Carlo Pierleoni

List of Publications by Year
in descending order

98 papers	3,566 citations	136950 32 h-index	138484 58 g-index
100 all docs	100 docs citations	100 times ranked	2077 citing authors

#	Article	IF	Citations
1	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	1.8	79
2	Multi-scale simulation of the adsorption of lithium ion on graphite surface: From quantum Monte Carlo to molecular density functional theory. Journal of Chemical Physics, 2022, 156, 094709.	3.0	6
3	Electronic energy gap closure and metal-insulator transition in dense liquid hydrogen. Physical Review B, 2020, 102, .	3.2	13
4	Quantum Monte Carlo determination of the principal Hugoniot of deuterium. Physical Review B, 2020, 102, .	3.2	3
5	Characterization of molecular-atomic transformation in fluid hydrogen under pressure via long-wavelength asymptote of charge density fluctuations. Journal of Molecular Liquids, 2020, 312, 113274.	4.9	6
6	Energy Gap Closure of Crystalline Molecular Hydrogen with Pressure. Physical Review Letters, 2020, 124, 116401.	7.8	24
7	Electronic band gaps from quantum Monte Carlo methods. Physical Review B, 2020, 101, .	3.2	26
8	Electronic structure and optical properties of quantum crystals from first principles calculations in the Bornâ€“Oppenheimer approximation. Journal of Chemical Physics, 2020, 153, 234117.	3.0	6
9	Velocity autocorrelations across the molecularâ€”atomic fluid transformation in hydrogen under pressure. Condensed Matter Physics, 2020, 23, 23607.	0.7	3
10	Filament flexibility enhances power transduction of F-actin bundles. Journal of Chemical Physics, 2019, 150, 185101.	3.0	3
11	Optical properties of high-pressure fluid hydrogen across molecular dissociation. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9770-9774.	7.1	28
12	Benchmarking vdWâ€DF firstâ€principles predictions against Coupled Electronâ€“Ion Monte Carlo for highâ€pressure liquid hydrogen. Contributions To Plasma Physics, 2019, 59, e201800185.	1.1	11
13	On the forceâ€“velocity relationship of a bundle of rigid bio-filaments. Journal of Chemical Physics, 2018, 148, 095101.	3.0	6
14	Local structure in dense hydrogen at the liquidâ€“liquid phase transition by coupled electronâ€“ion Monte Carlo. Contributions To Plasma Physics, 2018, 58, 99-106.	1.1	21
15	Coupled electron-ion Monte Carlo simulation of hydrogen molecular crystals. Journal of Chemical Physics, 2018, 148, 102314.	3.0	38
16	Electron localization properties in high pressure hydrogen at the liquid-liquid phase transition by Coupled Electron-Ion Monte Carlo. Journal of Physics: Conference Series, 2018, 1136, 012005.	0.4	6
17	A Review of Equation-of-State Models for Inertial Confinement Fusion Materials. High Energy Density Physics, 2018, 28, 7-24.	1.5	54
18	Particle-Based Modeling of Living Actin Filaments in an Optical Trap. Polymers, 2016, 8, 343.	4.5	1

