Karl F Freed

List of Publications by Year in Descending Order

600 papers	19,365 citations	68 h-index	98 g-index
626 ext. papers	20,055 ext. citations	4.1 avg, IF	6.75 L-index

#	Paper	IF	Citations
600	Lattice theory for binding of linear polymers to a solid substrate from polymer melts. II. Influence of van der Waals interactions and chain semiflexibility on molecular binding and adsorption. *Journal of Chemical Physics*, **2019**, 151, 124709	3.9	1
599	Lattice theory for binding of linear polymers to a solid substrate from polymer melts: I. Influence of chain connectivity on molecular binding and adsorption. *Journal of Chemical Physics*, **2019**, 151, 124706	3.9	2
598	On the Interpretation of Force-Induced Unfolding Studies of Membrane Proteins Using Fast Simulations. *Biophysical Journal*, **2019**, 117, 1429-1441	2.9	4
597	Lattice theory of competitive binding: Influence of van der Waals interactions on molecular binding and adsorption to a solid substrate from binary liquid mixtures. *Journal of Chemical Physics*, **2018**, 149, 044704	3.9	4
596	Dielectric virial expansion of polarizable dipolar spheres. *Journal of Chemical Physics*, **2018**, 149, 163332	3.9	1
595	A Membrane Burial Potential with H-Bonds and Applications to Curved Membranes and Fast Simulations. *Biophysical Journal*, **2018**, 115, 1872-1884	2.9	5
594	Accurate calculation of side chain packing and free energy with applications to protein molecular dynamics. *PLoS Computational Biology*, **2018**, 14, e1006342	5	11
593	Trajectory-based training enables protein simulations with accurate folding and Boltzmann ensembles in cpu-hours. *PLoS Computational Biology*, **2018**, 14, e1006578	5	15
592	Response to Comment on "Innovative scattering analysis shows that hydrophobic disordered proteins are expanded in water". *Science*, **2018**, 361,	33.3	25
591	Influence of Pressure on Glass Formation in a Simulated Polymer Melt. *Macromolecules*, **2017**, 50, 2585-2598	5.9	21
590	Comparative Study of the Collective Dynamics of Proteins and Inorganic Nanoparticles. *Scientific Reports*, **2017**, 7, 41671	4.9	10
589	Innovative scattering analysis shows that hydrophobic disordered proteins are expanded in water. *Science*, **2017**, 358, 238-241	33.3	116
588	Mixtures of two self- and mutually-associating liquids: Phase behavior, second virial coefficients, and entropy-enthalpy compensation in the free energy of mixing. *Journal of Chemical Physics*, **2017**, 147, 064909	3.9	10
587	Image method for electrostatic energy of polarizable dipolar spheres. *Journal of Chemical Physics*, **2017**, 147, 064908	3.9	7
586	ENTROPY THEORY OF POLYMER GLASS-FORMATION IN VARIABLE SPATIAL DIMENSION. *Advances in Chemical Physics*, **2016**, 443-497		18
585	Influence of Cohesive Energy on the Thermodynamic Properties of a Model Glass-Forming Polymer Melt. *Macromolecules*, **2016**, 49, 8341-8354	5.5	47
584	Influence of Cohesive Energy on Relaxation in a Model Glass-Forming Polymer Melt. *Macromolecules*, **2016**, 49, 8355-8370	5.5	40

583	Image method for induced surface charge from many-body system of dielectric spheres. *Journal of Chemical Physics*, **2016**, 145, 124903	3.9	18
582	Relation Between Solvent Quality and Phase Behavior of Ternary Mixtures of Polymers and Two Solvents that Exhibit Cononsolvency. *Journal of Physical Chemistry B*, **2016**, 120, 5753-8	3.4	9
581	A theory of interactions between polarizable dielectric spheres. *Journal of Colloid and Interface Science*, **2016**, 469, 237-241	9.3	26
580	Self-assembly and glass-formation in a lattice model of telechelic polymer melts: Influence of stiffness of the sticky bonds. *Journal of Chemical Physics*, **2016**, 144, 214903	3.9	2
