Curriculum Vitae of Carlo Pierleoni

(May 2022)

General Information

- Name: **Carlo Pierleoni**
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- E-Mail: `Carlo.Pierleoni@aquila.infn.it`
- Academic Position: Full Professor in Condensed Matter Physics at the University of L'Aquila.

Degrees and Academic career

- from April 2020: Full Professor in Condensed Matter Physics at the Faculty of Sciences, University of L'Aquila.
- January 2005: Associate Professor in Condensed Matter Physics at the Faculty of Sciences, University of L'Aquila.
- 21 September 2001: habilitation as Associate Professor in Condensed Matter Physics at the University of Padova
- June 1994-December 2004: researcher in Condensed Matter Physics (B03X) at the Physics Department, University of L'Aquila.
- March 1994 - May 1994 : Post Doc at CECAM, ENS Lyon (France).
- October 1993- February 1994 : INFM Post Doc position at the Physics Department, University of Rome "La Sapienza".
- June 1992 - September 1993 : associate researcher of the *Centre National de la Recherche Scientifique (CNRS)*, at the Laboratoire de Physique Theorique des Liquids, University of Paris VI, Place Jussieu, Parigi, France.
- May 1992 : Ph.D. in Sciences (Physics) with full marks (la plus grande distinction avec felicitations) at the Free University of Brussels (ULB). Title of the dissertation: "Scaling laws in dilute polymer solutions at equilibrium and in flow by Molecular Dynamics Simulation".
- June 1989 - May 1992 : research contract (Allocation Research Contract n.SC1*0059) of the EEC at the Free University of Brussels(ULB), Belgium.
- October 1988 - May 1989 : research fellow at the Fusion Department, ENEA Research Center in Frascati, Rome.
- October 1987 - September 1988 : military service
- February 1987 : "laurea in fisica cum laude" at the University of Roma "La Sapienza".

International awards

- November 2016-October 2020: ANR research grant "Accueil de Chercheurs de Haut Niveau" 2015 edition. PI of the project: "Physics of hydrogen and other light elements under extreme conditions" (HyLightExtreme).
- September 2016: Visiting scientist at the "Laboratoire de Physique et Modélisation des Milieux Condensés", CNRS Grenoble
- December 2009: Visiting Professor at the Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore India
- August-December 2008: Visiting Professor at the Physics Department, University of Illinois at Urbana-Champaig (USA).
- April-May 2007: award of the Royal Society of London at the Department of Theoretical Chemistry, University of Cambridge (UK).
- September-December 2005: Schlumberger Visiting Professor at the Department of Theoretical Chemistry, University of Cambridge (UK).
- October 2001-January 2002: research associate CNRS at CECAM, ENS Lione.

Research experience:

Molecular Modelling and Computational Methods in Condensed Matter

Classical Systems

– simple fluids at equilibrium and out-of-equilibrium
– models of polymeric fluids: scaling laws and rheology
– surfactants in acqueous solutions: self-assembling and structure
– confined water: structure and dynamics
– selfassembling and micro-phase separations in polymeric fluids
– coarse-grained models of polymeric fluids

Quantum systems

– Path Integral formalism and simulation methods for fermions in the ground state and at finite temperature.
– Hydrogen and hydrogen-helium mixtures at extreme conditions
– Strongly coupled electron-phonon systems: single and many-body systems.

Methodological expertise

– Molecular dynamics techniques for simple systems at equilibrium and out-of-equilibrium.
– Molecular dynamics of all-atom models of surfactants in water.
– Monte Carlo methods for simple systems and polymers.
– Free energy methods.
– Path Integral Monte Carlo method for quantum many-body systems including fermions.
– Quantum Monte Carlo methods for ground state many-body systems.
– Coupled Electron-Ion Monte Carlo method.
– Methods for Quantum Dynamics and for dynamical properties (excited states).
– Ab-initio Molecular Dynamics.

Organizational and managerial experiences

- 2018-: member of the Program Committee of the Physics of NonIdeal Plasmas (PNP) conference series.L
- 2014– : delegate of the Rector UNIVAQ in the council of the CECAM-SIMUL Node.
- 2012-2017: member of the Scientific Council of CINECA.
- 2015-2016: member of the Programming Commission of DSFC - UNIVAQ.
- 2015–: member of the Board of Professors of the PhD program of DSFC, UNIVAQ.
- E-CAM State of the Art Workshop "Improving the accuracy of ab-initio prediction for materials", 17-20 September 2018, Paris. organizers: D. Alfé, Michele Casula, D. M. Ceperley, C. Pierleoni.
- CECAM Tutorial on “Continuum Quantum Monte Carlo Methods”, 20-24 September 2011, Losanna. organizers: D. Ceperley, B. Clark, J. Kim, C. Pierleoni, L. Schulenburger
- International Conference on Computational Physics CCP2004, Genova 1-4 September 2004. Chairman G. Ciccotti, scientific organizers: M. Ferrario, S. Melchionna, C. Pierleoni.
- CECAM workshop on “Ab-Initio Simulation Method beyond Density Functional Theory”, 23-25 September 2005. organizers: C. Pierleoni e L. Mitas.

