Michele Parrinello

List of Publications by Year in Descending Order

448 papers	81,516 citations	117 h-index	281 g-index
466 ext. papers	92,005 ext. citations	7 avg, IF	8.31 L-index

#	Paper	IF	Citations
448	Prediction of a Supersolid Phase in High-Pressure Deuterium.. *Physical Review Letters*, **2022**, 128, 045301	7.4	3
447	Discover, Sample, and Refine: Exploring Chemistry with Enhanced Sampling Techniques.. *Journal of Physical Chemistry Letters*, **2022**, 1424-1430	6.4	1
446	Deep learning the slow modes for rare events sampling. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	17
445	Using metadynamics to build neural network potentials for reactive events: the case of urea decomposition in water. *Catalysis Today*, **2021**,	5.3	18
444	A combined molecular dynamics and experimental study of two-step process enabling low-temperature formation of phase-pure □FAPbI. *Science Advances*, **2021**, 7,	14.3	17
443	Confinement effects and acid strength in zeolites. *Nature Communications*, **2021**, 12, 2630	17.4	29
442	Solubility Prediction of Organic Molecules with Molecular Dynamics Simulations. *Crystal Growth and Design*, **2021**, 21, 5198-5205	3.5	4
441	The role of water in host-guest interaction. *Nature Communications*, **2021**, 12, 93	17.4	11
440	A modified nudged elastic band algorithm with adaptive spring lengths. *Journal of Chemical Physics*, **2021**, 155, 074103	3.9	
439	Water-Triggered, Irreversible Conformational Change of SARS-CoV-2 Main Protease on Passing from the Solid State to Aqueous Solution. *Journal of the American Chemical Society*, **2021**, 143, 12930-12934	16.4	4
438	Liquid-Liquid Critical Point in Phosphorus. *Physical Review Letters*, **2021**, 127, 080603	7.4	8
437	From Enhanced Sampling to Reaction Profiles. *Journal of Physical Chemistry Letters*, **2021**, 12, 8621-8626	6.4	2
436	Targeted Free Energy Perturbation Revisited: Accurate Free Energies from Mapped Reference Potentials. *Journal of Physical Chemistry Letters*, **2021**, 12, 9449-9454	6.4	3
435	Integrating NMR and simulations reveals motions in the UUCG tetraloop. *Nucleic Acids Research*, **2020**, 48, 5839-5848	20.1	5
434	Path integral molecular dynamics for fermions: Alleviating the sign problem with the Bogoliubov inequality. *Journal of Chemical Physics*, **2020**, 152, 171102	3.9	11
433	Ab initio phase diagram and nucleation of gallium. *Nature Communications*, **2020**, 11, 2654	17.4	46
432	Molecular Mechanism of Gas Solubility in Liquid: Constant Chemical Potential Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 5279-5286	6.4	4

