Michele Parrinello

List of Publications by Citations

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	Polymorphic transitions in single crystals: A new molecular dynamics method. *Journal of Applied Physics*, **1981**, 52, 7182-7190	2.5	10557
447	Unified approach for molecular dynamics and density-functional theory. *Physical Review Letters*, **1985**, 55, 2471-2474	7.4	8744
446	Canonical sampling through velocity rescaling. *Journal of Chemical Physics*, **2007**, 126, 014101	3.9	8131
445	Escaping free-energy minima. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 12562-6	11.5	3706
444	Quickstep: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach. *Computer Physics Communications*, **2005**, 167, 103-128	4.2	3322
443	Crystal Structure and Pair Potentials: A Molecular-Dynamics Study. *Physical Review Letters*, **1980**, 45, 1196-1199	7.4	2363
442	Generalized neural-network representation of high-dimensional potential-energy surfaces. *Physical Review Letters*, **2007**, 98, 146401	7.4	1638
441	Well-tempered metadynamics: a smoothly converging and tunable free-energy method. *Physical Review Letters*, **2008**, 100, 020603	7.4	1586
440	The nature of the hydrated excess proton in water. *Nature*, **1999**, 397, 601-604	50.4	1399
439	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. *Computer Physics Communications*, **2009**, 180, 1961-1972	4.2	1087
438	Metadynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 826-843	7.9	746
437	The nature and transport mechanism of hydrated hydroxide ions in aqueous solution. *Nature*, **2002**, 417, 925-9	50.4	738
436	A hybrid Gaussian and plane wave density functional scheme. *Molecular Physics*, **1997**, 92, 477-487	1.7	633
435	Efficient exploration of reactive potential energy surfaces using Car-Parrinello molecular dynamics. *Physical Review Letters*, **2003**, 90, 238302	7.4	629
434	On the Quantum Nature of the Shared Proton in Hydrogen Bonds. *Science*, **1997**, 275, 817-20	33.3	617
433	Autoionization in liquid water. *Science*, **2001**, 291, 2121-4	33.3	594
432	Ab initio molecular dynamics simulation of liquid water: Comparison of three gradient-corrected density functionals. *Journal of Chemical Physics*, **1996**, 105, 1142-1152	3.9	562

431	Study of an F center in molten KCl. *Journal of Chemical Physics*, **1984**, 80, 860-867	3.9	530
430	Water Molecule Dipole in the Gas and in the Liquid Phase. *Physical Review Letters*, **1999**, 82, 3308-3311	7.4	527
429	Structural, electronic, and bonding properties of liquid water from first principles. *Journal of Chemical Physics*, **1999**, 111, 3572-3580	3.9	522
428	Ab Initio Molecular Dynamics Simulation of the Solvation and Transport of H3O+ and OH- Ions in Water. *The Journal of Physical Chemistry*, **1995**, 99, 5749-5752		493
427	The Gaussian and augmented-plane-wave density functional method for ab initio molecular dynamics simulations. *Theoretical Chemistry Accounts*, **1999**, 103, 124-140	1.9	435
426	The influence of temperature and density functional models in ab initio molecular dynamics simulation of liquid water. *Journal of Chemical Physics*, **2005**, 122, 14515	3.9	417
425	Assessing the accuracy of metadynamics. *Journal of Physical Chemistry B*, **2005**, 109, 6714-21	3.4	402
424	Efficient reconstruction of complex free energy landscapes by multiple walkers metadynamics. *Journal of Physical Chemistry B*, **2006**, 110, 3533-9	3.4	389
423	Free-energy landscape for beta hairpin folding from combined parallel tempering and metadynamics. *Journal of the American Chemical Society*, **2006**, 128, 13435-41	16.4	378
422	From A to B in free energy space. *Journal of Chemical Physics*, **2007**, 126, 054103	3.9	361
421	Tunnelling and zero-point motion in high-pressure ice. *Nature*, **1998**, 392, 258-261	50.4	349
420	Effective force fields for condensed phase systems from ab initio molecular dynamics simulation: a new method for force-matching. *Journal of Chemical Physics*, **2004**, 120, 10896-913	3.9	349
419	Ab initio path integral molecular dynamics: Basic ideas. *Journal of Chemical Physics*, **1996**, 104, 4077-4082	3.9	348
418	Equilibrium Geometries and Electronic Structure of Iron Porphyrin Complexes: A Density Functional Study. *Journal of Physical Chemistry A*, **1997**, 101, 8914-8925	2.8	347
417	Structural, dynamical, and electronic properties of amorphous silicon: An ab initio molecular dynamics study. *Physical Review Letters*, **1988**, 60, 204-207	7.4	346
416	Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint. *Annual Review of Physical Chemistry*, **2016**, 67, 159-84	15.7	324
415	Maximally-localized Wannier functions for disordered systems: Application to amorphous silicon. *Solid State Communications*, **1998**, 107, 7-11	1.6	320
414	Liquid Water from First Principles: Investigation of Different Sampling Approaches. *Journal of Physical Chemistry B*, **2004**, 108, 12990-12998	3.4	309