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19	Phase Diagram and Structure of Mixtures of Large Colloids and Linear Polymers under Good-Solvent Conditions. Macromolecules, 2016, 49, 5266-5280.	4.8	8
20	On the properties of a bundle of flexible actin filaments in an optical trap. Journal of Chemical Physics, 2016, 144, 245102.	3.0	3
21	Liquidâ€“liquid phase transition in hydrogen by coupled electronâ€“ion Monte Carlo simulations. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4953-4957.	7.1	91
22	Theory of finite size effects for electronic quantum Monte Carlo calculations of liquids and solids. Physical Review B, 2016, 94, .	3.2	79
23	Probabilistic Derivation of Spatiotemporal Correlation Functions in the Hydrodynamic Limit. Journal of Physical Chemistry B, 2016, 120, 1996-2000.	2.6	2
24	Molecular-Atomic Transition along the Deuterium Hugoniot Curve with Coupled Electron-Ion Monte Carlo Simulations. Physical Review Letters, 2015, 115, 045301.	7.8	35
25	A semi-flexible model prediction for the polymerization force exerted by a living F-actin filament on a fixed wall. Journal of Chemical Physics, 2015, 143, 145101.	3.0	6
26	Coarse-graining polymer solutions: A critical appraisal of single- and multi-site models. European Physical Journal: Special Topics, 2015, 224, 2239-2267.	2.6	11
27	Integral equation analysis of single-site coarse-grained models for polymerâ€“colloid mixtures. Molecular Physics, 2015, 113, 2629-2642.	1.7	2
28	Accurate coarse-grained models for mixtures of colloids and linear polymers under good-solvent conditions. Journal of Chemical Physics, 2014, 141, 244905.	3.0	7
29	First Principles Methods: A Perspective from Quantum Monte Carlo. Entropy, 2014, 16, 287-321.	2.2	33
30	Benchmarking exchange-correlation functionals for hydrogen at high pressures using quantum Monte Carlo. Physical Review B, 2014, 89, .	3.2	72
31	Phase diagram of mixtures of colloids and polymers in the thermal crossover from good to Î¸ solvent. Journal of Chemical Physics, 2014, 141, 024902.	3.0	11
32	Quantum Monte Carlo Techniques and Applications for Warm Dense Matter. Lecture Notes in Computational Science and Engineering, 2014, , 123-149.	0.3	10
33	Depletion effects in colloidâ€“polymer solutions. Molecular Physics, 2013, 111, 3372-3393.	1.7	12
34	Personal Tribute. Molecular Physics, 2013, 111, 3341-3342.	1.7	0
35	Charge transport simulations of NaCl in an external magnetic field: the quest for the Hall effect. Molecular Physics, 2013, 111, 3651-3661.	1.7	7
36	Nuclear Quantum Effects and Nonlocal Exchange-Correlation Functionals Applied to Liquid Hydrogen at High Pressure. Physical Review Letters, 2013, 110, 065702.	7.8	150

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37	Towards a predictive first-principles description of solid molecular hydrogen with density functional theory. Physical Review B, 2013, 87, .	3.2	75
38	Predicting the thermodynamics by using state-dependent interactions. Journal of Chemical Physics, 2013, 138, 234107.	3.0	38
39	Consistent coarse-graining strategy for polymer solutions in the thermal crossover from good to Î, solvent. Journal of Chemical Physics, 2013, 139, 034901.	3.0	7
40	The properties of hydrogen and helium under extreme conditions. Reviews of Modern Physics, 2012, 84, 1607-1653.	45.6	425
41	Coarse-graining strategies in polymer solutions. Soft Matter, 2012, 8, 5151.	2.7	40
42	Polymers as compressible soft spheres. Journal of Chemical Physics, 2012, 136, 224905.	3.0	15
43	Consistent and transferable coarse-grained model for semidilute polymer solutions in good solvent. Journal of Chemical Physics, 2012, 137, 024901.	3.0	9
44	Free energy methods in coupled electron ion Monte Carlo. Molecular Physics, 2011, 109, 3029-3036.	1.7	20
45	Liquid-solid transition in fully ionized hydrogen at ultra-high pressures. Journal of Chemical Physics, 2011, 134, 184505.	3.0	13
46	Momentum Distribution of the Homogeneous Electron Gas. Physical Review Letters, 2011, 107, 110402.	7.8	64
47	Path integral based calculations of symmetrized time correlation functions. I.. Journal of Chemical Physics, 2010, 133, 164104.	3.0	17
48	Crystalline free energies of micelles of diblock copolymer solutions. Journal of Chemical Physics, 2010, 133, 204902.	3.0	2
49	Path integral based calculations of symmetrized time correlation functions. II. Journal of Chemical Physics, 2010, 133, 164105.	3.0	15
50	Equation of state of metallic hydrogen from coupled electron-ion Monte Carlo simulations. Physical Review E, 2010, 81, 021202.	2.1	69
51	Evidence for a first-order liquid-liquid transition in high-pressure hydrogen from ab initio simulations. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 12799-12803.	7.1	217
52	Transient hydrodynamical behavior by dynamical nonequilibrium molecular dynamics: The formation of convective cells. Journal of Chemical Physics, 2009, 131, 064106.	3.0	13
53	Electrical Conductivity of High-Pressure Liquid Hydrogen by Quantum MonteÂCarlo Methods. Physical Review Letters, 2009, 103, 256401.	7.8	30
54	Phase separation in hydrogenâ€“helium mixtures at Mbar pressures. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 1324-1329.	7.1	107