431	Gaussian Mixture-Based Enhanced Sampling for Statics and Dynamics. *Journal of Physical Chemistry Letters*, **2020**, 11, 5076-5080	6.4	16
430	Rethinking Metadynamics: From Bias Potentials to Probability Distributions. *Journal of Physical Chemistry Letters*, **2020**, 11, 2731-2736	6.4	38
429	Variationally Enhanced Sampling **2020**, 621-634		2
428	Data-Driven Collective Variables for Enhanced Sampling. *Journal of Physical Chemistry Letters*, **2020**, 11, 2998-3004	6.4	35
427	Metadynamics of Paths. *Physical Review Letters*, **2020**, 125, 026001	7.4	6
426	How Collective Phenomena Impact CO Reactivity and Speciation in Different Media. *Journal of Physical Chemistry A*, **2020**, 124, 3963-3975	2.8	7
425	A metadynamics perspective on the reduction mechanism of the Pt(IV) asplatin prodrug. *Journal of Computational Chemistry*, **2020**, 41, 290-294	3.5	0
424	Atomistic Mechanism of the Nucleation of Methylammonium Lead Iodide Perovskite from Solution. *Chemistry of Materials*, **2020**, 32, 529-536	9.6	24
423	Accuracy of Molecular Simulation-Based Predictions of Values: A Metadynamics Study. *Journal of Physical Chemistry Letters*, **2020**, 11, 6373-6381	6.4	14
422	Unified Approach to Enhanced Sampling. *Physical Review X*, **2020**, 10,	9.1	16
421	Tautomeric Equilibrium in Condensed Phases. *Journal of Chemical Theory and Computation*, **2020**, 16, 6027-6031	6.4	2
420	Neural networks-based variationally enhanced sampling. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 17641-17647	11.5	58
419	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. *Angewandte Chemie - International Edition*, **2019**, 58, 3976-3980	16.4	17
418	Accurate Quantum Chemical Free Energies at Affordable Cost. *Journal of Physical Chemistry Letters*, **2019**, 10, 3727-3731	6.4	11
417	Temperature Dependence of Homogeneous Nucleation in Ice. *Physical Review Letters*, **2019**, 122, 245501	7.4	30
416	A local fingerprint for hydrophobicity and hydrophilicity: From methane to peptides. *Journal of Chemical Physics*, **2019**, 150, 204103	3.9	1
415	Exhaustive Search of Ligand Binding Pathways via Volume-Based Metadynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 3495-3499	6.4	31
414	Naphthalene crystal shape prediction from molecular dynamics simulations. *CrystEngComm*, **2019**, 21, 3280-3288	3.3	9

413	Making the Best of a Bad Situation: A Multiscale Approach to Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2019**, 15, 2187-2194	6.4	11
412	Chasing the Full Free Energy Landscape of Neuroreceptor/Ligand Unbinding by Metadynamics Simulations. *Journal of Chemical Theory and Computation*, **2019**, 15, 3354-3361	6.4	31
411	Improving collective variables: The case of crystallization. *Journal of Chemical Physics*, **2019**, 150, 094509	3.9	22
410	Multithermal-Multibaric Molecular Simulations from a Variational Principle. *Physical Review Letters*, **2019**, 122, 050601	7.4	10
409	Kinetics of Aqueous Media Reactions via Ab Initio Enhanced Molecular Dynamics: The Case of Urea Decomposition. *Journal of Physical Chemistry B*, **2019**, 123, 6851-6856	3.4	5
408	Blind Search for Complex Chemical Pathways Using Harmonic Linear Discriminant Analysis. *Journal of Chemical Theory and Computation*, **2019**, 15, 4507-4515	6.4	13
407	Calculation of phase diagrams in the multithermal-multibaric ensemble. *Journal of Chemical Physics*, **2019**, 150, 244119	3.9	16
406	Path integral molecular dynamics for bosons. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 21445-21449	11.5	12
405	Molecular Dynamics Simulations of Crystal Nucleation from Solution at Constant Chemical Potential. *Journal of Chemical Theory and Computation*, **2019**, 15, 6923-6930	6.4	15
404	Enhanced Sampling of Transition States. *Journal of Chemical Theory and Computation*, **2019**, 15, 2454-2459	6.4	10
403	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. *Angewandte Chemie*, **2019**, 131, 4016-4020	3.6	7
402	Microscopic description of acid-base equilibrium. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 4054-4057	11.5	16
401	Enhanced Sampling of Protein Conformational Transitions via Dynamically Optimized Collective Variables. *Journal of Chemical Theory and Computation*, **2019**, 15, 1393-1398	6.4	8
400	Solvent-mediated morphology selection of the active pharmaceutical ingredient isoniazid: Experimental and simulation studies. *Chemical Engineering Science*, **2019**, 204, 320-328	4.4	23
399	Accelerating the Calculation of Protein-Ligand Binding Free Energy and Residence Times Using Dynamically Optimized Collective Variables. *Journal of Chemical Theory and Computation*, **2019**, 15, 743-750	6.4	27
398	A Cannibalistic Approach to Grand Canonical Crystal Growth. *Journal of Chemical Theory and Computation*, **2018**, 14, 2678-2683	6.4	14
397	Searching for Entropically Stabilized Phases: The Case of Silver Iodide. *Journal of Physical Chemistry C*, **2018**, 122, 1786-1790	3.8	12
396	Refining Collective Coordinates and Improving Free Energy Representation in Variational Enhanced Sampling. *Journal of Chemical Theory and Computation*, **2018**, 14, 2889-2894	6.4	13