413	Equilibrium free energies from nonequilibrium metadynamics. *Physical Review Letters*, **2006**, 96, 090601	7.4	304
412	Ab initio infrared spectrum of liquid water. *Chemical Physics Letters*, **1997**, 277, 478-482	2.5	298
411	Large scale electronic structure calculations. *Physical Review Letters*, **1992**, 69, 3547-3550	7.4	297
410	Efficient and accurate Car-Parrinello-like approach to Born-Oppenheimer molecular dynamics. *Physical Review Letters*, **2007**, 98, 066401	7.4	295
409	Structural and electronic properties of amorphous carbon. *Physical Review Letters*, **1989**, 62, 555-558	7.4	275
408	Efficient and general algorithms for path integral Car-Parrinello molecular dynamics. *Journal of Chemical Physics*, **1996**, 104, 5579-5588	3.9	272
407	From metadynamics to dynamics. *Physical Review Letters*, **2013**, 111, 230602	7.4	270
406	Dispersion corrections to density functionals for water aromatic interactions. *Journal of Chemical Physics*, **2004**, 120, 2693-9	3.9	266
405	A time-independent free energy estimator for metadynamics. *Journal of Physical Chemistry B*, **2015**, 119, 736-42	3.4	263
404	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
403	Equilibrium structures and finite temperature properties of silicon microclusters from ab initio molecular-dynamics calculations. *Physical Review Letters*, **1988**, 60, 271-274	7.4	258
402	Hydrogen bonding in water. *Physical Review Letters*, **2003**, 91, 215503	7.4	253
401	The role and perspective of ab initio molecular dynamics in the study of biological systems. *Accounts of Chemical Research*, **2002**, 35, 455-64	24.3	248
400	Reconstructing the equilibrium Boltzmann distribution from well-tempered metadynamics. *Journal of Computational Chemistry*, **2009**, 30, 1615-21	3.5	237
399	Nucleation mechanism for the direct graphite-to-diamond phase transition. *Nature Materials*, **2011**, 10, 693-7	27	235
398	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
397	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
396	Flexible docking in solution using metadynamics. *Journal of the American Chemical Society*, **2005**, 127, 2600-7	16.4	230

395	General and efficient algorithms for obtaining maximally localized Wannier functions. *Physical Review B*, **2000**, 61, 10040-10048	3.3	229
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393	Molecular dynamics in low-spin excited states. *Journal of Chemical Physics*, **1998**, 108, 4060-4069	3.9	219
392	Isothermal-isobaric molecular dynamics using stochastic velocity rescaling. *Journal of Chemical Physics*, **2009**, 130, 074101	3.9	215
391	Ab initio molecular dynamics with excited electrons. *Physical Review Letters*, **1994**, 73, 2599-2602	7.4	213
390	A recipe for the computation of the free energy barrier and the lowest free energy path of concerted reactions. *Journal of Physical Chemistry B*, **2005**, 109, 6676-87	3.4	210
389	Freezing of a Lennard-Jones fluid: from nucleation to spinodal regime. *Physical Review Letters*, **2006**, 97, 105701	7.4	207
388	Efficient stochastic thermostatting of path integral molecular dynamics. *Journal of Chemical Physics* , **2010**, 133, 124104	3.9	203
387	Anisotropy of Earth's D'' layer and stacking faults in the MgSiO3 post-perovskite phase. *Nature*, **2005**, 438, 1142-4	50.4	203
386	A New ab-Initio Approach for NMR Chemical Shifts in Periodic Systems. *Journal of Physical Chemistry A*, **2001**, 105, 1951-1958	2.8	199
385	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
384	Ab initio path-integral molecular dynamics. *European Physical Journal B*, **1994**, 95, 143-144	1.2	196
383	First Principles Molecular Dynamics Study of Ziegler Natta Heterogeneous Catalysis. *Journal of the American Chemical Society*, **1998**, 120, 2746-2752	16.4	194
382	Accurate sampling using Langevin dynamics. *Physical Review E*, **2007**, 75, 056707	2.4	193
381	Enhanced sampling in the well-tempered ensemble. *Physical Review Letters*, **2010**, 104, 190601	7.4	188
380	An Efficient Real Space Multigrid QM/MM Electrostatic Coupling. *Journal of Chemical Theory and Computation*, **2005**, 1, 1176-84	6.4	186
379	Ab initio Molecular Dynamics Simulation of Laser Melting of Silicon. *Physical Review Letters*, **1996**, 77, 3149-3152	7.4	186
378	Crystal structure transformations in SiO2 from classical and ab initio metadynamics. *Nature Materials*, **2006**, 5, 623-6	27	183

