List of Publications of Carlo Pierleoni

(May 2022)

Complete list of Publications.

References

2016-present

[1] M. Ruggeri, K. Reeves, Tzu-Yao Hsu, G. Jeanmairet, M. Salanne and **C. Pierleoni**, "Multi-scale simulation of the adsorption of lithium ion on graphite surface: From quantum Monte Carlo to molecular density functional theory", J. Chem. Phys. **156**, 094709 (2022).

[2] L. Boeri et al, "The 2021 Room-Temperature Superconductivity Roadmap", J. Phys. Cond. Matt. **34**, 18300210, (2022).

[3] V. Gorelov, D. M. Ceperley, M. Holzmann and **C. Pierleoni**, "Electronic structure and optical properties of quantum crystals from first principles calculations in the Born–Oppenheimer approximation", *J. Chem Phys* **153**, 234117 (2020).

[4] V. Gorelov, D. M. Ceperley, M. Holzmann and **C. Pierleoni**, "Electronic energy gap closure and metal-insulator transition in dense liquid hydrogen", *Phys. Rev. B* **102**, 195133 (2020).

[5] M. Ruggeri, M. Holzmann, D.M. Ceperley and **C. Pierleoni**, "Quantum Monte Carlo determination of the principal Hugoniot of deuterium", *Phys. Rev. B* **102**, 144108 (2020).

[6] G. Ruocco, T. Bryk, **C. Pierleoni** and A.P. Seitsonen, "Velocity autocorrelations across the molecular-atomic fluid transformation in hydrogen under pressure", *Condensed Matter Physics* **23**, 23607 (2020).

[7] T. Bryk, **C. Pierleoni**, G. Ruocco and A. P. Seitsonen,"Characterization of molecular-atomic transformation in fluid hydrogen under pressure via long-wavelength asymptote of charge density fluctuations", *Journal of Molecular Liquids* **312**, 113274 (2020).

[8] V. Gorelov, M. Holzmann, D.M. Ceperley and **C. Pierleoni**, "Energy Gap Closure of Crystalline Molecular Hydrogen with Pressure", *Phys. Rev. Letts.* **124**, 116401 (2020); arXiv:1911.06135.

[9] Y. Yang, V. Gorelov, **C. Pierleoni**, D.M. Ceperley and M. Holzmann, "Electronic band gaps from Quantum Monte Carlo methods", *Phys. Rev B* **101**, 085115(2020); arXiv:1910.07531.

[10] G. Rillo, M.A. Morales, D.M. Ceperley and **C. Pierleoni**, "Optical properties of liquid hydrogen across molecular dissociation", *PNAS* **116** 9770 (2019).

[11] A. Perilli, **C. Pierleoni** and J.P. Ryckaert, "Filament flexibility enhances power transduction of F-actin bundles", *J. Chem. Phys.* **150**, 185101 (2019).

[12] V. Gorelov, **C. Pierleoni** and D.M. Ceperley, "Benchmarking vdW-DF first-principles predictions against Coupled Electron-Ion Monte Carlo for high-pressure liquid hydrogen". *Contributions to Plasma Physics* (2019); e201800185. https://doi.org/10.1002/ctpp.201800185

[13] J.A. Gaffney et al, "A Review of Equation-of-State Models for Inertial Confinement Fusion Materials", *High Energy-Density Physics* **28**, 7-24 (2018).

[14] **C. Pierleoni**, G. Rillo, M. Holzmann and D.M. Ceperley, "Electron localization properties in high pressure hydrogen at the liquid-liquid phase transition by Coupled Electron-Ion Monte Carlo", *J. Phys.: Conf. Ser.* **1136**, 012005 (2018).

[15] **C. Pierleoni**, M. Holzmann and D.M. Ceperley, "Local structure in dense hydrogen at the fluid-fluid phase transition by Coupled Electron-Ion Monte Carlo", *Contribution to Plasma Physics*, **58**, 99–106 (2018).

[16] A. Perilli, **C. Pierleoni**, G. Ciccotti, J.P. Ryckaert, "On the force–velocity relationship of a bundle of rigid living filaments", *J. Chem Phys.* **148**, 095101 (2018); doi: 10.1063/1.5001124.