Research grants

- 1994-1997: CNR National Project “Parallel Computing in Condensed Matter", principal investigator (PI) of the research unit at University of L’Aquila.
- 1999-2001: INFM postdoctoral grant on the project “Strongly coupled electron-phonon systems”.
- 2001-2003: PRIN2001 on “Statistical Physics of classical and quantum complex systems", investigator of the research team at University of L’Aquila.
- 2003-2005: PRIN2003 on “Complex systems and many body problem", investigator of the research team at University of L’Aquila.

- 2005-2007: PRIN2005 on “High temperature superconductivity and strongly correlated systems", principal investigator (PI) of the research team at University of L’Aquila.
- 2008-2010: PRIN2009 on “Superconductivity and coherence in non conventional and strongly correlated systems", principal investigator (PI) of the research team at University of L’Aquila.
- 2009-2011: IIT grant SEED “Advanced Computational Methods for Biophysics, Drug Design and Energy Research”, University of Rome “Sapienza”, co-PI.
- 2016-2020: ANR grant “Accueil de Chercheurs de Haut Niveau" 2015 edition. Project: “Physics of hydrogen and other light elements under extreme conditions" (HiLightExtreme), PI.
- 2016-2019: HPC Centre of Excellence (CoE) E-CAM, coordinated by CECAM-Losanna. Member of the team CECAM-SIMUL. One year of Post-Doc.
- 2019-2021: HPC CoE EoCoE2, coordinated by CEA-Saclay. member of the CEA team. Two years of PostDoc.

Competitive Computer Allocation grants

- 2008-2009: INCITE grant at the National Center for Computational Science (NCCS, Oak-Ridge) of 20M core-hours on the project “Simulations of Quantum Systems", co-PI.
- 2009-2010: CASPUR Competitive HPC Grant 2009 of 1M core-hours on the project “Coupled Electron-Ion Monte Carlo Study of High Pressure Hydrogen", PI.
- 2009-2010: DEISA Extreme Computing Initiative (DECI-5) grant of 600K core-hours on the project HiPHyQMC, PI.
- 2010-2011: ISCRA class A grant di 600K core-hours at CINECA on the project HP10A1QFJC, PI.
- 2011-2012: INCITE grant at NCCS (Oak-Ridge), 28M core-hours, “Quantum Monte Carlo simulations of light elements at high pressures", co-PI.
- 2012-2013: PRACE Tier-0 grant n 2011050781, 51M core-hours, “Quantum Monte Carlo simulation of hydrogen at high pressure”, PI.
- 2014-1015: PRACE Tier-0 grant n 2013091918, 30M core-hours, “PHHP - Phases of hydrogen at high pressure”, PI.
- 2016-2017: PRACE Tier-0 grant n 2016143296, 65M core-hours, “PHHP - Phases of hydrogen at high pressure", PI.
- 2016-2017: INCITE Tier-0 grant, 40M core-hours, “Simulation of dense hydrogen and helium", co-PI.
- 2017-2020: DARI Tier-1 grant, 10M core-hours, “Metalization and melting of crystalline hydrogen”, PI.
- 2018-2019: ISCRA B grant of 4M core hours, “Metallization and Melting of Crystalline Hydrogen", PI.
- 2020-2021: ISCRA B grant of 2M core hours, “First principle simulation of high pressure hydrogen", PI.

Evaluation activity

- 2016 - expert evaluator for the The Icelandic Centre for Research - RANNES.
- from 2013, expert evaluator for the Swiss National Science Foundation- SNSF.
- 2012-2017: member of the Scientific Council of CINECA.
- 2011 expert eevaluator for the Academy of Finland and the Research Council for Natural Sciences and Engineering.
- expert evaluator of PRIN2008 projects
- expert evaluator, University of Milan, research projects 2010, 2017.
- expert evaluator, University Sapienza of Rome, 2018.
- expert evaluator of FIRB projects “Futuro in ricerca”, 2009.
- member of the evaluation committee for a research position in Condensed Matter Physics, University of Messina, 2001
- member of the evaluation committee for a RTDA position, Campus Biomedico Rome, 2016.
- member of the evaluation committee for a RTDB position, Campus Biomedico Rome, 2019.
- expert evaluator and member of evaluation committee for the final exam for the PhD program in Electrical Engineering, Sapienza University of Rome, 2011.
- member of the admission committee at the XXX course of the Doctorate School at DSFC, UNIVAQ, 2014.
- expert evaluator of 2 PhD theses, Sorbonne University, Paris 2106.
- expert evaluator and member of the evaluation committee for the final exam for the PhD program in Theoretical and Applied Mechanics, Sapienza University of Rome, 2018.
- member of the evaluation committee for the final exam for the PhD school, XXX course, DSFC, UNIVAQ, 2018.

- expert evaluator of a PhD thesis in Physics, Sapienza University of Rome, 2019.
- board of the referees of the PRACE and DECI, HPC initiatives.
- in the board of the referees of the following International Journals: Physical Review Letters, Physical Review X, Physical Review E, Physical Review B, Nature, Nature Physics, Nature Communications, The Journal of Chemical Physics, The Journal of Physical Chemistry B, Langmuir, Macromolecules, Europhysics Letters, The European Physical Journal B e D, Macromolecular Theory and Simulation, The Journal of Computational Chemistry, Journal of Statistical Mechanics: theory and experiment, Soft Matter, etc.