395	Collective Variables from Local Fluctuations. *Journal of Physical Chemistry Letters*, **2018**, 9, 2776-2781	6.4	58
394	Folding a small protein using harmonic linear discriminant analysis. *Journal of Chemical Physics*, **2018**, 149, 194113	3.9	20
393	Silicon Liquid Structure and Crystal Nucleation from Ab□Initio Deep Metadynamics. *Physical Review Letters*, **2018**, 121, 265701	7.4	59
392	Variationally Enhanced Sampling **2018**, 1-14		1
391	Quantum Symmetry from Enhanced Sampling Methods. *Physical Review Letters*, **2018**, 121, 140602	7.4	3
390	Combining Metadynamics and Integrated Tempering Sampling. *Journal of Physical Chemistry Letters* , **2018**, 9, 6426-6430	6.4	16
389	Metadynamics with Discriminants: A Tool for Understanding Chemistry. *Journal of Chemical Theory and Computation*, **2018**, 14, 5040-5044	6.4	28
388	Predicting polymorphism in molecular crystals using orientational entropy. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 10251-10256	11.5	36
387	Chemical potential calculations in non-homogeneous liquids. *Journal of Chemical Physics*, **2018**, 149, 072305	3.9	7
386	Frequency adaptive metadynamics for the calculation of rare-event kinetics. *Journal of Chemical Physics*, **2018**, 149, 072309	3.9	33
385	Molecular dynamics simulations of liquid silica crystallization. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 5348-5352	11.5	47
384	Variational Flooding Study of a S2 Reaction. *Journal of Physical Chemistry Letters*, **2017**, 8, 580-583	6.4	19
383	Analyzing and Driving Cluster Formation in Atomistic Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 1317-1327	6.4	48
382	Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E2136-E2145	11.5	74
381	1,3,5-tris(4-bromophenyl)-benzene Nucleation: From Dimers to Needle-like Clusters. *Crystal Growth and Design*, **2017**, 17, 4137-4143	3.5	7
380	Unbinding Kinetics of a p38 MAP Kinase Type II Inhibitor from Metadynamics Simulations. *Journal of the American Chemical Society*, **2017**, 139, 4780-4788	16.4	115
379	Coarse graining from variationally enhanced sampling applied to the Ginzburg-Landau model. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 3370-3374	11.5	23
378	Concentration gradient driven molecular dynamics: a new method for simulations of membrane permeation and separation. *Chemical Science*, **2017**, 8, 3858-3865	9.4	43