[17] G. Rillo, M.A. Morales, D.M. Ceperley and **C. Pierleoni**, "Coupled electron-ion Monte Carlo simulation of hydrogen molecular crystals", *J. Chem Phys.* **148**, 102314 (2018).

[18] T.A. Hunt, S. Mogurampelly, G. Ciccotti, **C. Pierleoni** and J.P. Ryckaert (2016). "Particle-based modeling of living actin filaments in an optical trap", *Polymers* **8** 343 (2016).

[19] G. Ciccotti, S. Bonella, M. Ferrario and **C. Pierleoni**, "Probabilistic Derivation of Spatiotemporal Correlation Functions in the Hydrodynamic Limit", *J. Phys. Chem. B* **120**, 1996-2000 (2016).

[20] M. Holzmann, R.C. Clay, M.A. Morales, N.M. Tubman, D.M. Ceperley and **C. Pierleoni**, "Theory of finite size effects for electronic quantum Monte Carlo calculations of liquids and solids", *Phys. Rev. B* **94** 035126 (2016).

[21] G. D'Adamo, A. Pelissetto, **C. Pierleoni**, "Phase Diagram and Structure of Mixtures of Large Colloids and Linear Polymers under Good-Solvent Conditions", *Macromolecules* **49** 5266-5280 (2016).

[22] A. Perilli, **C. Pierleoni**, G. Ciccotti, J.P. Ryckaert, "On the properties of a bundle of flexible actin filaments in an optical trap", *J. Chem Phys.* **144**, 245102 (2016).

[23] **C. Pierleoni**, M.A. Morales, G. Rillo, M. Holzmann, D.M. Ceperley, "Liquid-liquid transition in high pressure hydrogen by Coupled Electron-Ion Monte Carlo", *PNAS* **113**, 4953-4957 (2016).

2011-2015

[24] G D'Adamo, R Menichetti, A Pelissetto, **C Pierleoni** "Coarse-graining polymer solutions: a critical appraisal of single-and multi-site models", *Eur. Phys. J.- Special Topics* **224**, 2239 (2015).

[25] N.M. Tubman, E. Liberatore, **C. Pierleoni**, M. Holzmann, D.M. Ceperley, "Molecular-Atomic Transition along the Deuterium Hugoniot Curve with Coupled Electron Ion Monte Carlo Simulations", *Phys. Rev. Letts.* **115**, 045301 (2015).

[26] **C. Pierleoni**, G. Ciccotti, J.P. Ryckaert, "A semi-flexible model prediction for the polymerization force exerted by a living F-actin filament on a fixed wall", *J. Chem. Phys.* **143**,145101 (2015).

[27] R Menichetti, A Pelissetto, G D'Adamo, **C Pierleoni**, "Integral-equation analysis of single-site coarse-grained models for polymer-colloid mixtures", *Mol. Phys.* **113**, 2629 (2015).

[28] R.C. Clay III, J. Mcminis, J.M. McMahon, **C. Pierleoni**, D.M. Ceperley and M.A. Morales, "Benchmarking exchange-correlation functionals for hydrogen at high pressures using quantum Monte Carlo", *Phys. Rev.* B 89, 184106 (2014).

[29] G D'Adamo, A Pelissetto, **C Pierleoni**, "Phase diagram of mixtures of colloids and polymers in the thermal crossover from good to θ solvent", *J. Chem Phys* 141 (2), 024902 (2014).

[30] G D'Adamo, A Pelissetto, **C Pierleoni**, "Accurate coarse-grained models for mixtures of colloids and linear polymers under good-solvent conditions", *J. Chem Phys* 141 (24), 244905 (2014).

[31] E. Brown, M. A. Morales, **C. Pierleoni**, D.M. Ceperley, "Quantum Monte Carlo techniques and applications for warm dense matter", in Frontiers and Challenges in Warm Dense Matter, F. Graziani, M.P. Desjarlais, R. Redmer and S.B. Trickey eds., Lecture Notes in Computational Science and Engineering, vol 96, pg.123-149 (Springer, 2014).

[32] M. A. Morales, J. M. McMahon, **C. Pierleoni**, D. M. Ceperley, "Nuclear Quantum Effects and Nonlocal Exchange–Correlation Functionals Applied to Liquid Hydrogen at High Pressure", *Phys Rev Letts.* **110**, 065702 (2013).