Research activity

My research activity started with a Non-Equilibrium Molecular Dynamics (NEMD) investigation of thermal transport coefficients for Coulomb systems. Later, during my PhD training, I studied polymer solutions always using Molecular Dynamics. After these experiences with classical fluids I addressed my research towards quantum fluids and in particular electron fluids, by employing and developing Quantum Monte Carlo (QMC) methods. However I have always followed the development in the field of classical fluids and soft matter where recently I have given interesting contributions.
I have authored more than 90 publications on international journals, some rather prestigious. These are my current bibliometric indices (Decembre 2019)

- WoS:
  – number of publications 96
  – H-index 31 (average citations per item 31.64)
  – number of citations: 3037
- SCOPUS:
  – number of publications 96
  – H-index 31 (average citations per item 32.33)
  – number of citations: 3104

My research activity can be presented along two distinct lines: i) classical systems (simple and complex fluids, equilibrium and out of equilibrium properties); ii) quantum many-body systems.

1. Classical fluids and polymers

I have studied Coulomb fluids and polymer solutions at equilibrium and out-of-equilibrium, using standard Molecular Dynamics (MD) and NEMD, and Monte Carlo (MC) methods to sample the configuration space of long linear chains and to compute free energies [97, 96, 95, 94, 93, 92, 91, 90, 89, 86, 83, 82, 80, 79, 65, 62, 60, 56, 54, 53, 52, 50, 41, 40, 39, 37, 36, 35, 34, 30, 29, 27, 24, 21, 19] (the numbers refer to the list of publications enclosed below). Relevant results in chronological order are:

1. MD validation of the Zimm scaling for the dynamical relaxation of a single chain in explicit solvent (with J.P. Ryckaert) [94, 91].

2. non-linear response of dilute polymer solutions under flow of various geometries with NEMD (with J.P. Ryckaert)[89, 86, 82, 79, 95].

3. investigation of the appearance of Pincus blobs in a stretched linear chain with Configurational Biased MC (with J.P. Ryckaert et al.) [83, 80, 74].

4. development of a thermodynamically consistent, multi-scale coarse-graining strategy for solution of homopolymers and copolymers (with J.P. Hansen, A. Pelissetto et al.) [65, 62, 53, 52, 50, 41, 40, 39, 36, 35, 34, 30, 29, 27, 24, 21]

Moreover, in collaboration with an experimental group in Rome and a groups in CEA Saclay, I studied the self-assembling of nonionic surfactants in aqueous solutions by "all-atom" MD simulation [76, 71, 68, 64, 63, 59, 55]. Our specific interest was in studying the microscopic structure of the extended interface in those systems and the confining effects on the structure and dynamics of water molecules, as support to interpret experiments. The most relevant result was a study of the temperature dehydration of the interface of a spherical micelle of $C_{12}E_6$ which helped in interpreting in a coherent manner experimental results from different methods in apparent disagreement [71].

In the last three years I started investigating statistical mechanical models for actin filaments and bundles of filaments at various level of coarse-graining. The aim of this investigation is to enter in this new (to me) field with a clear theoretical framework of the biomechanics of filopodia and actin molecular motors and to try to interpret debated experiments. We have set up a clear statistical mechanical framework for a single growing filament [26], and for a bundle of filaments including the non-equilibrium properties [22, 18, 16, 11]. This work is in collaboration with J.P. Ryckaert (ULB, Belgium)

and G. Ciccotti (Sapienza, Rome).

2. Many-body quantum systems

I have developed the Path Integral Monte Carlo method (PIMC) for the simulation of many-body quantum systems at finite temperature, including fermions, and I have introduced and developed a QMC-based "ab-initio" method for nuclei and electrons [88, 87, 85, 84, 78, 77, 75, 73, 72, 70, 69, 67, 66, 61, 58, 57, 51, 47, 46, 45, 44, 42, 38, 33, 32, 31, 28, 25, 23, 20, 17, 10, 15, 14, 13, 12]. This latter method, known as "Coupled Electron-Ion Monte Carlo" method (CEIMC) is the first "ab-initio" method based on correlated electron techniques which allows to study the thermodynamic behavior of systems of many electrons and ions in the Born-Oppenheimer approximation. The accuracy of CEIMC is superior to that of the standard "ab-initio" methods based on Density Functional Theory (DFT) and can be used to study physical phenomena out of reach of DFT. An example is the metallization in fluid phase. The system to which I have devoted most of my effort is the hydrogen at high pressure which has a reach physics still largely unknown.
The most relevant results obtained in this field, in chronological order, are:

1. the development of PIMC for a mixture of protons and electrons and the first PIMC study of hydrogen phase diagram at high pressure and temperature (with D.M. Ceperley et al.) [88, 87, 85, 84] .

2. the development of PIMC for Fröhlich polarons and the study of the single polaron free energy (with S. Ciuchi et al.) [78, 77].