579	Stringlike Cooperative Motion Explains the Influence of Pressure on Relaxation in a Model Glass-Forming Polymer Melt. *ACS Macro Letters*, **2016**, 5, 1375-1380	6.6	14
578	Generalized entropy theory of glass-formation in fully flexible polymer melts. *Journal of Chemical Physics*, **2016**, 145, 234509	3.9	24
577	Cooperative folding near the downhill limit determined with amino acid resolution by hydrogen exchange. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 4747-52	11.5	5
576	Even with nonnative interactions, the updated folding transition states of the homologs Proteins G & L are extensive and similar. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 8302-7	11.5	17
575	Generalized Entropy Theory of Glass Formation in Polymer Melts with Specific Interactions. *Macromolecules*, **2015**, 48, 2333-2343	5.5	23
574	Theory of competitive solvation of polymers by two solvents and entropy-enthalpy compensation in the solvation free energy upon dilution with the second solvent. *Journal of Chemical Physics*, **2015**, 142, 214906	3.9	8
573	Lattice cluster theory for dense, thin polymer films. *Journal of Chemical Physics*, **2015**, 142, 134901	3.9	2
572	Communication: The simplified generalized entropy theory of glass-formation in polymer melts. *Journal of Chemical Physics*, **2015**, 143, 051102	3.9	3
571	Communication: Cosolvency and cononsolvency explained in terms of a Flory-Huggins type theory. *Journal of Chemical Physics*, **2015**, 143, 131101	3.9	62
570	Lattice model of linear telechelic polymer melts. I. Inclusion of chain semiflexibility in the lattice cluster theory. *Journal of Chemical Physics*, **2015**, 143, 024901	3.9	4
569	Lattice model of linear telechelic polymer melts. II. Influence of chain stiffness on basic thermodynamic properties. *Journal of Chemical Physics*, **2015**, 143, 024902	3.9	3
568	Phase behavior and second osmotic virial coefficient for competitive polymer solvation in mixed solvent solutions. *Journal of Chemical Physics*, **2015**, 143, 194901	3.9	9
567	The meaning of the "universal" WLF parameters of glass-forming polymer liquids. *Journal of Chemical Physics*, **2015**, 142, 014905	3.9	30
566	Benchmarking all-atom simulations using hydrogen exchange. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 15975-80	11.5	61

565	Loss of conformational entropy in protein folding calculated using realistic ensembles and its implications for NMR-based calculations. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 15396-401	11.5	81
564	Influence of Cohesive Energy and Chain Stiffness on Polymer Glass Formation. *Macromolecules*, **2014**, 47, 6990-6997	5.5	49
563	Advances in the generalized entropy theory of glass-formation in polymer melts. *Journal of Chemical Physics*, **2014**, 141, 234903	3.9	30
562	Two glass transitions in miscible polymer blends?. *Journal of Chemical Physics*, **2014**, 140, 244905	3.9	24
561	Perturbative many-body expansion for electrostatic energy and field for system of polarizable charged spherical ions in a dielectric medium. *Journal of Chemical Physics*, **2014**, 141, 034115	3.9	13
560	Communication: Towards first principles theory of relaxation in supercooled liquids formulated in terms of cooperative motion. *Journal of Chemical Physics*, **2014**, 141, 141102	3.9	34
559	Concentration fluctuations in miscible polymer blends: influence of temperature and chain rigidity. *Journal of Chemical Physics*, **2014**, 140, 194901	3.9	8
558	Lattice cluster theory for polymer melts with specific interactions. *Journal of Chemical Physics*, **2014**, 141, 044909	3.9	27
557	Simplified protein models: predicting folding pathways and structure using amino acid sequences. *Physical Review Letters*, **2013**, 111, 028103	7.4	26