[33] M. A. Morales, J. M. McMahon, **C. Pierleoni**, D. M. Ceperley, "Toward a Predictive First-Principles Description of Solid Molecular Hydrogen with Density-Functional Theory", *Phys Rev B* **87**, 184107 (2013).

[34] G. D'Adamo, A. Pelissetto, **C. Pierleoni**, "Predicting the thermodynamics by using state-dependent interactions", *J. Chem. Phys.* **138**, 234107 (2013).

[35] G. D'Adamo, A. Pelissetto, **C. Pierleoni**, "Consistent Coarse-graining strategy for polymer solutions in the thermal crossover from good to theta solvent" *J. Chem. Phys.* **139**, 034901 (2013).

[36] G. D'Adamo, A. Pelissetto, **C. Pierleoni**, "Depletion effects in colloid-polymer solutions", *Mol. Phys.*, 111 (22-23), 3372-3393 (2013).

[37] F Mouhat, S Bonella, C Pierleoni, "Charge transport simulations of NaCl in an external magnetic field: the quest for the Hall effect", *Mol. Phys.* 111 (22-23), 3651-3661 (2013).

[38] M.A. Morales, R. C. Clay III, **C. Pierleoni**, D.M. Ceperley, "First principles methods: A perspective from quantum Monte Carlo", *Entropy* 16 (1), 287-321 (2013).

[39] G. D'Adamo, A. Pelissetto, **C. Pierleoni**, "Coarse-graining strategies in polymer solutions", *Soft Matter*, **8**, 5151-5167 (2012).

[40] G. D'Adamo, A. Pelissetto, **C. Pierleoni**, "Polymers as compressible soft spheres", *J. Chem. Phys.*, **136**, 224905 (2012).

[41] G. D'Adamo, A. Pelissetto, **C. Pierleoni**, "Consistent and transferrable coarse-grained model for semidilute polymer solutions in good solvent", *J. Chem. Phys.*. **137**, 024901 (2012).

[42] J. M. McMahon, M.A. Morales, **C. Pierleoni**, D. M. Ceperley, "The properties of Hydrogen and Helium under Extreme Conditions", *Rev. Mod. Phys.*, **Invited Article**, **84**, 1607 (2012).

[43] E. Liberatore, **C. Pierleoni**, D.M. Ceperley, "Liquid-Solid transition in fully ionized hydrogen at ultra-high pressure", *J. Chem. Phys.* **134**, 184505 (2011).

[44] M. Holzmann, B. Bernu, **C. Pierleoni**, J. McMinis, D.M. Ceperley, V. Olevano, L. Delle Site, "The momentum distribution of the homogeneous electron gas", *Phys. Rev. Letts.* **107**, 110402 (2011).

[45] E. Liberatore, M. A. Morales, D.M. Ceperley, **C. Pierleoni**, "Free energy methods in Coupled Electron-Ion Monte Carlo", *Mol. Phys.*, **109**, 3029-3036 (2011), **Invited Article**.

2006-2010

[46] M.A.Morales, **C. Pierleoni**, E. Schwegler, D.M. Ceperley, "Evidence for a first-order liquid-liquid transition in high-pressure hydrogen from ab-initio simulations", *PNAS*, **108**, 12799 (2010).

[47] M.A. Morales, **C. Pierleoni** and D. M. Ceperley, "Equation of state of metallic hydrogen from Coupled Electron-Ion Monte Carlo simulations", *Phys. Rev. E* **81**, 021202 (2010).

[48] S. Bonella, M. Monteferrante, **C. Pierleoni**, G. Ciccotti, "Path Integral based calculations of symmetrized time correlation functions I : general formulation", *J. Chem. Phys.* **133**, 164104 (2010).

[49] S. Bonella, M. Monteferrante, **C. Pierleoni**, G. Ciccotti, "Path Integral based calculations of symmetrized time correlation functions II : a numerical algorithm", *J. Chem. Phys.* **133**, 164105 (2010).

[50] G. D'Adamo, **C. Pierleoni**, "Crystalline free energies of micelles of diblock copolymer solutions ", *J. Chem. Phys.* **133**, 204902 (2010).