377	Dimer Metadynamics. *Journal of Chemical Theory and Computation*, **2017**, 13, 425-430	6.4	5
376	Entropy based fingerprint for local crystalline order. *Journal of Chemical Physics*, **2017**, 147, 114112	3.9	47
375	Identifying Slow Molecular Motions in Complex Chemical Reactions. *Journal of Physical Chemistry Letters*, **2017**, 8, 4197-4200	6.4	8
374	Prion protein 2-2 loop conformational landscape. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 9617-9622	11.5	16
373	Conformational Entropy as Collective Variable for Proteins. *Journal of Physical Chemistry Letters*, **2017**, 8, 4752-4756	6.4	11
372	The impact of methylphenidate and its enantiomers on dopamine synthesis and metabolism in vitro. *Progress in Neuro-Psychopharmacology and Biological Psychiatry*, **2017**, 79, 281-288	5.5	9
371	Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations. *Physical Review Letters*, **2017**, 119, 015701	7.4	48
370	A variational conformational dynamics approach to the selection of collective variables in metadynamics. *Journal of Chemical Physics*, **2017**, 147, 204109	3.9	63
369	Hierarchical Protein Free Energy Landscapes from Variationally Enhanced Sampling. *Journal of Chemical Theory and Computation*, **2016**, 12, 5751-5757	6.4	4
368	Enhanced, targeted sampling of high-dimensional free-energy landscapes using variationally enhanced sampling, with an application to chignolin. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 1150-5	11.5	34
367	General Protein Data Bank-Based Collective Variables for Protein Folding. *Journal of Chemical Theory and Computation*, **2016**, 12, 29-35	6.4	4
366	The interaction with gold suppresses fiber-like conformations of the amyloid (16-22) peptide. *Nanoscale*, **2016**, 8, 8737-48	7.7	45
365	Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint. *Annual Review of Physical Chemistry*, **2016**, 67, 159-84	15.7	324
364	A variational approach to nucleation simulation. *Faraday Discussions*, **2016**, 195, 557-568	3.6	12
363	Application to large systems: general discussion. *Faraday Discussions*, **2016**,	3.6	4
362	Communication: Role of explicit water models in the helix folding/unfolding processes. *Journal of Chemical Physics*, **2016**, 145, 121101	3.9	5
361	Overcoming time scale and finite size limitations to compute nucleation rates from small scale well tempered metadynamics simulations. *Journal of Chemical Physics*, **2016**, 145, 211925	3.9	29
360	Bespoke Bias for Obtaining Free Energy Differences within Variationally Enhanced Sampling. *Journal of Chemical Theory and Computation*, **2016**, 12, 2162-9	6.4	10

359	Characterization of Vanadium Species in Mixed Chloride–Sulfate Solutions: An Ab Initio Metadynamics Study. *Journal of Physical Chemistry C*, **2016**, 120, 10791-10798	3.8	17
358	Chemical potential calculations in dense liquids using metadynamics. *European Physical Journal: Special Topics*, **2016**, 225, 1621-1628	2.3	14
357	Kinetics of protein-ligand unbinding: Predicting pathways, rates, and rate-limiting steps. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E386-91	11.5	234
356	Heterogeneous Crystallization of the Phase Change Material GeTe via Atomistic Simulations. *Journal of Physical Chemistry C*, **2015**, 119, 6428-6434	3.8	25
355	Insight into the nucleation of urea crystals from the melt. *Chemical Engineering Science*, **2015**, 121, 51-59	4.4	53
354	Well-Tempered Variational Approach to Enhanced Sampling. *Journal of Chemical Theory and Computation*, **2015**, 11, 1996-2002	6.4	37
353	Urea homogeneous nucleation mechanism is solvent dependent. *Faraday Discussions*, **2015**, 179, 291-307	3.6	41
352	Metadynamics studies of crystal nucleation. *IUCrJ*, **2015**, 2, 256-66	4.7	64
351	Molecular dynamics simulations of solutions at constant chemical potential. *Journal of Chemical Physics*, **2015**, 142, 144113	3.9	45
350	de Broglie Swapping Metadynamics for Quantum and Classical Sampling. *Journal of Chemical Theory and Computation*, **2015**, 11, 5114-9	6.4	6
349	A time-independent free energy estimator for metadynamics. *Journal of Physical Chemistry B*, **2015**, 119, 736-42	3.4	263
348	Variationally Optimized Free-Energy Flooding for Rate Calculation. *Physical Review Letters*, **2015**, 115, 070601	7.4	25
347	A perturbative solution to metadynamics ordinary differential equation. *Journal of Chemical Physics* , **2015**, 143, 234112	3.9	9
346	Energetics and structural characterization of the large-scale functional motion of adenylate kinase. *Scientific Reports*, **2015**, 5, 8425	4.9	36
345	Molecular-dynamics simulations of urea nucleation from aqueous solution. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E6-14	11.5	113
344	Probing the Unfolded Configurations of a β-Hairpin Using Sketch-Map. *Journal of Chemical Theory and Computation*, **2015**, 11, 1086-93	6.4	19
343	Combustion chemistry via metadynamics: benzyl decomposition revisited. *Journal of Physical Chemistry A*, **2015**, 119, 978-89	2.8	17
342	Path Integral Metadynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 1383-8	6.4	15