556	A novel implicit solvent model for simulating the molecular dynamics of RNA. *Biophysical Journal*, **2013**, 105, 1248-57	2.9	14
555	Phase field method for nonequilibrium dynamics of reversible self-assembly systems. *Journal of Chemical Physics*, **2013**, 139, 134904	3.9	
554	Molecular origins of cofilin-linked changes in actin filament mechanics. *Journal of Molecular Biology*, **2013**, 425, 1225-40	6.5	36
553	Theoretical studies of the ground and excited state structures of stilbene. *Journal of Physical Chemistry A*, **2013**, 117, 9424-34	2.8	13
552	Thermodynamic scaling of dynamics in polymer melts: predictions from the generalized entropy theory. *Journal of Chemical Physics*, **2013**, 138, 234501	3.9	16
551	Solvation of polymers as mutual association. I. General theory. *Journal of Chemical Physics*, **2013**, 138, 164901	3.9	6
550	Solvation of polymers as mutual association. II. Basic thermodynamic properties. *Journal of Chemical Physics*, **2013**, 138, 164902	3.9	11
549	Lattice cluster theory of associating polymers. II. Enthalpy and entropy of self-assembly and Flory-Huggins interaction parameter for solutions of telechelic molecules. *Journal of Chemical Physics*, **2012**, 136, 064903	3.9	10
548	Can the Miscibility of Telechelic Polymer Solutions Increase with Polymer Chain Length?. *ACS Macro Letters*, **2012**, 1, 88-91	6.6	5

547	The folding transition state of protein L is extensive with nonnative interactions (and not small and polarized). *Journal of Molecular Biology*, **2012**, 420, 220-34	6.5	25
546	Context and force field dependence of the loss of protein backbone entropy upon folding using realistic denatured and native state ensembles. *Journal of the American Chemical Society*, **2012**, 134, 15929-36	10.4	25
545	On docking, scoring and assessing protein-DNA complexes in a rigid-body framework. *PLoS ONE*, **2012**, 7, e32647	3.7	8
544	Modeling large regions in proteins: applications to loops, termini, and folding. *Protein Science*, **2012**, 21, 107-21	6.3	17
543	Cooperativity in self-limiting equilibrium self-associating systems. *Journal of Chemical Physics*, **2012**, 137, 204906	3.9	3
542	Lattice cluster theory of associating polymers. I. Solutions of linear telechelic polymer chains. *Journal of Chemical Physics*, **2012**, 136, 064902	3.9	10
541	Influence of small rings on the thermodynamics of equilibrium self-assembly. *Journal of Chemical Physics*, **2012**, 136, 244904	3.9	9
540	Lattice cluster theory of associating telechelic polymers. III. Order parameter and average degree of self-assembly, transition temperature, and specific heat. *Journal of Chemical Physics*, **2012**, 136, 194902	3.9	5
539	Lattice cluster theory of associating polymers. IV. Phase behavior of telechelic polymer solutions. *Journal of Chemical Physics*, **2012**, 136, 194903	3.9	2
538	Local Backbone Preferences and Nearest-Neighbor Effects in the Unfolded and Native States **2012**, 79-98		7
537	De novo prediction of protein folding pathways and structure using the principle of sequential stabilization. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 17442-7	11.5	35
536	Theoretical aids in screening candidates for atomic clocks: Illustration for Yb II. *Europhysics Letters*, **2012**, 98, 23002	1.6	2
535	Automated real-space refinement of protein structures using a realistic backbone move set. *Biophysical Journal*, **2011**, 101, 899-909	2.9	26
534	Modeling the hydration layer around proteins: applications to small- and wide-angle x-ray scattering. *Biophysical Journal*, **2011**, 101, 2061-9	2.9	58
533	Entropy-enthalpy compensation in chemical reactions and adsorption: an exactly solvable model. *Journal of Physical Chemistry B*, **2011**, 115, 1689-92	3.4	45
