



Claudio Attaccalite

PhD

Personal

Name **Claudio Attaccalite**
Sex **Male**
Date of birth: **8th July 1977**
Place of birth: **Rome (Italy)**
Affiliation: **CNRS, CINaM
Campus de Luminy
13288 Marseille Cedex 9 (France)**
Phone: **+33-4-91172806**
Fax: **+33-4-91418916**
Email: **claudio.attaccalite@gmail.com**
Web: **www.attaccalite.com**

Education

- 1997–2001 **B. S. Degree in Physics**,
"La Sapienza" University, Rome (Italy),
thesis title: "Correlation energy and spin polarization in the 2D electron gas"
supervisors: G. Bachelet and S. Moroni.
- 2001–2002 **M. S. Degree in Condensed Matter Physics**,
International School for Advanced Studies (SISSA/ISAS), Trieste (Italy),
title: "Properties of Gutzwiller wave-functions for multi-band models"
supervisor: M. Fabrizio.
- 2002–2005 **PhD in Condensed Matter Physics**,
International School for Advanced Studies (SISSA/ISAS), Trieste (Italy),
title: "RVB phase of hydrogen at high pressure: towards the first *ab-initio* Molecular Dynamics by Quantum Monte Carlo"
supervisor: S. Sorella.

Awards and Honors

- 2017 **Habilitation à Diriger des Recherches (arXiv:1609.09639)**, February 2017.
- 2016 **Prime d'installation chercheur**, Ville de Marseille.
- 2013 **Abilitazione scientifica nazionale**, professore di seconda fascia 02/B2.
- 2011 **Prime d'excellence scientifique**, CNRS (France).
- 2010 **Volker Heine Young Investigator Award**, *selected among the five finalists*, PSI-k conference (Germany).
- 2009 **Research Fellow "Juan de la Cierva"**, by Spanish Ministry of Education and Science (Spain).

Experience

Vocational

- 2017-present **Visiting Researcher**, *Tor-Vergata University*, Rome (Italy).
- since 2015 **Researcher CR1**, *CINaM Aix-Marseille Université, CNRS*, Marseille (France).
- 2010-2014 **Researcher CR2**, *Institute Neel, CNRS*, Grenoble (France).
- 2008-2009 **PostDoc**, *Universidad del Pais Vasco*, San Sebastian (Spain).
- 2007 **Visiting Researcher**, *Universidad del Pais Vasco*, San Sebastian (Spain).
- 2006-2007 **PostDoc**, *Institute for Electronics, Microelectronics, and Nanotechnology*, Lille (France).
- 2005-2006 **Visiting Researcher**, *CNR-INFN Democritos and SISSA*, Trieste (Italy).
- 1997-2000 **Web developer**, Rome (Italy).

Research Activities

- **Optical properties and excited states:** part of my research activity is devoted to the study of optical properties and excited states in molecules and bulk materials. In particular I investigated molecules and solids with possible applications in photovoltaic[37,33,31,24,22,21], the role of defects on the optical properties of solids and nanostructures[30,20, patent 1] and the optical response beyond the linear regime[36,34,32,40]. All these studies were performed by means of many-body Green's function theory and Time-Dependent Density Functional Theory.
- **Electronic structure and electron-phonon coupling:** in collaboration with different experimental groups, I investigated the electronic structure and the coupling between electronic and atomic degrees of freedom in different materials[41,27,26,18,13,11,9]. Then I investigated how correlation effects enhance electron-phonon coupling for particular phonon modes and my predictions were later experimentally verified[35,16,15,14].

- **Methodological and numerical developments:** a large part of my research activity consists in the development and the implementation of new methodologies to study complex materials. In recent years I developed a new approach in real-time [39,38,32,32] to study response functions beyond the linear regime, where correlation effects were derived from Green's function theory. Other works include faster methods to solve equations[28] and a new algorithm for ab-initio molecular dynamics[8].
- **Quantum Monte Carlo:** I used Quantum Monte Carlo approach to study different correlated materials, in particular: the phase diagram of the two-dimensional electron gas[1,2], resonance valence bonds in molecules [4,5], liquid hydrogen at high pressure[8] and metal to Mott-insulator cross-over in one dimensional systems[23].