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376	Metadynamics simulations of the high-pressure phases of silicon employing a high-dimensional neural network potential. *Physical Review Letters*, **2008**, 100, 185501	7.4	181
375	The conformational free energy landscape of beta-D-glucopyranose. Implications for substrate preactivation in beta-glucoside hydrolases. *Journal of the American Chemical Society*, **2007**, 129, 10686-93	16.4	177
374	Water structure as a function of temperature from X-ray scattering experiments and ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2003**, 5, 1981	3.6	173
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372	Structural quantum effects and three-centre two-electron bonding in CH+5. *Nature*, **1995**, 375, 216-218	50.4	172
371	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
370	Colored-Noise Thermostats la Carte. *Journal of Chemical Theory and Computation*, **2010**, 6, 1170-1180	6.4	166
369	Generalized variational density functional perturbation theory. *Journal of Chemical Physics*, **2000**, 113, 7102-7109	3.9	165
368	Ab initio molecular-dynamics simulation of K+ solvation in water. *Journal of Chemical Physics*, **1999**, 111, 1587-1591	3.9	165
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366	First Principles Study of Propene Polymerization in ZieglerNatta Heterogeneous Catalysis. *Journal of the American Chemical Society*, **2000**, 122, 501-509	16.4	160
365	Nuclear quantum effects in solids using a colored-noise thermostat. *Physical Review Letters*, **2009**, 103, 030603	7.4	158
364	Integrating the CarParrinello equations. I. Basic integration techniques. *Journal of Chemical Physics* , **1994**, 101, 1302-1315	3.9	158
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360	Variational approach to enhanced sampling and free energy calculations. *Physical Review Letters*, **2014**, 113, 090601	7.4	154

359	Metadynamics with Adaptive Gaussians. *Journal of Chemical Theory and Computation*, **2012**, 8, 2247-54	6.4	149
358	Hydrolysis at stepped MgO surfaces. *Physical Review Letters*, **1994**, 73, 504-507	7.4	149
357	Electronic structure of wet DNA. *Physical Review Letters*, **2002**, 89, 108102	7.4	148
356	Signature of tetrahedral Ge in the Raman spectrum of amorphous phase-change materials. *Physical Review Letters*, **2010**, 104, 085503	7.4	147
355	First-principles molecular-dynamics simulations of a hydrated electron in normal and supercritical water. *Physical Review Letters*, **2003**, 90, 226403	7.4	147
354	Pulling monatomic gold wires with single molecules: an Ab initio simulation. *Physical Review Letters*, **2002**, 89, 186402	7.4	147
353	Langevin equation with colored noise for constant-temperature molecular dynamics simulations. *Physical Review Letters*, **2009**, 102, 020601	7.4	144
352	Ab initio molecular dynamics of ion solvation. The case of Be2+ in water. *Chemical Physics Letters*, **1997**, 273, 360-366	2.5	144
351	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
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349	Reconstructing the density of states by history-dependent metadynamics. *Physical Review Letters*, **2004**, 92, 170601	7.4	137
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346	Hydrogen bonding and dipole moment of water at supercritical conditions: a first-principles molecular dynamics study. *Physical Review Letters*, **2000**, 85, 3245-8	7.4	134
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336	Microscopic struture of amorphous covalent alloys probed by ab initio molecular dynamics: SiC. *Physical Review Letters*, **1992**, 68, 3044-3047	7.4	120
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329	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
328	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
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315	A molecular dynamics study of the early stages of calcium carbonate growth. *Journal of Physical Chemistry B*, **2009**, 113, 11680-7	3.4	97
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303	The role of the peripheral anionic site and cation-pi interactions in the ligand penetration of the human AChE gorge. *Journal of the American Chemical Society*, **2005**, 127, 9147-55	16.4	87
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290	Density-functional study of hydration of sodium in water clusters. *Journal of Chemical Physics*, **1998**, 109, 6839-6843	3.9	77
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