532	General approach to polymer chains confined by interacting boundaries. II. Flow through a cylindrical nano-tube. *Journal of Chemical Physics*, **2011**, 135, 144902	3.9	19
531	Prediction of electronic structure of organic radicaloid anions using efficient, economical multireference gradient approach. *Physical Chemistry Chemical Physics*, **2011**, 13, 7514-23	3.6	18
530	The descent into glass formation in polymer fluids. *Accounts of Chemical Research*, **2011**, 44, 194-203	24.3	32

529	Geometry optimization of radicaloid systems using improved virtual orbital-complete active space configuration interaction (IVO-CASCI) analytical gradient method. *Journal of Physical Chemistry A*, **2011**, 115, 3665-78	2.8	31
528	Comparison of Calculated and Measured Critical Flow Rates for Dragging Linear Polymer Chains through a Small Cylindrical Tube. *Macromolecules*, **2011**, 44, 9863-9866	5.5	19
527	Application of an efficient multireference approach to free-base porphin and metalloporphyrins: ground, excited, and positive ion states. *Journal of Chemical Physics*, **2011**, 135, 084118	3.9	16
526	A probabilistic and continuous model of protein conformational space for template-free modeling. *Journal of Computational Biology*, **2010**, 17, 783-98	1.7	14
525	Dynamics of electronic dephasing in the Fenna□Matthews□Olson complex. *New Journal of Physics*, **2010**, 12, 065042	2.9	49
524	Molecular applications of analytical gradient approach for the improved virtual orbital-complete active space configuration interaction method. *Journal of Chemical Physics*, **2010**, 132, 034105	3.9	12
523	Electrostatic solvation energy for two oppositely charged ions in a solvated protein system: salt bridges can stabilize proteins. *Biophysical Journal*, **2010**, 98, 470-7	2.9	22
522	Modeling the hydration layer around proteins: HyPred. *Biophysical Journal*, **2010**, 99, 1611-9	2.9	51
521	Plasticization and antiplasticization of polymer melts diluted by low molar mass species. *Journal of Chemical Physics*, **2010**, 132, 084504	3.9	64
520	Extended structures in RNA folding intermediates are due to nonnative interactions rather than electrostatic repulsion. *Journal of Molecular Biology*, **2010**, 397, 1298-306	6.5	16
519	General approach to polymer chains confined by interacting boundaries. *Journal of Chemical Physics* , **2010**, 133, 094901	3.9	22
518	Protein structure prediction enhanced with evolutionary diversity: SPEED. *Protein Science*, **2010**, 19, 520-34	6.3	21
517	Langevin-Debye model for nonlinear electrostatic screening of solvated ions. *Physical Review Letters*, **2009**, 102, 057603	7.4	42
516	Crowding induced self-assembly and enthalpy-entropy compensation. *Physical Review Letters*, **2009** , 103, 135701	7.4	51
515	An exactly solvable model of hierarchical self-assembly. *Journal of Chemical Physics*, **2009**, 130, 224906	3.9	14
514	Mimicking the folding pathway to improve homology-free protein structure prediction. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 3734-9	11.5	56
513	Competition between self-assembly and surface adsorption. *Journal of Chemical Physics*, **2009**, 130, 084903	3.9	14
512	Extension of lattice cluster theory to strongly interacting, self-assembling polymeric systems. *Journal of Chemical Physics*, **2009**, 130, 061103	3.9	16

511	Equilibrium polymerization models of re-entrant self-assembly. *Journal of Chemical Physics*, **2009**, 130, 164905	3.9	18
510	Third-order quasidegenerate many-body perturbation theory calculations for valence state correlation energies of the nitrogen and oxygen atoms and their ions. *International Journal of Quantum Chemistry*, **2009**, 20, 21-31	2.1	1