[51] M.A. Morales, E. Schwegler, D.M. Ceperley, **C. Pierleoni**, S. Hamel and K. Capsersen, "Phase separation in hydrogen-helium mixtures at Mbar pressures", *PNAS* **106**, 1324 (2009).

[52] B. Capone, **C. Pierleoni**, J.P. Hansen and V. Krakoviak, "Entropic self-assembly of diblock copolymers into disordered and ordered micellar phases", *J. Phys. Chem. B* **113**, 3629 (2009).

[53] J.J. Molina, **C. Pierleoni**, B. Capone, J.P. Hansen and I.S. Santos de Oliveira, "Crystal Stability of Diblock Copolymer Micelles in Solution", *Molecular Physics* **107**, 535 (2009), **Invited Article**.

[54] M.L. Mugnai, S. Caprara, G. Ciccotti, **C. Pierleoni** and M. Mareschal, "Transient hydrodynamical behavior by dynamical nonequilibrium molecular dynamics: The formation of convective cells ', *J. Chem. Phys* **131**, 064106 (2009).

[55] F. Sterpone, G. Briganti and **C. Pierleoni**, "Sphere vs Rod: the effect of packing on micellar structure", *Langmuir* **25**, 8960 (2009).

[56] M Mareschal, S. Vantieghem, M.L. Mugnai, S. Caprara, G. Ciccotti, **C. Pierleoni**, "Compressible Convective Instability by Molecular Dynamics", *Progress of Theoretical Physics Supp*, **178**, 15 (2009).

[57] F. Lin, M.A. Morales, K.T. Delaney, **C. Pierleoni**, R.M. Martin, D.M. Ceperley, "Electrical conductivity of high-pressure liquid hydrogen by quantum Monte Carlo methods". *Phys. Rev. Letts.* **103**, 256401 (2009).

[58] **C. Pierleoni**, K.T. Delaney, M.A. Morales, D.M. Ceperley and M. Holzmann, "Trial wave functions for High-Pressure Metallic Hydrogen", *Comp. Phys. Comm.* **179**, 89 (2008).

[59] 1F. Sterpone, G. Briganti, S. Melchionna e **C. Pierleoni**, "Pressure induced core packing and interfacial dehydration in nonionic $C_{12}E_6$ micelle in aqueous solution", *Langmuir*, **24** 6067 (2008).

[60] P.L. Palla, **C. Pierleoni** and G. Ciccotti, "Bulk viscosity of the Lennard-Jones system at triple point by nonequilibrium Molecular Dynamics", *Phys. Rev. E* **78**, 021204 (2008).

[61] **C. Pierleoni**, K.T. Delaney, M.A. Morales, D.M. Ceperley and M. Holzmann, "Progress in Coupled Electron-Ion Monte Carlo Simulations of High-Pressure Hydrogen", In: *Advances in Quantum Many-Body Theories* eds. Astrakharchik G. E., Boronat J., Mazzanti F., World Scientific (Singapore, 2008).

[62] **C. Pierleoni**, B. Capone and J.P. Hansen, "A soft effective segment representation of semi-dilute polymer solutions", *J. Chem. Phys.* **127**, 171102 (2007).

[63] F. Sterpone, G. Marchetti,**C. Pierleoni** and M. Marchi "Molecular modeling and simulation of water near model micelles: Diffusion, rotational dynamics and structure of the hydration interface", *J of Physical Chemistry* B **110**, 11504 (2006).

[64] F. Sterpone, **C. Pierleoni**, G. Briganti and M. Marchi "Structure and Dynamics of hydrogen bonds in the interface of a $C_{12}E_6$ spherical micelle in water solution", *J. of Physical Chemistry* B**110**, 18254 (2006).

[65] **C. Pierleoni**, C. Addison, J.P. Hansen and V. Krakoviack, "Multi-scale coarse-graining of diblock copolymer self-assembly: from monomers to ordered micelles", *Phys. Rev. Letts.* **96**, 128302 (2006).

[66] K. Delaney, **C. Pierleoni** and D.M. Ceperley, "Quantum Monte Carlo Simulation of the High-Pressure Molecular-Atomic Transition in Fluid Hydrogen", *Phys Rev Letts.* **97**, 235702 (2006).