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55	Compressible Convective Instability by Molecular Dynamics. Progress of Theoretical Physics Supplement, 2009, 178, 15-23.	0.1	1
56	Entropic Self-Assembly of Diblock Copolymers into Disordered and Ordered Micellar Phases. Journal of Physical Chemistry B, 2009, 113, 3629-3638.	2.6	32
57	Sphere versus Cylinder: The Effect of Packing on the Structure of Nonionic C₁₂E₆ Micelles. Langmuir, 2009, 25, 8960-8967.	3.5	25
58	Crystal stability of diblock copolymer micelles in solution. Molecular Physics, 2009, 107, 535-548.	1.7	8
59	Trial wave functions for high-pressure metallic hydrogen. Computer Physics Communications, 2008, 179, 89-97.	7.5	21
60	Bulk viscosity of the Lennard-Jones system at the triple point by dynamical nonequilibrium molecular dynamics. Physical Review E, 2008, 78, 021204.	2.1	17
61	Pressure-Induced Core Packing and Interfacial Dehydration in Nonionic C12E6 Micelle in Aqueous Solution. Langmuir, 2008, 24, 6067-6071.	3.5	7
62	PROGRESS IN COUPLED ELECTRON-ION MONTE CARLO SIMULATIONS OF HIGH-PRESSURE HYDROGEN. , 2008, , .		0
63	A soft effective segment representation of semidilute polymer solutions. Journal of Chemical Physics, 2007, 127, 171102.	3.0	53
64	Molecular Modeling and Simulation of Water near Model Micelles:Â Diffusion, Rotational Relaxation and Structure at the Hydration Interface. Journal of Physical Chemistry B, 2006, 110, 11504-11510.	2.6	40
65	Structure and Dynamics of Hydrogen Bonds in the Interface of a C12E6Spherical Micelle in Water Solution:Â A MD Study at Various Temperatures. Journal of Physical Chemistry B, 2006, 110, 18254-18261.	2.6	8
66	Quantum MonteÂCarlo Simulation of the High-Pressure Molecular-Atomic Crossover in Fluid Hydrogen. Physical Review Letters, 2006, 97, 235702.	7.8	62
67	Multiscale Coarse Graining of Diblock Copolymer Self-Assembly: From Monomers to Ordered Micelles. Physical Review Letters, 2006, 96, 128302.	7.8	64
68	The Coupled Electron-Ion Monte Carlo Method. , 2006, , 641-683.		17
69	Hydration and thermodynamic equilibrium of non-ionic surfactant in solution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2005, 261, 93-99.	4.7	2
70	Computational Methods in Coupled Electron-Ion Monte Carlo Simulations. ChemPhysChem, 2005, 6, 1872-1878.	2.1	33
71	Coupled Electronâ€“Ion Monte Carlo calculations of atomic hydrogen. Computer Physics Communications, 2005, 169, 421-425.	7.5	4
72	Coupled Electron-Ion Monte Carlo Calculations of Dense Metallic Hydrogen. Physical Review Letters, 2004, 93, 146402.	7.8	76

