140.	3.3	135
41	New views on phototransduction from atomic force microscopy and single molecule force spectroscopy on native rods. Scientific Reports, 2017, 7, 12000.	3.3	5
42	Predicting Amino Acid Substitution Probabilities Using Single Nucleotide Polymorphisms. Genetics, 2017, 207, 643-652.	2.9	1
43	fMRI single trial discovery of spatioâ€temporal brain activity patterns. Human Brain Mapping, 2017, 38, 1421-1437.	3.6	6
44	Non-Markovian effects on protein sequence evolution due to site dependent substitution rates. BMC Bioinformatics, 2016, 17, 258.	2.6	7
45	Metadynamics surfing on topology barriers: the CP Nâ^'1 case. Journal of High Energy Physics, 2016, 2016, 1.	4.7	24
46	Permeability Coefficients of Lipophilic Compounds Estimated by Computer Simulations. Journal of Chemical Theory and Computation, 2016, 12, 4093-4099.	5.3	22
47	Protein-protein structure prediction by scoring molecular dynamics trajectories of putative poses. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1312-1320.	2.6	11
48	Sampling Molecular Conformers in Solution with Quantum Mechanical Accuracy at a Nearly Molecular-Mechanics Cost. Journal of Chemical Theory and Computation, 2016, 12, 4385-4389.	5.3	15
49	Fusing simulation and experiment: The effect of mutations on the structure and activity of the influenza fusion peptide. Scientific Reports, 2016, 6, 28099.	3.3	10
50	Markov state modeling of sliding friction. Physical Review E, 2016, 94, 053001.	2.1	5
51	In Silico Design of Short Peptides as Sensing Elements for Phenolic Compounds. ACS Sensors, 2016, 1, 279-286.	7.8	14
52	Role of Enzyme Flexibility in Ligand Access and Egress to Active Site: Bias-Exchange Metadynamics Study of 1,3,7-Trimethyluric Acid in Cytochrome P450 3A4. Journal of Chemical Theory and Computation, 2016, 12, 2101-2109.	5.3	44
53	The inverted free energy landscape of an intrinsically disordered peptide by simulations and experiments. Scientific Reports, 2015, 5, 15449.	3.3	118
54	QMMMW: A wrapper for QM/MM simulations with Quantum ESPRESSO Âand LAMMPS. Computer Physics Communications, 2015, 195, 191-198.	7.5	6

#	Article	IF	Citations
55	Native fold and docking pose discrimination by the same residueâ€based scoring function. Proteins: Structure, Function and Bioinformatics, 2015, 83, 621-630.	2.6	17
56	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	47.7	530
57	Designing High-Affinity Peptides for Organic Molecules by Explicit Solvent Molecular Dynamics. Journal of Physical Chemistry B, 2015, 119, 12963-12969.	2.6	17
58	A structural, functional, and computational analysis suggests pore flexibility as the base for the poor selectivity of CNG channels. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3619-28.	7.1	35
59	Metadynamics Simulations Reveal a Na+ Independent Exiting Path of Galactose for the Inward-Facing Conformation of vSGLT. PLoS Computational Biology, 2014, 10, e1004017.	3.2	20
60	Shape and area fluctuation effects on nucleation theory. Journal of Chemical Physics, 2014, 140, 094501.	3.0	34
61	Sodium-Galactose Transporter: The First Steps of the Transport Mechanism Investigated by Molecular Dynamics. Biophysical Journal, 2014, 106, 365a-366a.	0.5	0
62	Mechanism of Ionic Permeation in the Mimics of CNG Channels: A Structural, Functional and Computational Analysis. Biophysical Journal, 2014, 106, 758a.	0.5	0
63	Clustering by fast search and find of density peaks. Science, 2014, 344, 1492-1496.	12.6	3,709
64	Nucleation Process of a Fibril Precursor in the C-Terminal Segment of Amyloid-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math>. Physical Review Letters, 2013, 110, 168103.	7.8	53
65	A Candidate Ion-Retaining State in the Inward-Facing Conformation of Sodium/Galactose Symporter: Clues from Atomistic Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1240-1246.	5.3	26
66	Designing Short Peptides with High Affinity for Organic Molecules: A Combined Docking, Molecular Dynamics and Monte Carlo Approach. Biophysical Journal, 2013, 104, 556a.	0.5	10
67	Thermodynamics of an Intrinsically Disordered Protein by Atomistic Simulations. Biophysical Journal, 2013, 104, 55a.	0.5	1
68	A fingerprint of surface-tension anisotropy in the free-energy cost of nucleation. Journal of Chemical Physics, 2013, 138, 064508.	3.0	27
