



- Quantum Monte Carlo Methods: Coupled Electron-Ion Monte Carlo
- High Pressure Hydrogen
- Path Integral Monte Carlo of continuum polaron models
- Polymer solutions at equilibrium and in flows
- Self-assembling of polymers in solutions: coarse grained and atomistic models

### ***Selected Publications***

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- J.M. McMahon, M.A. Morales, C. Pierleoni, D.M. Ceperley, "The properties of hydrogen and helium under extreme conditions", *Reviews of Modern Physics*, vol. 84, p. 1607-1653 (2012). **Invited article.** <http://dx.doi.org/10.1103/RevModPhys.84.1607>
- 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). [10.1063/1.4732851](http://dx.doi.org/10.1063/1.4732851)
- G. D'Adamo, A. Pelissetto, C. Pierleoni, "Coarse-graining strategies in polymer solutions", *Soft Matter*, 8, 5151 (2012). [doi: 10.1039/c2sm07174f](http://dx.doi.org/10.1039/c2sm07174f)
- 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).
- 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).
- 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).
- C. Pierleoni, B. Capone and J.P. Hansen, "A soft effective segment representation of semi-dilute polymer solutions", *J. Chem. Phys.* 127, 171102 (2007).
- K. Delaney, C. Pierleoni and D.M. Ceperley, "Quantum Monte Carlo Simulation of the High-Pressure Molecular-Atomic Crossover in Fluid Hydrogen", *Phys. Rev. Lett.* 97, 235702 (2006), <http://xxx.lanl.gov/abs/cond-mat/0603750>
- C. Pierleoni and D.M. Ceperley, "The coupled electron-ion Monte Carlo method " proceedings of the Internation School of Solid State Physics 34th course: "Computer Simulations in Condensed Matter: from Materials to Chemical Biology", *Lecture Notes in Physics* (2006), <http://xxx.lanl.gov/abs/physics/0510254>
- 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),

<http://xxx.lanl.gov/abs/cond-mat/0601417>

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    - C. Pierleoni, D.M. Ceperley and M. Holzmann "Coupled Electron-Ion Monte Carlo Calculations of Dense Metallic Hydrogen", Phys. Rev. Letts. 93, 146402 (2004),  
<http://xxx.lanl.gov/abs/physics/0405056>
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    - F. Sterpone, C. Pierleoni, G. Briganti and M. Marchi: "Molecular Dynamics study of temperature dehydration of a C<sub>12</sub>E<sub>6</sub> spherical micelle", Langmuir, 20, 4311 (2004, USA).
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    - 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), <http://xxx.lanl.gov/abs/cond-mat/0010386>
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    - 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).
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    - W. R. Magro, D. M. Ceperley, C. Pierleoni and B. Bernu, "Dissociation in hot, dense hydrogen", Phys. Rev. Lett. 76, 1240 (1996, USA).
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