Curriculum Vitae di Carlo Pierleoni

Informazioni generali

- Name: **Carlo Pierleoni**
- Address: Dipartimento di Scienze Fisiche e Chimiche, Università dell'Aquila, Via Vetoio 10, 67100 L'Aquila
- [redacted]
- [redacted]
- E-Mail: `Carlo.Pierleoni@aquila.infn.it`

- Posizione accademica: Professore ordinario, SSD FIS/03.

formazione e carriera accademica

- da Aprile 2020: professore di I fascia per il settore scientifico disciplinare FIS03, presso il Dipartimento di Scienze Fisiche e Chimiche dell'Università di L'Aquila.
- da Gennaio 2005: professore di ruolo di II fascia per il settore scientifico disciplinare FIS03, presso la facoltà di Scienze dell'Università di L'Aquila.
- 21 settembre 2001: conseguita l'idoneità a professore universitario di seconda fascia, settore scientifico disciplinare B03X-Struttura della Materia, presso l'Università di Padova
- giugno 1994-Dicembre 2014: ricercatore in Materia Condensata (B03X-FIS03) presso il Dipartimento di Fisica dell'Università di L'Aquila..
- 01 marzo 1994 / 20 maggio 1994 : contratto di ricerca post-dottorale al CECAM, Scuola Normale Superiore in Lione (Francia).
- 01 ottobre 1993 / 28 febbraio 1994 : borsa di studio del Consorzio INFM, sezione G, presso il Dipartimento di Fisica dell'Università La Sapienza in Roma.
- 01 giugno 1992 / 30 settembre 1993 : contratto di Chercheur associé al *Centre National de la Recherche Scientifique (CNRS)*, presso il Laboratorio di Fisica Teorica dei Liquidi, Università di Parigi VI, Place Jussieu, Parigi, Francia.
- 27 maggio 1992 : conseguimento a pieni voti (la plus grande distinction avec felicitations) del titolo di Dottore in Scienze (Fisica) presso l'Università Libera di Bruxelles.Titolo della dissertazione originale : "*Scaling laws in dilute polymer solutions at equilibrium and in flow by Molecular Dynamics Simulation"*.
- 6 dicembre 1990 : vincitore di una borsa di studio per l'estero del Consiglio Nazionale Ricerche (CNR). Non ne ha usufruito per incompatibilità con altri sussidi.
- 01 giugno 1989 / 31 maggio 1992 : contratto di ricerca (Allocation Research Contract n.SC1*0059) della Comunità Economica Europea presso l'Università Libera di Bruxelles (ULB), Belgio.
- 19 ottobre 1988 / 31 maggio 1989 : borsa di studio SIF-ENEA presso il Dipartimento Fusione del Centro Ricerche ENEA di Frascati.
- 15 ottobre 1987 / 14 ottobre 1988 : servizio militare di leva.
- 26 febbraio 1987 : laurea in fisica con lode presso l'Università di Roma "La Sapienza".

Riconoscimenti internazionali

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

Esperienze organizzative e gestionali

- 2014– : rappresentate UNIVAQ delegato del rettore nel consiglio del Nodo CECAM-SIMUL.
- 2012-2017: membro del Consiglio Scientifico del CINECA.
- 2015-2016: membro della Commissione Programmazione del DSFC - UNIVAQ.
- 2015– : membro del Collegio dei Docenti del Corso di Dottorato in Scienze Fisiche e Chimiche, DSFC, UNIVAQ.
- E-CAM State of the Art Workshop "Improving the accuracy of ab-initio predictions 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.

Grant di ricerca

- 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, coordinato dal CECAM-Losanna. Membro del team CECAM-SIMUL. Un anno di finanziamento di una posizione Post-Doc.
- 2019-2021: HPC CoE EoCoE2, coordinato dal CEA-Saclay. Membro del team del CEA. Due anni di finanziamento di una posizione 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.

Attività valutativa

- 2016 - valutatore for the The Icelandic Centre for Research - RANNES.
- from 2013, valutatore for the Swiss National Science Foundation- SNSF.
- 2011 valutatore per l'Academy of Finland and the Research Council for Natural Sciences and Engineering.
- valutatore progetti PRIN2008
- valutatore progetti di ricerca per l'Università di Milano, 2010, 2017.
- valutatore progetti di ricerca per l'Università Sapienza di Roma, 2018.
- progetti FIRB "Futuro in ricerca", 2009.
- commissario di concorso da ricercatore presso l'Università di Messina, 2001.
- commissario di concorso per RTDA pressi il Campus Biomedico di Roma, 2016.
- commissario di concorso per RTDB presso il Campus Biomedico di Roma, 2019.
- valutatore esterno di una tesi di dottorato e membro della commissione di valutazioen per l'esame finale del dottorato in Ingegneria Elettrica, Università Sapienza di Roma, 2011.
- membro della Commissione di valutazione per l'esame finale del Dottorato di Fisica della Materia, XXVI ciclo, Università Sapienza di Roma, 2013.
- membro della commissione di ammissione al XXX ciclo del dottorato in Scienze Fisiche e Chimiche, DSFC, UNIVAQ 2014.
- Valutatore esterno di 2 tesi di dottorato, Università Sorbonne Parigi, 2016.
- Membro della Commissione per l'esame finale del Dottorato di Meccanica Teorica e Applicata, Università Sapienza di Roma, 2018.
- membro della commissione di valutazione per l'esame finale del dottorato XXX ciclo, UNIVAQ, 2018.
- Valutatore esterno di una tesi di dottorato in Fisica, Università Sapienza di Roma, 2019.
- board dei referees di PRACE e DECI, iniziative Europee per HPC.
- nel board dei referees delle seguenti riviste internazionali: Nature Physics, Nature Communications, PNAS, Physical Review Letters, Physical Review E, Physical Review X, Physical Review B, 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.