69	BACHSCORE. A tool for evaluating efficiently and reliably the quality of large sets of protein structures. Computer Physics Communications, 2013, 184, 2860-2865.	7.5	20
70	Characterization of the free-energy landscapes of proteins by NMR-guided metadynamics. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6817-6822.	7.1	122
71	Absolute Transition Rates for Rare Events from Dynamical Decoupling of Reaction Variables. Physical Review Letters, 2012, 109, 150601.	7.8	9
72	A simple and efficient statistical potential for scoring ensembles of protein structures. Scientific Reports, 2012, 2, .	3.3	48

#	Article	IF	Citations
73	Atomistic Structure of Cobalt-Phosphate Nanoparticles for Catalytic Water Oxidation. ACS Nano, 2012, 6, 10497-10504.	14.6	62
74	Simulation of Amyloid Nucleation with Bias-Exchange Metadynamics. Biophysical Journal, 2012, 102, 242a.	0.5	2
75	Protein Folding and Ligand-Enzyme Binding from Bias-Exchange Metadynamics Simulations. Current Physical Chemistry, 2012, 2, 79-91.	0.2	44
76	Multidimensional View of Amyloid Fibril Nucleation in Atomistic Detail. Journal of the American Chemical Society, 2012, 134, 3886-3894.	13.7	78
77	Systematic Improvement of Classical Nucleation Theory. Physical Review Letters, 2012, 108, 225701.	7.8	88
78	A Novel Approach to the Investigation of Passive Molecular Permeation through Lipid Bilayers from Atomistic Simulations. Journal of Physical Chemistry B, 2012, 116, 8714-8721.	2.6	63
79	Designing Short Peptides with High Affinity for Organic Molecules: A Combined Docking, Molecular Dynamics, And Monte Carlo Approach. Journal of Chemical Theory and Computation, 2012, 8, 1121-1128.	5.3	24
80	METAGUI. A VMD interface for analyzing metadynamics and molecular dynamics simulations. Computer Physics Communications, 2012, 183, 203-211.	7.5	92
81	Protein Folding and Ligand-Enzyme Binding from Bias-Exchange Metadynamics Simulations. Current Physical Chemistry, 2012, 2, 79-91.	0.2	6
82	Initial stages of salt crystal dissolution determined with ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2011, 13, 13162.	2.8	51
83	Cytoskeletal actin networks in motile cells are critically self-organized systems synchronized by mechanical interactions. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 13978-13983.	7.1	44
84	Finite Temperature Properties of Clusters by Replica Exchange Metadynamics: The Water Nonamer. Journal of the American Chemical Society, 2011, 133, 2535-2540.	13.7	11
85	Conformations of the Huntingtin N-term in aqueous solution from atomistic simulations. FEBS Letters, 2011, 585, 3086-3089.	2.8	24
86	Which similarity measure is better for analyzing protein structures in a molecular dynamics trajectory?. Physical Chemistry Chemical Physics, 2011, 13, 10421.	2.8	25
87	Theory of the reentrant quantum rotational phase transition in high-pressure HD. Physical Review B, 2011, 84, .	3.2	10
88	Metadynamics convergence law in a multidimensional system. Physical Review E, 2010, 81, 055701.	2.1	73
89	Exploring the Universe of Protein Structures beyond the Protein Data Bank. PLoS Computational Biology, 2010, 6, e1000957.	3.2	62
90	Force Generation in Lamellipodia Is a Probabilistic Process with Fast Growth and Retraction Events. Biophysical Journal, 2010, 98, 979-988.	0.5	29

#	Article	IF	Citations
91	Optimizing the Performance of Bias-Exchange Metadynamics: Folding a 48-Residue LysM Domain Using a Coarse-Grained Model. Journal of Physical Chemistry B, 2010, 114, 3259-3265.	2.6	40
92	Calculating thermodynamics properties of quantum systems by a non-Markovian Monte Carlo procedure. Physical Review E, 2009, 80, 015702.	2.1	4
93	A Kinetic Model of Trp-Cage Folding from Multiple Biased Molecular Dynamics Simulations. PLoS Computational Biology, 2009, 5, e1000452.	3.2	246
94	A Collective Variable for the Efficient Exploration of Protein Beta-Sheet Structures: Application to SH3 and GB1. Journal of Chemical Theory and Computation, 2009, 5, 2197-2201.	5.3	153
95	The Energy Gap as a Universal Reaction Coordinate for the Simulation of Chemical Reactions. Journal of Physical Chemistry B, 2009, 113, 7867-7873.	2.6	36
96	Tracing the Entropy along a Reactive Pathway: The Energy As a Generalized Reaction Coordinate. Journal of Chemical Theory and Computation, 2009, 5, 2193-2196.	5.3	15