3. the development of a systematic method to improve trial wave functions in the ground state QMC (with D.M. Ceperley et al) [73, 58].

4. the introduction of an efficient sampling algorithm for Reptation MC, known as "the bounce algorithm" (with D.M. Ceperley) [70].

5. the introduction and development of the CEIMC (with D.M. Ceperley) [75, 72, 69, 67, 66, 61, 58, 47, 45, 44, 42, 38, 32, 31, 28, 25, 23, 20, 17, 10, 12].

6. the first "ab-initio" quantitative study, by free energy methods, of the demixing phenomenon in hydrogen-helium mixtures in thermodynamic conditions interesting to planetary physics [51].

7. the "ab-initio" study (both BOMD and CEIMC) of the metallization and molecular dissociation in liquid hydrogen under pressure [66, 46, 32, 23, 17, 10, 15, 14, 12].

Computing dynamical properties of quantum many body systems is still an open problem with modern computational methods, even for systems of few degrees of freedom. In general computing real time correlation functions requires an amount of computer time which scales exponentially with the number of degrees of freedom. The problem is very different if the system is in the semiclassical regime or near its ground state. In the former case the starting point is a Path Integral formulation and one introduces stationary phase or a linearization approximation in the real time dynamics, in the latter case one needs a methods to compute the first low-lying excited states participating into the dynamics.
My contributions in this area are:

1. the introduction of a Wigner-Liouville formalism in the semiclassical approximation (with G. Ciccotti et al.) [81].

2. the development of a mixed imaginary time Path Integral-linearized real time dynamics method for time correlation functions (with S. Bonella and G. Ciccotti) [48, 49].

3. the application of a Projection QMC method for low energy excited states (many-body) to compute the electrical conductivity of high pressure hydrogen (with D.M. Ceperley et al.) [57].

In the last years I have developed a method to compute electronic band gaps by Grand-Canonical Quantum Monte Carlo. This method solves the infamous gap problem present in the DFT formulation and provide benchmark gap values for less fundamental theories[9]. Moreover it can be easily applied to disordered systems, like quantum crystals and liquid [8]. We are presently extending the approach to compute optical properties with QMC accuracy [10, 57]

Teaching experience

undergraduate level

- Advanced Simulation Techniques, Master Degree, University of L'Aquila since 2020/21.
- Spectroscopy, Master Degree, University of L'Aquila since 2020/21.
- Many-Body theory in Condensed Matter (6CFU), Master Degree, University of L'Aquila since 2020/21.
- Mathematical Methods for Physics II (6CFU), Physics degree, University of L'Aquila, 2015/16.
- Structure of Matter (6CFU), Physics Degree, University of L'Aquila, since 2009/10.

- Physics of Fluids (6CFU), Physics Degree, University of L'Aquila, 2008/09-2019/20.
- Laboratory of Computational Physics (9CFU), Physics Degree, University of L'Aquila, 2005/06-2009/10.
- Computational Methods in Condensed Matter Physics (6CFU), Master Degree in Physics, University of L'Aquila, 2002/03-2012/13.
- Statistical Mechanics (6CFU), Master Degree in Physics, University of L'Aquila, 2000/01.
- Molecular Physics (6CFU), Physics Degree, University of Rome "La Sapienza", 1997/98.
- teaching assistant, Mathematical Methods for Physics, Physics Degree, University of l'Aquila, 1995/96-2006/07.
- teaching assistant, General Physics II (electromagnetism), Computer Science degree, University of L'Aquila, 1994-95.
- teaching assistant, Physics Laboratory, Degree in Biology, University of L'Aquila, 1994-95.

graduate level and advanced courses

- IGRTG 1524 SSNI tutorial on "Methods and physics of high pressure hydrogen and hydrogen-helium mixtures", June 2012, Technische Universitat Berlin.
- Lecturer at the CECAM Tutorial on "Continuum Quantum Monte Carlo", 20-24 Settembre 2011, Losanna.
- Lecturer at the International School on "Multiscale Modeling and Simulations of Hard and Soft Materials", Dec 7 - 16 2009, Bangalore, India.
- Lecturer at the International School of Solid State Physics 34^{th} course "Computer Simulation in Condenses Matter: From Materials to Chemical Biology", organized by G. Ciccotti and K. Binder, 20 July-1 August 2005, Erice, Italy.
- Lecturer at the Joint DEMOCRITOS-ICTP School on "Continuum Quantum Monte Carlo Methods", organized by S. Baroni, D.M. Ceperley, S. Moroni, 13-23 January 2004, ICTP, Trieste , Italy.
- Lecturer at the SIMU Tutorial on "Quantum Monte Carlo: Mostly Path Integral" organized by D.M. Ceperley, 22-26 October 2001, CECAM, Lyon (France).
- Graduate course on "Quantum Monte Carlo Methods for continuum systems", University of L'Aquila, 2000/01-2003/04.
- Graduate course on "Path Integral Monte Carlo Methods", University of Rome "La Sapienza", 2000/01-2011/12.
- Lecturer at the IV School INFM-INCM-CNR of Material Science, organized by P. Rolla and G. Granozzi, 18-29 October 1993 in Mesagne, Brindisi, Italy.