341	Aqueous solutions: state of the art in ab initio molecular dynamics. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2014**, 372, 20120482	3	104
340	Anomalous water diffusion in salt solutions. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 3310-5	11.5	95
339	Well-tempered metadynamics converges asymptotically. *Physical Review Letters*, **2014**, 112, 240602	7.4	182
338	Assessing the Reliability of the Dynamics Reconstructed from Metadynamics. *Journal of Chemical Theory and Computation*, **2014**, 10, 1420-5	6.4	122
337	Variational approach to enhanced sampling and free energy calculations. *Physical Review Letters*, **2014**, 113, 090601	7.4	154
336	Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-the-Fly Transition Barrier Estimation. *Journal of Chemical Theory and Computation*, **2014**, 10, 3626-33	6.4	47
335	1,3,5-Tris(4-bromophenyl)benzene prenucleation clusters from metadynamics. *Acta Crystallographica Section C, Structural Chemistry*, **2014**, 70, 132-6	0.8	19
334	The role of the umbrella inversion mode in proton diffusion. *Chemical Physics Letters*, **2014**, 599, 133-138	2.5	27
333	G-triplex structure and formation propensity. *Nucleic Acids Research*, **2014**, 42, 13393-404	20.1	51
332	The role of quantum effects on structural and electronic fluctuations in neat and charged water. *Journal of Physical Chemistry B*, **2014**, 118, 13226-35	3.4	42
331	Evaluating functions of positive-definite matrices using colored-noise thermostats. *Physical Review E*, **2014**, 89, 023302	2.4	4
330	Mechanistic insight into ligand binding to G-quadruplex DNA. *Nucleic Acids Research*, **2014**, 42, 5447-55	20.1	65
329	Transient Polymorphism in NaCl. *Journal of Chemical Theory and Computation*, **2013**, 9, 2526-30	6.4	36
328	Chiral, Racemic, and Meso-Lithium Tartrate Framework Polymorphs: A Detailed Structural Analysis. *Crystal Growth and Design*, **2013**, 13, 3705-3715	3.5	23
327	The G-Triplex DNA. *Angewandte Chemie*, **2013**, 125, 2325-2329	3.6	25
326	Controlling and predicting crystal shapes: the case of urea. *Angewandte Chemie - International Edition*, **2013**, 52, 13369-72	16.4	70
325	Density functional simulations of hexagonal Ge2Sb2Te5 at high pressure. *Physical Review B*, **2013**, 87,	3.3	5
324	Nuclear quantum effects and hydrogen bond fluctuations in water. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 15591-6	11.5	170