509	Energy dependence of nonradiative decay in polyatomic molecules. *International Journal of Quantum Chemistry*, **2009**, 6, 267-277	2.1	8
508	Self-assembly in a polymer matrix and its impact on phase separation. *Journal of Physical Chemistry B*, **2009**, 113, 3920-31	3.4	18
507	Psi-constrained simulations of protein folding transition states: implications for calculating. *Journal of Molecular Biology*, **2009**, 386, 920-8	6.5	11
506	Application of the entropy theory of glass formation to poly(alpha-olefins). *Journal of Chemical Physics*, **2009**, 131, 114905	3.9	82
505	A Probabilistic Graphical Model for Ab Initio Folding. *Lecture Notes in Computer Science*, **2009**, 5541, 59-73	3.9	7
504	Generalized Entropy Theory of Polymer Glass Formation. *Advances in Chemical Physics*, **2008**, 125-222		105
503	Quantifying the structural requirements of the folding transition state of protein A and other systems. *Journal of Molecular Biology*, **2008**, 381, 1362-81	6.5	30
502	Self-assembly by mutual association: basic thermodynamic properties. *Journal of Physical Chemistry B*, **2008**, 112, 16193-204	3.4	34
501	Benchmarking implicit solvent folding simulations of the amyloid beta(10-35) fragment. *Journal of Physical Chemistry B*, **2008**, 112, 6175-86	3.4	28
500	Solvation effect on conformations of 1,2:dimethoxyethane: charge-dependent nonlinear response in implicit solvent models. *Journal of Chemical Physics*, **2008**, 128, 034501	3.9	44
499	Potential energy curve for isomerization of N2H2 and C2H4 using the improved virtual orbital multireference M□ller-Plesset perturbation theory. *Journal of Chemical Physics*, **2008**, 128, 144304	3.9	43
498	Lattice model of equilibrium polymerization. VII. Understanding the role of "cooperativity" in self-assembly. *Journal of Chemical Physics*, **2008**, 128, 224901	3.9	61
497	Improved virtual orbital multireference M□ller-Plesset study of the ground and excited electronic states of protonated acetylene, C2H3+. *Journal of Chemical Physics*, **2008**, 129, 054308	3.9	10
496	Multistep relaxation in equilibrium polymer solutions: a minimal model of relaxation in "complex" fluids. *Journal of Chemical Physics*, **2008**, 129, 094901	3.9	32
495	Influence of nonlinear electrostatics on transfer energies between liquid phases: charge burial is far less expensive than Born model. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 11146-51	11.5	47
494	Reappraisal of cis effect in 1,2-dihaloethenes: an improved virtual orbital multireference approach. *Journal of Chemical Physics*, **2008**, 129, 064101	3.9	23

493	Polypeptide motions are dominated by peptide group oscillations resulting from dihedral angle correlations between nearest neighbors. *Biochemistry*, **2007**, 46, 669-82	3.2	23
492	The Algebra of Effective Hamiltonians and Operators: Exact Operators. *Advances in Chemical Physics*, **2007**, 465-541		24
491	Actin polymerization under pressure: a theoretical study. *Journal of Chemical Physics*, **2007**, 126, 024908	3.9	5
490	Analysis and Evaluation of Ionization Potentials, Electron Affinities, and Excitation Energies by the Equations of Motion Green's Function Method. *Advances in Chemical Physics*, **2007**, 1-69		169
489	Geometry optimization using improved virtual orbitals: a complete active space numerical gradient approach. *Journal of Chemical Physics*, **2007**, 126, 114103	3.9	14
488	Reduced C(beta) statistical potentials can outperform all-atom potentials in decoy identification. *Protein Science*, **2007**, 16, 2123-39	6.3	35
487	Lattice model of equilibrium polymerization. VI. Measures of fluid "complexity" and search for generalized corresponding states. *Journal of Chemical Physics*, **2007**, 127, 224901	3.9	23