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73	Molecular Dynamics Study of Temperature Dehydration of a C12E6Spherical Micelle. Langmuir, 2004, 20, 4311-4314.	3.5	50
74	Backflow correlations for the electron gas and metallic hydrogen. Physical Review E, 2003, 68, 046707.	2.1	94
75	Single chain elasticity and thermoelasticity of polyethylene. Journal of Chemical Physics, 2002, 117, 9028-9036.	3.0	8
76	Restricted Path Integral Monte Carlo Calculations of Hot, Dense Hydrogen. , 2002, , 337-340.		1
77	The Coupled Electronic-Ionic Monte Carlo Simulation Method. Lecture Notes in Physics, 2002, , 473-500.	0.7	11
78	Molecular Dynamics Study of Spherical Aggregates of Chain Molecules at Different Degrees of Hydrophilicity in Water Solution. Langmuir, 2001, 17, 5103-5110.	3.5	32
79	Free Energy of the FrÃ¶hlich Polaron in Two and Three Dimensions. Physical Review Letters, 2001, 87, 206406.	7.8	23
80	Induced charge in a FrÃ¶hlich polaron: Sum rule and spatial extent. Physical Review B, 2000, 62, 4426-4430.	3.2	8
81	Excluded volume effects on the structure of a linear polymer under shear flow. Journal of Chemical Physics, 2000, 113, 5545.	3.0	10
82	Different statistical mechanical ensembles for a stretched polymer. Physical Review E, 1999, 60, 7010-7021.	2.1	37
83	Wigner approach to the semiclassical dynamics of a quantum many-body system: the dynamic scattering function of 4He. Computer Physics Communications, 1999, 121-122, 452-459.	7.5	14
84	Polymer Solutions in Flow: A Non-Equilibrium Molecular Dynamics Approach. , 1999, , 5-40.		1
85	On the Signature of Tensile Blobs in the Scattering Function of a Stretched Polymer. Physical Review Letters, 1997, 79, 2990-2993.	7.8	15
86	Molecular Dissociation in Hot, Dense Hydrogen. Physical Review Letters, 1996, 76, 1240-1243.	7.8	215
87	Deformation and Orientation of Flexible Polymers in Solution under Shear Flow: A New Picture for Intermediate Reduced Shear Rates. Macromolecules, 1995, 28, 5097-5108.	4.8	48
88	Isotopic shift of helium melting pressure: Path integral Monte Carlo study. Physical Review Letters, 1994, 72, 1854-1857.	7.8	48
89	Equation of State of the Hydrogen Plasma by Path Integral Monte Carlo Simulation. Physical Review Letters, 1994, 73, 2145-2149.	7.8	153
90	Scaling analysis for a chain molecule in shear flow by molecular dynamics simulation. Physical Review Letters, 1993, 71, 1724-1727.	7.8	21

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91	Liquid chlorine in shear and elongational flows: A nonequilibrium molecular dynamics study. Journal of Chemical Physics, 1992, 97, 9335-9344.	3.0	43
92	On the use of the NosÃ©-Hoover thermostat in the simulation of dynamic properties of a single chain molecule in solvent. Molecular Physics, 1992, 75, 731-737.	1.7	15
93	Molecular dynamics investigation of dynamic scaling for dilute polymer solutions in good solvent conditions. Journal of Chemical Physics, 1992, 96, 8539-8551.	3.0	57
94	Theoretical Foundation and Rheological Application of Non-Equilibrium Molecular Dynamics. NATO ASI Series Series B: Physics, 1992, , 25-45.	0.2	30
95	Non-Newtonian viscosity of atomic fluids in shear and shear-free flows. Physical Review A, 1991, 44, 5314-5317.	2.5	16
96	Relaxation of a single chain molecule in good solvent conditions by molecular-dynamics simulation. Physical Review Letters, 1991, 66, 2992-2995.	7.8	49
97	Thermotransport coefficients of a classical binary ionic mixture by non-equilibrium molecular dynamics. Journal of Physics Condensed Matter, 1990, 2, 1315-1324.	1.8	11
98	Thermal Conductivity of the Classical One-Component Plasma by Nonequilibrium Molecular Dynamics. Europhysics Letters, 1987, 4, 1115-1120.	2.0	35