323	From metadynamics to dynamics. *Physical Review Letters*, **2013**, 111, 230602	7.4	270
322	Proton transfer through the water gossamer. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 13723-8	11.5	260
321	Water Release from Pyrophyllite during the Dehydroxylation Process Explored by Quantum Mechanical Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 7526-7532	3.8	7
320	Funnel metadynamics as accurate binding free-energy method. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 6358-63	11.5	234
319	The G-triplex DNA. *Angewandte Chemie - International Edition*, **2013**, 52, 2269-73	16.4	113
318	Combining metadynamics simulation and experiments to characterize dendrimers in solution. *Soft Matter*, **2013**, 9, 2593	3.6	34
317	Demonstrating the Transferability and the Descriptive Power of Sketch-Map. *Journal of Chemical Theory and Computation*, **2013**, 9, 1521-32	6.4	93
316	Thermodynamical Description of a Quasi-First-Order Phase Transition from the Well-Tempered Ensemble. *Journal of Chemical Theory and Computation*, **2013**, 9, 5267-76	6.4	11
315	The allosteric communication pathways in KIX domain of CBP. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 14237-42	11.5	52
314	Free-energy landscape of protein oligomerization from atomistic simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, E4708-13	11.5	62
313	Controlling and Predicting Crystal Shapes: The Case of Urea. *Angewandte Chemie*, **2013**, 125, 13611-13614	3.6	5
312	Sampling protein motion and solvent effect during ligand binding. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 1467-72	11.5	86
311	Uncovering molecular details of urea crystal growth in the presence of additives. *Journal of the American Chemical Society*, **2012**, 134, 17221-33	16.4	142
310	Counterion Redistribution upon Binding of a Tat-Protein Mimic to HIV-1 TAR RNA. *Journal of Chemical Theory and Computation*, **2012**, 8, 688-94	6.4	22
309	Investigating the mechanism of substrate uptake and release in the glutamate transporter homologue Glt(Ph) through metadynamics simulations. *Journal of the American Chemical Society*, **2012**, 134, 453-63	16.4	60
308	Combined Computational and Experimental NMR Study of Calix[4]arene Derivatives. *Journal of Physical Chemistry C*, **2012**, 116, 23441-23452	3.8	1
307	Metadynamics with Adaptive Gaussians. *Journal of Chemical Theory and Computation*, **2012**, 8, 2247-54	6.4	149
306	The fuzzy quantum proton in the hydrogen chloride hydrates. *Journal of the American Chemical Society*, **2012**, 134, 8557-69	16.4	41

305	Microscopic origins of the anomalous melting behavior of sodium under high pressure. *Physical Review Letters*, **2012**, 108, 115701	7.4	53
304	Locating binding poses in protein-ligand systems using reconnaissance metadynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 5170-5	11.5	39
303	Using sketch-map coordinates to analyze and bias molecular dynamics simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 5196-201	11.5	115
302	Replica Temperatures for Uniform Exchange and Efficient Roundtrip Times in Explicit Solvent Parallel Tempering Simulations. *Journal of Chemical Theory and Computation*, **2011**, 7, 2025-7	6.4	54
301	Effect of urea on the β-hairpin conformational ensemble and protein denaturation mechanism. *Journal of the American Chemical Society*, **2011**, 133, 17200-6	16.4	53
300	On the recombination of hydronium and hydroxide ions in water. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 20410-5	11.5	123
299	Nucleation mechanism for the direct graphite-to-diamond phase transition. *Nature Materials*, **2011**, 10, 693-7	27	235
298	Metadynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 826-843	7.9	746
297	A chirality-based metrics for free-energy calculations in biomolecular systems. *Journal of Computational Chemistry*, **2011**, 32, 2627-37	3.5	20
296	Intramolecular weak interactions in the thermodynamic stereoselectivity of copper(II) complexes with carnosine-trehalose conjugates. *Chemistry - A European Journal*, **2011**, 17, 9448-55	4.8	22
295	Accelerating the convergence of path integral dynamics with a generalized Langevin equation. *Journal of Chemical Physics*, **2011**, 134, 084104	3.9	119
294	Static disorder and structural correlations in the low-temperature phase of lithium imide. *Physical Review B*, **2011**, 83,	3.3	10
293	Structural Diversity and Energetics in Anhydrous Lithium Tartrates: Experimental and Computational Studies of Novel Chiral Polymorphs and Their Racemic and Meso Analogues. *Crystal Growth and Design*, **2011**, 11, 221-230	3.5	39
292	First-Principles Study of the High-Temperature Phase of Li2NH. *Journal of Physical Chemistry C*, **2011**, 115, 7076-7080	3.8	5
291	Hydrogen oxidation reaction at the Ni/YSZ anode of solid oxide fuel cells from first principles. *Physical Review Letters*, **2011**, 107, 206103	7.4	33
290	Exploring the free energy surfaces of clusters using reconnaissance metadynamics. *Journal of Chemical Physics*, **2011**, 135, 114109	3.9	20
289	Momentum distribution, vibrational dynamics, and the potential of mean force in ice. *Physical Review B*, **2011**, 83,	3.3	32
288	From the Cover: Simplifying the representation of complex free-energy landscapes using sketch-map. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 13023-8	11.5	198