graduate students

1. Vitaly Gorelov, Maison de la Simulation, University of Paris-Saclay, France, in progress, advisor.
2. Alessia Perilli, Physics Department, Sapienza University of Rome, 2018, advisor.
3. Giovanni Rillo, Physics Department, Sapienza University of Rome, 2017, "A Quantum Monte Carlo study of high pressure solid and liquid hydrogen", advisor.
4. Giuseppe D'Adamo, Physics Department, University of L'Aquila, 2012, "Coarse-Graining Strategies in Polymer Solutions", advisor.
5. Elisa Liberatore, Physics Department, University of Rome "La Sapienza", 2011, "Monte Carlo simulations of high pressure hydrogen", advisor.
6. Miguel A. Morales, Physics Department, University of Illinois at Urbana-Champaign (USA), 2008, "First Principles Simulations of Hydrogen and Helium at high pressures.", coadvisor.
7. John T. Titantah, Physics Department, Free University of Brussels (ULB), 1999, coadvisor.

master students

1. 2020-21, Mauro Pulzone, Master in Physics, University of L'Aquila, in progress.
2. 2016-17, Vitaly Gorelov, Erasmus Mundus Master program ATOSIM, ENS-Lyon, title "Determination of the electronic band gap of crystalline molecular hydrogen by Quantum Monte Carlo methods", advisor.
3. 2013-14, Alessia Perilli, Master in Physics, University of L'Aquila, title "Biomechanics of a Bundle of Actin Filaments in Super-critical Conditions", advisor.
4. 2012-13, Giovanni Rillo, Master in Physics, University of Rome Sapienza, title "Dynamic properties of hydrogen under extreme conditions", advisor.
5. 2008-09, Giuseppe D'Adamo, Master in Physics, University of L'Aquila, title "Calcoli di energia libera per cristalli di clusters", advisor.

6. 2007-08, John J. Molina, Master AtoSim in Atomic Scale Modelling of Physical, Chemical and Biomolecular Systems, University of Rome “La Sapienza” and Ecole Normale Superieur, Lyon (France), title “Relative stability of various crystalline phases of spherical micelles in diblock copolymer solutions”, advisor.
7. 2006-07, Mauro Lorenzo Mugnai, Master in Physics Condensed Matter, University of Rome “La Sapienza”, title “Simulazione microscopica di instabilità idrodinamiche: le celle di Benard”, coadvisor.
8. 2006-07, Jamileh Seyed Yazdi, Master AtoSim in Atomic Scale Modelling of Physical, Chemical and Biomolecular Systems, University of Rome “La Sapienza” and Ecole Normale Superieur, Lyon (France), title “Non-equilibrium molecular dynamic simulation: the case of inter-diffusion”, coadvisor.
9. 2006-07, Igor Saulo Santos De Oliveira, Master AtoSim in Atomic Scale Modelling of Physical, Chemical and Biomolecular Systems, University of Rome “La Sapienza” and Ecole Normale Superieur, Lyon (France), title “Effective interactions and crystalline phases of spherical micelles in di-block copolymer solutions”, advisor.
10. 2005-06, Elisa Liberatore, Master in Physics, Condensed Matter, University of L’Aquila, title: “Potenziali effettivi nei liquidi: applicazione all’idrogeno metallico”, advisor.
11. 2004-05, Pier Luca Palla, Laurea in Physics (4 years), University of Rome “La Sapienza”, title: “Calcolo della Bulk viscosity di un fluido Lennard-Jones con la Dinamica Molecolare di Non Equilibrio”, coadvisor.
12. 1997-98, Fabrizio Capuani, Laurea in Physics (4 years), University of Rome “La Sapienza”, title: “La dinamica semiclassica di un sistema a molti corpi quantistico con il metodo di Wigner”, coadvisor.
13. 1997-98, Fabio Sterpone, Laurea in Physics (4 years), University of Rome “La Sapienza”, title “Caratterizzazione mediante dinamica molecolare di surfattanti non ionici a differenti gradi di idrofilicità”, advisor.

laurea (bachelor) students

1. 2020-21, Mattia di Muzio, Laurea in Physics (3 years), University of L’Aquila, title “Integrali di cammino di Feynman in Meccanica Quantistica non relativistica”, advisor.
2. 2020-21, Matteo Venturi, Laurea in Physics (3 years), University of L’Aquila, title “Dai cammini aleatori al moto Browniano”, advisor.
3. 2020-21, Leonardo Masci, Laurea in Physics (3 years), University of L’Aquila, title “L’esperimento di Fermi-Pasta-Ulam”, advisor.
4. 2013-14, Ettore Lauri, Laurea in Physics (3 years), University of L’Aquila, title “Applicazione del Metodo Monte Carlo Variazionale per lo stato fondamentale della molecola di idrogeno”, advisor.
5. 2010-11, Raffaele Del Grande, Laurea in Physics (3 years), University of L’Aquila, title “L’esperimento di Fermi-Pasta-Ulam”, co-advisor.
6. 2008-09, Armando Di Matteo, Laurea in Physics (3 years), University of L’Aquila, title “Il metodo Monte Carlo di Metropolis con energie rumorose”, advisor.
7. 2005-06, Giuseppe D’Adamo, Laurea in Physics (3 years), University of L’Aquila, title “Studio Monte Carlo di un sistema unidimensionale con interazione Lennard-Jones”, advisor.
8. 2004-05, Paolo Giammatteo, Laurea in Physics (3 years), University of L’Aquila, title: “Studi numerici di sistemi non lineari: l’esperimento di Fermi-Pasta-Ulam”, advisor.