Esperienza di ricerca:

Modellistica molecolare e metodi di simulazione in Materia Condensata

Sistemi classici

– fluidi semplici all'equilibrio e fuori dall'equilibrio
– modelli di fluidi polimerici: leggi di scala e reologia
– surfattanti in soluzione acquosa: autoaggregazione e struttura
– acqua confinata: struttura e dinamica
– autoaggregazione e microseparazione di fase in fluidi polimerici
– metodi di coarse-graining per fluidi polimerici

Sistemi quantistici

– Sistemi di molti fermioni a temperatura finita: formalismo degli integrali di cammino e metodi di simulazione.
– Fisica dell'idrogeno e delle miscele idrogeno-elio in condizioni estreme.
– Sistemi di elettroni e fononi accoppiati: polarone di Frohlich e sistemi di molti polaroni.

Esperienza metodologica

– Dinamica Molecolare per modelli di fluidi semplici all'equilibrio e lontano dall'equilibrio.
– Dinamica Molecolare per modelli "all-atoms" di surfattanti in acqua.
– Metodi Monte Carlo per fluidi semplici e polimerici.
– Metodi per il calcolo dell'energia libera.
– Path Integral Monte Carlo per sistemi a molti corpi quantistici a temperatura finita, inclusi i fermioni.
– Quantum Monte Carlo per lo stato fondamentale di sistemi a molti corpi quantistici.
– Metodo Coupled Electron-Ion Monte Carlo.
– Metodi per la dinamica quantistica e per le il calcolo delle proprietà dinamiche.
– Dinamica Molecolare Ab-initio.

post-doc associates

1. [redacted], Maison de la Simulation, CEA, Paris-Saclay, 2019-2021, project title "Development of CEIMC for heavier elements", advisor.
2. [redacted], Maison de la Simulation, CEA, Paris Saclay, 2016-2018, project title "Development of CEIMC for heavier elements", advisor.
3. [redacted], Physics Department, Sapienza University of Rome, 2014-15, project title "Stochastic dynamic modelling of actin bundles in an optical trap", advisor.
4. [redacted], Physics Department, University of Rome, Sapienza, 2014-16, project title "Biomechanics of actin bundles", co-advisor.
5. [redacted] Physics Department, University of Rome, Sapienza, 2012-13, project title "Biomechanics of actin bundles", co-advisor.
6. [redacted], Physics Department, Sapienza University of Rome, 2012-13, project title "Coarse-graining strategy for colloid-polymer solutions", advisor.
7. [redacted], Physics Department, University of L'Aquila, 1999-2001, project title "Strongly coupled electron-phonon systems", co-advisor.

Invited talks at Conferences

1. *Monte Carlo methods in high pressure research: high pressure hydrogen*, July 2019, **invited speaker**, 5-th Conference "Statistical Physics: Modern Trends and Applications", to be held on 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. *High Pressure Liquid Hydrogen across molecular dissociation*, contributed talk, SIF2019, September 2019, L'Aquila, Italy.
2. *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.
3. *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.
4. *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.
5. *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.
6. *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).
7. *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.
8. *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.
9. *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.
10. *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.
11. *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.
12. *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.
13. *First principle simulations of Warm Dense Hydrogen and Helium*, invited talk, International Workshop on Warm Dense Matter 2013, Saint Malo, June 2013, France.
14. *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.

15. *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.
16. *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.
17. *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).
18. *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).
19. *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).
20. *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).
21. *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).
22. *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).
23. *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).
24. *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).
25. *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).
26. *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).
27. *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).
28. *Leggi di scala per una catena lineare in soluzione sotto shear*, 18 September 1996, INFM national school, Villa Gualino, Torino (Italy).
29. *Hydrogen plasma equation of state by Path Integral Monte Carlo*, 10 April 1995, Annual Meeting of Theoretical Physics, Fai della Paganella, Trento (Italy).
30. *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).
31. *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).
32. *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).
33. *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).
34. *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).
35. *Dinamica Molecolare di sistemi complessi: il caso dei polimeri in soluzione*, 23 January 1992, Annual Meeting GNSM/CNR (ex settore "Proprietà Collettive"), Firenze (Italy).
36. *Thermal Conductivity of One-Component Plasma by Nonequilibrium Molecular Dynamics*, 23 August 1986, CE-

CAM Workshop on “Non-equilibrium Molecular Dynamics”, organized by G. Ciccotti and W.Hoover, Orsay (France).

Complete list of Publications.

References

2016-present

[1] 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).

[2] 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).

[3] 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).

[4] 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).

[5] 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).

[6] 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.

[7] 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.

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

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

[10] 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

[11] 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).

[12] **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).

[13] **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).

[14] 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.

[15] 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).

[16] 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).

[17] 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).

[18] 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).

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