[67] **C. Pierleoni** and D.M. Ceperley, "The coupled electron-ion Monte Carlo method", *Lecture Notes in Physics* **703**, 641-683 (2006).

2001-2005

[68] G. Briganti, G D'Arrigo, M. Maccarini, **C. Pierleoni** and S. Sterpone "Hydration and thermodynamical equilibrium of non ionic surfactants in solutions", *Colloids and Surfaces A* **261**, 93-99 (2005).

[69] M. Holzmann, **C. Pierleoni** and D.M. Ceperley, "Zero-point energy of atomic hydrogen by Coupled Electron-Ion Monte Carlo Method", *Computer Physics Communications* **169**, 421-425 (2005).

[70] **C. Pierleoni** and D.M. Ceperley "Computational Methods in Coupled Electron-Ion Monte Carlo", ChemPhysChem **6**, 1872-1878 (2005).

[71] F. Sterpone, **C. Pierleoni**, G. Briganti and M. Marchi, "Molecular Dynamics study of temperature dehydration of a $C_{12}E_6$ spherical micelle", *Langmuir*, **20**, 4311 (2004, USA).

[72] **C. Pierleoni**, D.M. Ceperley and M. Holzmann "Coupled Electron-Ion Monte Carlo Calculations of Dense Metallic Hydrogen", *Phys. Rev. Letts.* **93**, 146402 (2004), physics/0405056.

[73] M. Holzmann., D.M.Ceperley, **C. Pierleoni** and K. Esler "Backflow correlation in the electron gas and metallic hydrogen" *Phys. Rev. E* **68**, 046707 (2003, USA).

[74] J.T. Titantah, **C. Pierleoni** and J.-P. Ryckaert, "Single chain elasticity and thermoelasticity of polyethylene", *J. Chem. Phys.* **117**, 9028 (2002 USA), cond-mat/0209130.

[75] D.M. Ceperley, M. Dewing and **C. Pierleoni** "The coupled Electronic-Ionic Monte Carlo simulation method", *Lecture Notes in Physics*, **605**, 473-499 (2002).

[76] F. Sterpone, G. Briganti, **C. Pierleoni** "Molecular Dynamics study of Spherical aggregates of chain molecules at different degree of hydrophilicity in aqueous solution", *Langmuir* **17**, 5103 (2001, USA).

[77] J.T. Titantah, **C. Pierleoni** and S. Ciuchi "Free energy of the Fröhlich polaron in two and three dimensions", *Phys. Rev. Lett.* **87** 206406 (2001, USA).

1987-2000

[78] S. Ciuchi, J. Lorenzana and **C. Pierleoni** "Induced charge in a Frohlich polaron: Sum rule and spatial extent", *Phys Rev B* **62**, 4426 (2000, USA).

[79] **C. Pierleoni** and J.-P. Ryckaert "Excluded volume effects on the structure of a linear polymer under shear flow", *J. Chem. Phys.* **113**, 5545 (2000, USA).

[80] J.T. Titantah, **C. Pierleoni** and J.-P. Ryckaert "Different statistical mechanical ensembles for a stretched polymer", *Phys. Rev.* **E**, **60**, 7010 (1999, USA).

[81] G. Ciccotti, **C. Pierleoni**, F. Capuani and V. S. Filinov "Wigner approach to the semiclassical dynamics of a quantum many-body system: the dynamic scattering function of ^4He", *Comp. Phys. Comm.*, **121-122**, 452 (1999, Holland).

[82] J.-P. Ryckaert and **C. Pierleoni**, "Polymer solutions in flow: a non-equilibrium molecular dynamics approach", in *Flexible Polymer Chains in Elongational Flow: Theories and Experiments* eds. T.Q. Nguyen and H.H. Kausch, Springer Verlag (Berlin 1999).

[83] **C. Pierleoni**, G. Arialdi and J.-P. Ryckaert, "On the signature of tensile blobs in the scattering function of a stretched polymer", *Phys. Rev. Lett.*, **79**, 2990 (1997, USA).

[84] W. R. Magro, D. M. Ceperley, **C. Pierleoni** and B. Bernu, "Dissociation in hot, dense hydrogen", *Phys. Rev. Lett.* **76**, 1240 (1996, USA).