486	Functional Integrals and Polymer Statistics. *Advances in Chemical Physics*, **2007**, 1-128		196
485	Photodissociation of Diatomic Molecules to Open Shell Atoms. *Advances in Chemical Physics*, **2007**, 1-113		46
484	Lattice Cluster Theory of Multicomponent Polymer Systems: Chain Semiflexibility and Specific Interactions. *Advances in Chemical Physics*, **2007**, 335-390		48
483	Collisional Effects on Electronic Relaxation Processes. *Advances in Chemical Physics*, **2007**, 207-269		35
482	Collision-Induced Intersystem Crossing. *Advances in Chemical Physics*, **2007**, 291-336		37
481	Does equilibrium polymerization describe the dynamic heterogeneity of glass-forming liquids?. *Journal of Chemical Physics*, **2006**, 125, 144907	3.9	70
480	Minimal model of relaxation in an associating fluid: viscoelastic and dielectric relaxations in equilibrium polymer solutions. *Journal of Chemical Physics*, **2006**, 125, 184905	3.9	16
479	Lattice model of equilibrium polymerization. V. Scattering properties and the width of the critical regime for phase separation. *Journal of Chemical Physics*, **2006**, 124, 144906	3.9	26
478	Entropy theory of polymer glass formation revisited. I. General formulation. *Journal of Chemical Physics*, **2006**, 124, 64901	3.9	79
477	Small proteins fold through transition states with native-like topologies. *Journal of Molecular Biology*, **2006**, 361, 755-70	6.5	32
476	Minimalist representations and the importance of nearest neighbor effects in protein folding simulations. *Journal of Molecular Biology*, **2006**, 363, 835-57	6.5	37

475	Ab initio description of the ground and excited states of cyanogen isomers. *Computational and Theoretical Chemistry*, **2006**, 768, 119-126		10
474	Generation of potential energy curves for the X1Sigma(+)g, B1Delta(+)g, and B'1Sigma(+)g states of C2 using the effective valence shell Hamiltonian method. *Journal of Chemical Physics*, **2005**, 122, 154310	3.9	10
473	The glass transition temperature of polymer melts. *Journal of Physical Chemistry B*, **2005**, 109, 21285-92	3.4	130
472	Fragility of glass-forming polymer liquids. *Journal of Physical Chemistry B*, **2005**, 109, 21350-6	3.4	102
471	Helix, sheet, and polyproline II frequencies and strong nearest neighbor effects in a restricted coil library. *Biochemistry*, **2005**, 44, 9691-702	3.2	150
470	A simple method for faster nonbonded force evaluations. *Journal of Computational Chemistry*, **2005**, 26, 691-8	3.5	13
469	Quadratic Pad approximants and the intruder state problem of multireference perturbation methods. *International Journal of Quantum Chemistry*, **2005**, 105, 18-33	2.1	5
468	Compressible models of equilibrium polymerization. *Journal of Chemical Physics*, **2005**, 123, 194906	3.9	14
467	Electronic structure of the calcium monohydroxide radical. *Journal of Chemical Physics*, **2005**, 122, 44317	3.9	26
466	Comparison of low-order multireference many-body perturbation theories. *Journal of Chemical Physics*, **2005**, 122, 134105	3.9	58
465	Relativistic effective valence shell Hamiltonian method: excitation and ionization energies of heavy metal atoms. *Journal of Chemical Physics*, **2005**, 122, 204111	3.9	20
464	Direct computation of characteristic temperatures and relaxation times for glass-forming polymer liquids. *Journal of Chemical Physics*, **2005**, 123, 111102	3.9	43
463	Statistical coil model of the unfolded state: resolving the reconciliation problem. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 13099-104	11.5	268
462	Flory-Huggins model of equilibrium polymerization and phase separation in the Stockmayer fluid. *Physical Review Letters*, **2004**, 92, 045502	7.4	59