97	Substrate Binding Mechanism of HIV-1 Protease from Explicit-Solvent Atomistic Simulations. Journal of the American Chemical Society, 2009, 131, 11811-11818.	13.7	132
98	Copper binding sites in the Câ€terminal domain of mouse prion protein: A hybrid (QM/MM) molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1084-1098.	2.6	21
99	Metadynamics: a method to simulate rare events and reconstruct the free energy in biophysics, chemistry and material science. Reports on Progress in Physics, 2008, 71, 126601.	20.1	1,334
100	Predicting the Effect of a Point Mutation on a Protein Fold: The Villin and Advillin Headpieces and Their Pro62Ala Mutants. Journal of Molecular Biology, 2008, 375, 460-470.	4.2	49
101	Optimal Langevin modeling of out-of-equilibrium molecular dynamics simulations. Journal of Chemical Physics, 2008, 129, 074105.	3.0	39
102	Vacancy-vacancy interaction and oxygen diffusion in stabilized cubic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ZrO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms first principles. Physical Review B, 2008, 78, .	3.2	69
103	Advillin Folding Takes Place on a Hypersurface of Small Dimensionality. Physical Review Letters, 2008, 101, 208101.	7.8	27
104	â€œSite Bindingâ€•of Ca2+Ions to Polyacrylates in Water:Â A Molecular Dynamics Study of Coiling and Aggregation. Macromolecules, 2007, 40, 3437-3442.	4.8	67
105	The Conformational Free Energy Landscape of Î²-<scp>d</scp>-Glucopyranose. Implications for Substrate Preactivation in Î²-Glucoside Hydrolases. Journal of the American Chemical Society, 2007, 129, 10686-10693.	13.7	196
106	Automated Parametrization of Biomolecular Force Fields from Quantum Mechanics/Molecular Mechanics (QM/MM) Simulations through Force Matching. Journal of Chemical Theory and Computation, 2007, 3, 628-639.	5.3	78
107	Free Energyab InitioMetadynamics:Â A New Tool for the Theoretical Study of Organometallic Reactivity? Example of the Câˆ'C and Câˆ'H Reductive Eliminations from Platinum(IV) Complexes. Organometallics, 2007, 26, 1241-1249.	2.3	37
108	A Bias-Exchange Approach to Protein Folding. Journal of Physical Chemistry B, 2007, 111, 4553-4559.	2.6	498

#	Article	IF	Citations
109	Dissociation Mechanism of Acetic Acid in Water. Journal of the American Chemical Society, 2006, 128, 11318-11319.	13.7	100
110	Stability and Structure of Oligomers of the Alzheimer Peptide AÎ²16â€“22: From the Dimer to the 32-Mer. Biophysical Journal, 2006, 91, 3217-3229.	0.5	102
111	Free-Energy Landscape for Î² Hairpin Folding from Combined Parallel Tempering and Metadynamics. Journal of the American Chemical Society, 2006, 128, 13435-13441.	13.7	458
112	Equilibrium Free Energies from Nonequilibrium Metadynamics. Physical Review Letters, 2006, 96, 090601.	7.8	355
113	An Efficient Linear-Scaling Electrostatic Coupling for Treating Periodic Boundary Conditions in QM/MM Simulations. Journal of Chemical Theory and Computation, 2006, 2, 1370-1378.	5.3	152
114	Computing Free Energies and Accelerating Rare Events with Metadynamics. , 2006, , 315-347.		34
115	Efficient Reconstruction of Complex Free Energy Landscapes by Multiple Walkers Metadynamicsâ€. Journal of Physical Chemistry B, 2006, 110, 3533-3539.	2.6	511
116	A comparative theoretical study of dipeptide solvation in water. Journal of Computational Chemistry, 2006, 27, 672-684.	3.3	37
117	A QUICKSTEP-based quantum mechanics/molecular mechanics approach for silica. Journal of Chemical Physics, 2006, 124, 154707.	3.0	11
118	Anisotropy of Earth's Dâ€³ layer and stacking faults in the MgSiO3 post-perovskite phase. Nature, 2005, 438, 1142-1144.	27.8	219
119	Ab Initio Simulations of Lewis-Acid-Catalyzed Hydrosilylation of Alkynes. ChemPhysChem, 2005, 6, 1772-1775.	2.1	15
120	Are structural biases at protein termini a signature of vectorial folding?. Proteins: Structure, Function and Bioinformatics, 2005, 62, 17-23.	2.6	15
121	QM/MM Simulation of the First Step of Vision. , 2005, , 237-243.		0
122	ELECTRON TRANSFER INDUCED DISSOCIATION OF CHLORO-CYANO-BENZENE RADICAL ANION: DRIVING CHEMICAL REACTIONS VIA CHARGE RESTRAINTS. Journal of Theoretical and Computational Chemistry, 2005, 04, 985-999.	1.8	2
123	Charge Localization in DNA Fibers. Physical Review Letters, 2005, 94, 158103.	7.8	53