[85] **C. Pierleoni**, W.R. Magro, D.M. Ceperley and B. Bernu, "Path Integral Monte Carlo Simulation of Hydrogen Plasma", in *Physics of Strongly Coupled Plasmas* eds. W.D. Kraeft and M. Schlanges, World Scientific, (Singapore 1996).

[86] **C. Pierleoni** and J.-P. Ryckaert, "Deformation and alignment of a flexible polymer under shear flow: a new picture for intermediate reduced shear rates", *Macromulecules* **28**, 5097 (1995, USA).

[87] M. Boninsegni, **C. Pierleoni** and D. M. Ceperley,"Isotopic shift of helium melting pressure: Path Integral Monte Carlo calculation", *Phys. Rev. Lett.*, **72**, 1854 (1994, USA).

[88] **C. Pierleoni**, D.M. Ceperley, B. Bernu and W.R. Magro, "Equation of state of the hydrogen plasma by Path Integral Monte Carlo", *Phys. Rev. Lett.* **73**, 2145 (1994, USA).

[89] **C. Pierleoni** and J.-P. Ryckaert,"Scaling analysis for a chain molecule in shear flow by molecular dynamics simulation", *Phys. Rev. Lett.*, **71**, 1724 (1993, USA).

[90] **C. Pierleoni** and J.-P. Ryckaert, "On the use of the Nosé-Hoover thermostat in the simulation of a single chain molecule in solvent", *Mol. Phys.* **75**, 731 (1992, United Kingdom).

[91] **C. Pierleoni** and J.-P. Ryckaert,"Molecular dynamics investigation of dynamic scaling for dilute polymer solutions in good solvent conditions", *J. Chem. Phys.* **96**, 8539 (1992, USA).

[92] M. N. Hounkonnou, **C. Pierleoni** and J.-P. Ryckaert,"Liquid chlorine in shear and elongational flows: a nonequilibrium molecular dynamics study", *J. Chem. Phys.*, **97**, 9335 (1992, USA).

[93] **C. Pierleoni** and J.-P. Ryckaert, "Non-Newtonian Viscosity of Atomic Fluids in Shear and Shearfree Flows", *Phys. Rev. A* **44**, 5314 (1991, USA).

[94] **C. Pierleoni** and J.-P. Ryckaert, "Relaxation of a single chain molecule in good solvent conditions by Molecular Dynamics simulation", *Phys. Rev. Lett.* **66**, 2992 (1991, USA).

[95] G. Ciccotti, **C. Pierleoni** and J.-P. Ryckaert, "Theoretical Foundation and Rheological Application of Nonequilibrium Molecular Dynamics", in *Microscopic Simulation of Complex Hydrodynamic Phenomena*, eds. M. Marechal and B. L. Holian, Plenum Press (New York USA, 1991).

[96] **C. Pierleoni** and G. Ciccotti, "Thermotransport Coefficients in a Binary Ionic Mixture by Non-Equilibrium Molecular Dynamics", *J. Phys. Condens. Matter* **2**, 1315 (1990, United Kingdom).

[97] **C. Pierleoni**, G. Ciccotti, B. Bernu, "Thermal Conductivity of Classical One-Component Plasma by Non-equilibrium Molecular Dynamics", *Europhysics Letters* **4**, 1115 (1987, Switzerland).

Edited books

[98] Proceedings of the Europhysics Conference on Computational Physics 2004, *Computer Physics Communications* **169**, issues 1-3, M. Ferrario, S. Melchionna and **C. Pierleoni** editors.

Publications in proceedings

[99] W. R. Magro, B. Militzer, D. M. Ceperley, B. Bernu and **C. Pierleoni** "Restricted Path Integral Monte Carlo calculations of hot, dense hydrogen", in *Strongly Coupled Coulomb Systems*, eds. G. J. Kalman, K.B. Blagoev and J.M. Rommel, Plenum Press (New York, 1998).

[100] **C. Pierleoni** and J.-P. Ryckaert,"Deformation and alignment of a chain molecule in solution subjected to a shear flow: a molecular dynamics simulation", *Polymer Preprints* **33**, 533 (1992, USA).

Technical reports

[101] P. Lindner, L. Mayer, **C. Pierleoni** and J.P. Ryckaert, ILL Report experiment 9-11-383 (1996).