461	Analytic density-functional self-consistent-field theory of diblock copolymers near patterned surfaces. *Journal of Chemical Physics*, **2004**, 120, 7174-82	3.9	10
460	Mixtures of lattice polymers with structured monomers. *Journal of Chemical Physics*, **2004**, 120, 6288-98	3.9	2
459	Influence of Frequency Shifts on Electron Transfer Processes. *Journal of Physical Chemistry B*, **2003**, 107, 10341-10343	3.4	22
458	Large-scale context in protein folding: villin headpiece. *Biochemistry*, **2003**, 42, 664-71	3.2	55

457	Computer Simulation of Met-Enkephalin Using Explicit Atom and United Atom Potentials: Similarities, Differences, and Suggestions for Improvement. *Journal of Physical Chemistry B*, **2003**, 107, 1685-1691	3.4	26
456	Investigations into sequence and conformational dependence of backbone entropy, inter-basin dynamics and the Flory isolated-pair hypothesis for peptides. *Journal of Molecular Biology*, **2003**, 331, 693-711	6.5	113
455	Folding and misfolding of the papillomavirus E6 interacting peptide E6ap. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 7087-92	11.5	9
454	A critical analysis of the ground and excited electronic states of transition metal nitrides using the relativistic effective Hamiltonian method. *Journal of Chemical Physics*, **2003**, 119, 5995-6002	3.9	9
453	Lattice model of equilibrium polymerization. IV. Influence of activation, chemical initiation, chain scission and fusion, and chain stiffness on polymerization and phase separation. *Journal of Chemical Physics*, **2003**, 119, 12645-12666	3.9	80
452	Influence of monomer molecular structure on the glass transition in polymers I. Lattice cluster theory for the configurational entropy. *Journal of Chemical Physics*, **2003**, 119, 5730-5739	3.9	35
451	The effective valence shell Hamiltonian for spin-orbit coupling. *Journal of Chemical Physics*, **2003**, 118, 8281-8289	3.9	6
450	Long time dynamics of Met-enkephalin: Tests of mode-coupling theory and implicit solvent models. *Journal of Chemical Physics*, **2003**, 118, 5143-5156	3.9	11
449	The polymerization of actin: Thermodynamics near the polymerization line. *Journal of Chemical Physics*, **2003**, 119, 4070-4084	3.9	38
448	Hydration structure of met-enkephalin: A molecular dynamics study. *Journal of Chemical Physics*, **2003**, 118, 1989-1995	3.9	9
447	All-atom fast protein folding simulations: the villin headpiece. *Proteins: Structure, Function and Bioinformatics*, **2002**, 49, 439-45	4.2	96
446	Lattice polymers with structured monomers: A Monte Carlo study of thermodynamic properties of melts and solutions. *Journal of Chemical Physics*, **2002**, 116, 10959-10966	3.9	9
445	Analytical solution for steady-state populations in the self-assembly of microtubules from nucleating sites. *Physical Review E*, **2002**, 66, 061916	2.4	11
444	Liquid-state theory derivation of surface accessible solvation potential models for proteins. *Journal of Chemical Physics*, **2002**, 116, 10475-10477	3.9	4
443	A comparison of self-assembly in lattice and off-lattice model amphiphile solutions. *Journal of Chemical Physics*, **2002**, 116, 4765	3.9	9
442	The Excited and Ion States of Allene. *ACS Symposium Series*, **2002**, 154-175	0.4	5
441	Beyond Flory-Huggins theory: new classes of blend miscibility associated with monomer structural asymmetry. *Physical Review Letters*, **2002**, 88, 095503	7.4	39
440	New patterns of polymer blend miscibility associated with monomer shape and size asymmetry. *Journal of Chemical Physics*, **2002**, 116, 9983-9996	3.9	33

439	Small angle neutron scattering studies of a polybutadiene/polystyrene blend with small additions of ortho-dichloro-benzene for varying temperatures and pressures. II. Phase boundaries and Flory–Huggins parameter. *Journal of Chemical Physics*, **2002**, 116, 2241-2250	3.9	8