post-doc associates

1. Michele Ruggeri, Maison de la Simulation, CEA, Paris-Saclay, 2019-2021, project title “Development of CEIMC for heavier elements”, advisor.
2. Dominik Domin, Maison de la Simulation, CEA, Paris Saclay, 2016-2018, project title “Development of CEIMC for heavier elements”, advisor.
3. Alessia Perilli, Physics Department, Sapienza University of Rome, 2014-15, project title “Stochastic dynamic modelling of actin bundles in an optical trap", advisor.
4. Tomas Hunt, Physics Department, University of Rome, Sapienza, 2014-16, project title “Biomechanics of actin bundles", co-advisor.
5. Santosh Mogurampelly, Physics Department, University of Rome, Sapienza, 2012-13, project title “Biomechanics of actin bundles", co-advisor.
6. Giuseppe D’Adamo, Physics Department, Sapienza University of Rome, 2012-13, project title “Coarse-graining strategy for colloid-polymer solutions", advisor.
7. John T. Titantah, Physics Department, University of L’Aquila, 1999-2001, project title “Strongly coupled electron-phonon systems", advisor.

Invited talks at Conferences

1. *Monte Carlo methods in high pressure research: high pressure hydrogen*, **invited speaker**, 5-th Conference "Statistical Physics: Modern Trends and Applications", July 3–6, 2019, in Lviv, Ukraine.
2. *Band gap closure and dissociation in crystalline molecular hydrogen by Quantum Monte Carlo methods*. July 2018, **invited speaker**, Gordon Research Conference on "Bridging Time-Scale, Temperature, and Pressure Gaps in High-Pressure Compressed-Matter Science", Holderness NH, USA.
3. *Coupled electron-ion Monte-Carlo methods for warm dense hydrogen*. August 2017, **keynote speaker**, Strongly Coupled Coulomb Systems , organized by Michael Bonitz and Patrick Ludwig, Kiel, Germany.
4. *Theory of the liquid-liquid phase transition in high pressure hydrogen*. September 2016, **invited speaker**, The 54th European High Pressure Research Group (EHPRG) International Meeting on High Pressure Science and Technology, organized by Leonid and Natalia Dubrovinsky, Bayreuth, Germany.
5. *First-principle simulations of high pressure hydrogen*, August 2013, **plenary speaker**, XXV IUPAP Conference on Computational Physics, organized by Lev Schur, Moscow, Russia.
6. *Coarse-graining strategies for polymer in solutions*, settembre 2011, **keynote speaker** at the 8^{th} EPS Liquid Matter Conference, organized by Chistof Dellago and Gerald Kahl, Wien, Austria.
7. *Coarse-grained model for diblock copolymers in solutions*, June 2010, **invited speaker**, International Conference "Multiscale Molecular Modelling: Molecular Dynamics, Computational Statistical Mechanics, and Simulation Algorithms", organized by B. Leimkuhler and L. Sarkisov, Edinburgh, UK.
8. *Coarse-graining models of Di-block Copolymer solutions*, December 2009, **invited speaker**, International Conference "Multiscale Modeling and Simulations of Hard and Soft Materials" organized by S. Kumar, S. Sastry and U. V. Waghmare , Bangalore India
9. *The phase diagram of hydrogen at extreme conditions*, 29 July 2008, **keynote speaker** at the International Conference on Strongly Coupled Coulomb Systems, organized by D. Nielsen e G. Senatore, Camerino (Italia).
10. *High-Pressure hydrogen: new predictions by coupled electron-ion Monte-Carlo*, 6 September 2007, **invited speaker**, International Conference in Computational Physics, organized by M. Mareschal, Brussels (Belgium).
11. *Coupled Electron-Ion Monte Carlo of High Pressure Hydrogen*, 18 July 2007, **invited speaker**, 14^{th} International Conference on "Recent Progress in Many Body Theory", organized by J. Boronat, Barcelona (Spain).
12. *Born-Oppenheimer Monte Carlo method and application to Hydrogen*, **invited speaker**, 20 September 2003, Annual Conference of the Italian Physics Society, Physics Dept, Università di Parma (Italy).
13. *Path Integral Monte Carlo study of a two dimensional polaron gas*, **invited speaker**, 13 September 2001, SIMU Conference "Bridging the time scale gap", organized by P. Nielaba, M. Mareschal and G. Ciccotti, University of Konstanz (Germany).
14. *Studio della transizione di plasma nell'idrogeno con il metodo Restricted Path Integral Monte Carlo*, 29 September 1998, **invited speaker**, Annual Conference of The Italian Physics Society (SIF), Physics Dept., University of Salerno (Italy).
15. *Plasma Phase Transition in Hydrogen by Restricted Path Integral Monte Carlo Simulation*, 2 July 1997, **invited speaker**, Adriatico Research Conference on "*Simple system at high pressures and temperatures: theory and experiments*", organized by P. Loubeyre, J. Kohanoff and E. Tosatti, ICTP Trieste (Italy).
16. *Study of the plasma phase transition in hydrogen by Path Integral Monte Carlo* , 11 September 1995, **invited speaker**, International Conference on "The Physics of Strongly Coupled Plasmas, organized by W. D. Kraeft and M. Schlanges, Binz (Germany).
17. *Path Integral Monte Carlo simulation of hydrogen plasma*, 22 September 1994, **invited speaker**, Euroconference on "Numerical Simulations of Quantum Many Body Systems" organized by R. Car, D.M. Ceperley, A. Muramatsu and L. Reatto, Elba International Physics Center, Marciana Marina (Italy).