124	A Recipe for the Computation of the Free Energy Barrier and the Lowest Free Energy Path of Concerted Reactionsâ€. Journal of Physical Chemistry B, 2005, 109, 6676-6687.	2.6	243
125	Assessing the Accuracy of Metadynamicsâ€. Journal of Physical Chemistry B, 2005, 109, 6714-6721.	2.6	446
126	Flexible Docking in Solution Using Metadynamics. Journal of the American Chemical Society, 2005, 127, 2600-2607.	13.7	266

#	Article	IF	Citations
127	Simulation of structural phase transitions by metadynamics. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	92
128	An Efficient Real Space Multigrid QM/MM Electrostatic Coupling. Journal of Chemical Theory and Computation, 2005, 1, 1176-1184.	5.3	224
129	Correlations among Hydrogen Bonds in Liquid Water. Physical Review Letters, 2004, 93, 087801.	7.8	65
130	A Molecular Spring for Vision. Journal of the American Chemical Society, 2004, 126, 15328-15329.	13.7	98
131	Azulene-to-Naphthalene Rearrangement: The Car-Parrinello Metadynamics Method Explores Various Reaction Mechanisms. ChemPhysChem, 2004, 5, 1558-1568.	2.1	78
132	Influence of DNA Structure on the Reactivity of the Guanine Radical Cation. Chemistry - A European Journal, 2004, 10, 4846-4852.	3.3	70
133	A Minimum Free Energy Reaction Path for the E2 Reaction between Fluoro Ethane and a Fluoride Ion. Journal of the American Chemical Society, 2004, 126, 9492-9493.	13.7	73
134	A Variational Definition of Electrostatic Potential Derived Charges. Journal of Physical Chemistry B, 2004, 108, 7963-7968.	2.6	40
135	Reconstructing the Density of States by History-Dependent Metadynamics. Physical Review Letters, 2004, 92, 170601.	7.8	149
136	Microscopic Mechanism of Antibiotics Translocation through a Porin. Biophysical Journal, 2004, 87, 58-64.	0.5	92
137	Molecular dynamics simulation of reconstructive phase transitions on an anhydrous zeolite. Physical Review B, 2004, 70, .	3.2	28
138	QM/MM Car-Parrinello Molecular Dynamics Study of the Solvent Effects on the Ground State and on the First Excited Singlet State of Acetone in Water. ChemPhysChem, 2003, 4, 1177-1182.	2.1	110
139	Reaction mechanism of caspases: Insights from QM/MM Car-Parrinello simulations. Proteins: Structure, Function and Bioinformatics, 2003, 52, 212-224.	2.6	47
140	Efficient Exploration of Reactive Potential Energy Surfaces Using Car-Parrinello Molecular Dynamics. Physical Review Letters, 2003, 90, 238302.	7.8	719
141	Characterization of the Dizinc Analogue of the Synthetic Diiron Protein DF1 Using ab Initio and Hybrid Quantum/Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2003, 107, 4182-4188.	2.6	43
142	Predicting Crystal Structures: The Parrinello-Rahman Method Revisited. Physical Review Letters, 2003, 90, 075503.	7.8	591
143	Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions. Chimia, 2002, 56, 13-19.	0.6	62
144	D-RESP:â€‰ Dynamically Generated Electrostatic Potential Derived Charges from Quantum Mechanics/Molecular Mechanics Simulations. Journal of Physical Chemistry B, 2002, 106, 7300-7307.	2.6	187

#	Article	IF	Citations
145	A Hamiltonian electrostatic coupling scheme for hybrid Carâ€“Parrinello molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 6941-6947.	3.0	588
146	Escaping free-energy minima. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12562-12566.	7.1	4,527
147	Physics of Iron at Earth's Core Conditions. Science, 2000, 287, 1027-1030.	12.6	341
148	Deciphering the folding kinetics of transmembrane helical proteins. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 14229-14234.	7.1	12
149	Physical Origin of Selectivity in Ionic Channels of Biological Membranes. Biophysical Journal, 1999, 76, 129-148.	0.5	70
150	Stepâ€“step interactions and correlations from 1D hard-core boson mapping. Surface Science, 1998, 402-404, 880-885.	1.9	0
151	Interacting hard-core bosons and surface preroughening. Physical Review B, 1998, 58, 13151-13162.	3.2	1
152	Quantum theory of frequency shifts of an electromagnetic wave interacting with a plasma. Physical Review E, 1997, 55, 7457-7461.	2.1	5
153	Interacting hard-core bosons and surface physics. Surface Science, 1997, 377-379, 514-518.	1.9	1
154	A third hypothesis on the origin of the redshift: Application to the Pioneer 6 data. Physics Letters, Section A: General, Atomic and Solid State Physics, 1995, 209, 277-284.	2.1	6