438	Vector properties of S(3P) and S(1D) in the photodissociation of SH: Quantum interference and overlapping resonance. *Journal of Chemical Physics*, **2002**, 116, 10656-10663	3.9	9
437	Long time dynamics of Met-enkephalin: comparison of explicit and implicit solvent models. *Biophysical Journal*, **2002**, 82, 1791-808	2.9	99
436	A critical comparison of theoretical and experimental electronic spectrum and potential energy curves of HF molecule and its positive and negative ions. *Computational and Theoretical Chemistry*, **2001**, 547, 83-96		15
435	Monte Carlo test of the lattice cluster theory: Thermodynamic properties of binary polymer blends. *Journal of Chemical Physics*, **2001**, 114, 1424-1431	3.9	13
434	Small-angle neutron scattering studies of polybutadiene/polystyrene blends as a function of pressure and microstructure: Comparison of experiment and theory. *Journal of Chemical Physics*, **2001**, 114, 5016-5025	3.9	19
433	Thermodynamic regulation of actin polymerization. *Journal of Chemical Physics*, **2001**, 114, 10573-10576	3.9	40
432	Quantum interference and asymptotic interactions in the photodissociation of SH: Total cross section and branching ratios. *Journal of Chemical Physics*, **2001**, 114, 5537-5544	3.9	13
431	The improved virtual orbital-complete active space configuration interaction method, a "packageable" efficient ab initio many-body method for describing electronically excited states. *Journal of Chemical Physics*, **2001**, 114, 2592-2600	3.9	90
430	Determination of conformational energy differences of propynlidyne isomers using the effective valence shell Hamiltonian method. *Journal of Chemical Physics*, **2000**, 112, 9301-9309	3.9	14
429	Thermodynamic properties of lattice polymers: Monte Carlo simulations and mean-field theories. *Journal of Chemical Physics*, **2000**, 112, 6040-6048	3.9	18
428	Lattice model of living polymerization. II. Interplay between polymerization and phase stability. *Journal of Chemical Physics*, **2000**, 112, 1002-1010	3.9	58
427	Polymer melts and polymer solutions near patterned surfaces. *Journal of Chemical Physics*, **2000**, 112, 6443-6451	3.9	19
426	Polymer blends near patterned surfaces. *Journal of Chemical Physics*, **2000**, 112, 6452-6460	3.9	16
425	Explanation for the Inversion of an UCST Phase Diagram to a LCST Diagram in Binary Polybutadiene Blends. *Macromolecules*, **2000**, 33, 9777-9781	5.5	26
424	Lattice Cluster Theory for Pedestrian. 2. Random Copolymer Systems. *Macromolecules*, **2000**, 33, 3467-3477	5.5	24
423	Lattice model of living polymerization. III. Evidence for particle clustering from phase separation properties and "bounding" of the dynamical clustering transition. *Journal of Chemical Physics*, **2000**, 113, 434-446	3.9	72
422	Theoretical Studies on Excited States of a Phenolate Anion in the Environment of Photoactive Yellow Protein. *Journal of Physical Chemistry A*, **2000**, 104, 2939-2952	2.8	25

421	Explanation for the Unusual Phase Behavior of Polystyrene-b-poly(n-alkyl methacrylate) Diblock Copolymers: Specific Interactions. *Macromolecules*, **2000**, 33, 5292-5299	5.5	33
420	Lattice cluster theory for pedestrians: models for random copolymer blends. *Macromolecular Symposia*, **2000**, 149, 11-16	0.8	2
419	Pragmatic analysis for the range of validity of the lattice cluster theory. *Journal of Chemical Physics*, **1999**, 110, 1307-1312	3.9	8
418	Lattice model of living polymerization. I. Basic thermodynamic properties. *Journal of Chemical Physics*, **1999**, 111, 7116-7130	3.9	103
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