Invited and contributed talks at workshops

1. *Energy gap closure and metal-insulator transition in solid and fluid hydrogen with pressure*, invited talk, CECAM workshop "Recent developments in quantum Monte Carlo", 21-22 October 2021, Rome Italy.
2. *Energy gap closure of crystalline molecular hydrogen with pressure*, invited on-line talk, SIF2020, Virtual meeting.
3. *Energy gap closure of crystalline molecular hydrogen with pressure*, contributed on-line talk, 58th European High Pressure Research Group International Conference, 6-11 September 2020, Tenerife, Spain.
4. *High Pressure Liquid Hydrogen across molecular dissociation*, contributed talk, SIF2019, September 2019, L'Aquila, Italy.

5. *High Pressure Liquid Hydrogen across molecular dissociation*, contributed talk, Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM, Lausanne, September 2019.
6. *Coupled Electron-Ion prediction for the Liquid-Liquid transition in high pressure hydrogen*, invited talk, 2019 Workshop on Recent Developments in Electronic Structure, NCSA, University of Illinois, May 2019.
7. *Phases of hydrogen: the never ending story*, invited talk,Computer Simulation in Physical & Life Sciences, organized by C. Domene, G. Ciccotti and M.L. Klein, October 26 2018, Temple University at Rome.
8. *Gap closure and dissociation in molecular hydrogen by Quantum Monte Carlo methods*, contributed talk, 16^{th} International Conference on the Physics of NonIdeal Plasmas, organized by J. Clerouin, September 24-28 2018, Saint-Malo, France.
9. *Coupled Electron-Ion Monte Carlo study of hydrogen under extreme conditions*, invited talk, July 2017, workshop on "Understanding Quantum Phenomena with Path Integrals: From Chemical Systems to Quantum Fluids and Solids", organized by M. Ceriotti and D.M. Ceperley, ICTP, Trieste (Italy).
10. *Theory of liquid-liquid phase transition in high pressure hydrogen*, invited talk, November 2016, workshop "Simple and molecular liquids at high pressures" organized by R.Vuilleumier, A.Seitsonen and T. Bryk, ENS Paris France.
11. *Coupled Electron-Ion Monte Carlo study of hydrogen under extreme conditions*, invited talk, June 2016, workshop 'Equations of state in quantum many-body systems", organized by S. Giorgini, M. Holzmann, F. Pederiva and G. Roati, ECT*, Trento Italy.
12. *Coarse-grained model for colloid-polymer solutions*, invited talk, September 2014, CECAM workshop "Scale-Bridging Techniques in Molecular Simulation: A Critical Appraisal", organized by L. Delle Site and C. Hartmann, Frei Universitat Berlin.
13. *Liquid-liquid phase transition in high pressure hydrogen*, invited talk, July 2014, International Workshop "Quantum Monte Carlo in the Apuan Alps IX", organized by M. Towler, The Apuan Alps Centre for Physics, Lucca Italy.
14. *Consistent and transferable coarse-grained model for colloid-polymer solutions*, invited talk, May 2014, workshop "Modeling Complex Systems in Soft Matter", organized by M. Sferrazza, Brussels, Belgium.
15. *Fully consistent and transferrable coarse-graining model for polymer solutions*, invited talk, December 2013, CECAM workshop in honor of Jean-Pierre Hansen, IHP, Paris France.
16. *First principle simulations of Warm Dense Hydrogen and Helium*, invited talk, International Workshop on Warm Dense Matter 2013, Saint Malo, June 2013, France.
17. *Crystalline free energy of a coarse-grained model of diblock copolymer solutions*, invited talk, CECAM workshop "Coarse-Graining Strategies and Methodologies for Polymeric and Biomolecular Assemblies", July 2011, Lyon, France.
18. *The coupled electron-ion: an ab-initio method with Quantum Monte Carlo accuracy*, invited talk, mini-symposium "Many-electron approaches in Material Science", organized by L. Delle Site, May 2011, MPI for Polymer Research, Mainz, Germany.
19. *The coupled electron-ion method and its application to the metal-insulating transition in fluid hydrogen at high pressure*, invited talk, workshop "New Approaches in Many-Electron Theory", organized by L. Delle Site and V. Bach, September 2010, MPI for Polymer Research, Mainz, Germany.
20. *Quantum Monte Carlo simulation of high pressure hydrogen* invited talk, miniworkshop "Quantum Monte Carlo Methods in Physics and Chemistry", organized by C. Filippi, S. Moroni, S. Sorella, C. Umrigar, S. Zhang, January 2008, ICTP (Italy).
21. *Multi-scale coarse-graining of diblock copolymer solutions*, invited talk, 27 September 2007, workshop "Polymers in Nanothecnology", organized by G. Milano, University of Salerno (Italy).
22. *High-Pressure hydrogen: new predictions by coupled electron-ion Monte-Carlo*, invited talk, 28 August 2007, CECAM workshop "Advances in continuum quantum Monte Carlo methods", organized by C. Filippi, W.M.C. Foulkes and R. Needs, Lyon (France).
23. *Coupled Electron-Ion Monte Carlo study of High Pressure Hydrogen*, invited talk, 18 May 2006, CECAM workshop "New developments for first principles molecular dynamics simulations in condensed matter and molecular physics", organized by Marie-Pierre Gaigeot , Rodolphe Vuilleumier, Joost VandeVondele and Ivano Tavernelli, Lyon (France).
24. *Coupled Electron-Ion Monte Carlo study of high pressure hydrogen*, invited talk, 12 January 2006, Workshop "Recent Developments in Computational Electronic Structure", organized by Richard Needs and Ali Alavi, University of Cambridge (UK).
25. *Idrogeno metallico con il metodo Coupled Electron-Ion Monte Carlo*, invited talk, 3 March 2005, Workshop "Sistemi ad alta pressione", organized by L. Ulivi, S. Scandolo, P. Postorino and R. Bini, Polo Scientifico CNR, Sesto Fiorentino (Italia).
26. *Path Integral Monte Carlo study of a two dimensional polaron gas*, 26 October 2001, SIMU Tutorial on "Quantum Monte Carlo Methods", organized by D.M.Ceperley, CECAM, Lyon (Francia).