287	Multiple routes and milestones in the folding of HIV-1 protease monomer. *PLoS ONE*, **2010**, 5, e13208	3.7	14
286	Displaced path integral formulation for the momentum distribution of quantum particles. *Physical Review Letters*, **2010**, 105, 110602	7.4	47
285	First-principles study of liquid and amorphous Sb2Te3. *Physical Review B*, **2010**, 81,	3.3	83
284	Nuclear quantum effects in ab initio dynamics: Theory and experiments for lithium imide. *Physical Review B*, **2010**, 82,	3.3	40
283	Molecular basis of cyclooxygenase enzymes (COXs) selective inhibition. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 5411-6	11.5	161
282	A self-learning algorithm for biased molecular dynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 17509-14	11.5	107
281	Signature of tetrahedral Ge in the Raman spectrum of amorphous phase-change materials. *Physical Review Letters*, **2010**, 104, 085503	7.4	147
280	Asprich peptides are occluded in calcite and permanently disorder biomineral crystals. *Journal of the American Chemical Society*, **2010**, 132, 11585-91	16.4	64
279	Colored-Noise Thermostats la Carte. *Journal of Chemical Theory and Computation*, **2010**, 6, 1170-1180	6.4	166
278	Linking well-tempered metadynamics simulations with experiments. *Biophysical Journal*, **2010**, 98, L44-6	2.9	50
277	Probing the mechanism of pH-induced large-scale conformational changes in dengue virus envelope protein using atomistic simulations. *Biophysical Journal*, **2010**, 99, 588-94	2.9	31
276	Efficient stochastic thermostatting of path integral molecular dynamics. *Journal of Chemical Physics* , **2010**, 133, 124104	3.9	203
275	Ab initio quality neural-network potential for sodium. *Physical Review B*, **2010**, 81,	3.3	103
274	Enhanced sampling in the well-tempered ensemble. *Physical Review Letters*, **2010**, 104, 190601	7.4	188
273	Graphite-diamond phase coexistence study employing a neural-network mapping of the ab initio potential energy surface. *Physical Review B*, **2010**, 81,	3.3	89
272	First Principles Study of the LiNH2/Li2NH Transformation. *Journal of Physical Chemistry C*, **2010**, 114, 15174-15183	3.8	31
271	Targeting biomolecular flexibility with metadynamics. *Current Opinion in Structural Biology*, **2010**, 20, 148-54	8.1	113
270	A Hybrid Approach to Fermi Operator Expansion **2009**,		11

269	Superionic conduction in substoichiometric LiAl alloy: an ab initio study. *Physical Review Letters*, **2009**, 103, 125901	7.4	17
268	Isothermal-isobaric molecular dynamics using stochastic velocity rescaling. *Journal of Chemical Physics*, **2009**, 130, 074101	3.9	215
267	Nucleotide-dependent conformational states of actin. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 12723-8	11.5	97
266	Reconstructing the equilibrium Boltzmann distribution from well-tempered metadynamics. *Journal of Computational Chemistry*, **2009**, 30, 1615-21	3.5	237
265	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. *Computer Physics Communications*, **2009**, 180, 1961-1972	4.2	1087
264	Protein conformational transitions: the closure mechanism of a kinase explored by atomistic simulations. *Journal of the American Chemical Society*, **2009**, 131, 244-50	16.4	114
263	A molecular dynamics study of the early stages of calcium carbonate growth. *Journal of Physical Chemistry B*, **2009**, 113, 11680-7	3.4	97
262	Langevin equation with colored noise for constant-temperature molecular dynamics simulations. *Physical Review Letters*, **2009**, 102, 020601	7.4	144
261	Nuclear quantum effects in solids using a colored-noise thermostat. *Physical Review Letters*, **2009**, 103, 030603	7.4	158
260	Ensemble of transition state structures for the cis-trans isomerization of N-methylacetamide. *Journal of Physical Chemistry B*, **2009**, 113, 12521-9	3.4	20
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