27. *Polyethylene elasticity and thermoelasticity*, 24 September 2001, CECAM Workshop on "Single molecules studies: from the experiments to their analysis", organized by A. Giansanti and M. Peyrard, CECAM, Lyon (France).
28. *Structure of a stretched and a sheared chain*, 4 October 1999, MPI Workshop on "Linking Different Length and Time Scales in (Macro-)Molecular Systems", organized by H. Pleiner, K. Kremer and B. Dünweg, Max Plank Institute for Complex Systems, Dresden (Germany).
29. *Hydrogen phase diagram and plasma phase transition by Restricted Path Integral Monte Carlo simulation*, 17 June 1998, CECAM Workshop on "Path Integral Simulation: From Physics to Chemistry", organized by D. Marx and D.M. Ceperley, ISI Torino (Italy).
30. *Path integral monte carlo study of the plasma-phase transition in hydrogen*, 19 September 1996, Workshop on "Quantum Monte Carlo simulations of many-body systems: Fermion systems and inhomogeneous systems", organized by L. Reatto and S. Fantoni, Scuola Normale Superiore, Pisa (Italy).
31. *Leggi di scala per una catena lineare in soluzione sotto shear*, 18 September 1996, INFM national school, Villa Gualino, Torino (Italy).
32. *Hydrogen plasma equation of state by Path Integral Monte Carlo*, 10 April 1995, Annual Meeting of Theoretical Physics, Fai della Paganella, Trento (Italy).
33. *Path Integral Monte Carlo simulation of high temperature/high density hydrogen*, 14 October 1994, CECAM Workshop on "Simulation of strongly coupled plasmas" organized by J.J. Kohanoff and J.P. Hansen, Lyon (France).
34. *Path Integral Quantum Monte Carlo simulation of high temperature/high density hydrogen*, 2 April 1993, CECAM Workshop on "Molecular Dynamics simulations of high pressure, high temperature systems", organized by D. Hohl and P. Ballone, Orsay (France).
35. *Single chain in solution subjected to various flows by Non Equilibrium Molecular Dynamics*, 24 July 1992, CECAM Workshop on "New trends in Polymer Simulation", organized by J-P. Ryckaert, A.J.C. Ladd and J.H.R. Clarke, Orsay (France).
36. *Dynamical relaxation of a single chain molecule in good solvent by Molecular Dynamics*, 21 July 1992, CECAM Workshop on "New trends in Polymer Simulation", organized by J-P. Ryckaert, A.J.C. Ladd and J.H.R. Clarke, Orsay (France).
37. *Leggi di scala per catene molecolari in soluzione: uno studio di Dinamica Molecolare*, 2 April 1992, Annual Meeting of Theoretical Physics, Fai della Paganella, Trento (Italy).
38. *Dinamica Molecolare di sistemi complessi: il caso dei polimeri in soluzione*, 23 January 1992, Annual Meeting GNSM/CNR (ex settore "Proprietà Collettive"), Firenze (Italy).
39. *Thermal Conductivity of One-Component Plasma by Nonequilibrium Molecular Dynamics*, 23 August 1986, CECAM Workshop on "Non-equilibrium Molecular Dynamics", organized by G. Ciccotti and W.Hoover, Orsay (France).

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).