Languages

Italian	Native
English	Fluent
Spanish	Fluent
French	Fluent

Computer skills

- **Programming Languages:** Fortran, C, C++, Python, Bash
- **Web Development:** PHP, HTML, SQL
- **Scientific Programs:** OCTOPUS, QuantumEspresso, Abinit, Yambo, TurboRVB, VMD and XCrySDen, MAPLE.
- **Libraries:** GSL, Blas, Lapack, numPy, sciPy, MPI, OpenMP, MathPlotLib
- **General Softwares:** Linux, LaTeX and LibreOffice.

Teaching Experience

- 2018 **Introduction to Statistical Mechanics**, *Tor Vergata University, Rome (Italy)*.
- 2017 **DFT and Quantum-Espresso (course at the PhD school)**, *Marseille, France*.
- 2013 **Yambo hands-on tutorial on electronic and optical excitations: from basic to advanced applications**, *Lausanne, Switzerland*.
- 2012 **Doctoral training: Second Les Houches school in computational physics: ab initio simulations in condensed matter**, *Les Houches, France*.
- 2010 **Time-Dependent Density-Functional Theory: Prospects and Applications**, *Benasque, Spain*.
- 2008 **Advanced Quantum Monte Carlo Methods**, *ICTP, Trieste (Italy)*.

Bibliometric parameters

H-index: 25
Citations: 2900
Articles: 50

Invited Seminars

1. *"MIFP March Meeting 2018"*, 2018 Rome, (Italy)
Invited Talk "Invisible excitations in hexagonal boron nitride"
2. *"2D layered materials for opto-electronics workshop"*, 2017 Rome, (Italy)
Invited Talk "Invisible excitations in hexagonal boron nitride"
3. *SFB/TRR 142 "Tailored Nonlinear Photonics"*, 2017 Paderborn, (Germany)
Invited Talk "Non-linear response in extended systems: a real-time approach"
4. *Korean-Physical Society*, 2016 Daejeon, (Korea)
Invited Talk "Non-linear response of bulk materials"
5. *Excited States Bridging Scale*, 2016 Marseille, (France)
Invited Talk "Electronic and optical excitations in molecules by means of Green's function theory"
6. *Theory Days*, 2015 Toulouse, (France)
Invited Talk "Nonlinear response of solids within the GW plus Bethe Salpeter approximation: application to second- and third-harmonic generation"
7. *PSI-K Conference*, 2010 Berlin (Germany)
Invited talk "Tunable electron-phonon coupling in doped graphene"
8. *PRACE Second Face to Face Meeting*, 2012 Paris (France)
Invited talk "Yambo: present, past and future"
9. *Total Energy*, 2009 Trieste (Italy)
Invited talk "Electron-phonon coupling in graphene"
10. *International Conference on Materials Discovery and Databases : Informatics and DFT*, 2008 University of Tlemcen (Algeria)
Plenary talk "*Ab-initio* band structure of graphene and graphite"

Other conferences and workshops

1. *ETSF meeting*, 2017 Rome, (Italy)
Talk "Lumen: an ab-initio code for non-linear response in solids"
2. *ETSF meeting*, 2017 Rome, (Italy)
Talk "Green Open Access Journals and SciPost"
3. *Marseille Condensed Matter 2016*, 2016 Marseille, (France)
Poster "Dielectrics in a time-dependent electric field: a density-polarization functional theory approach"
4. *PSI-k conference*, 2015 San-Sebastian, (Spain)
Talk "Nonlinear response of solids within the GW plus Bethe-Salpeter approximation "
5. *Computer Simulations for Condensed Matter Systems*, 2015 Rome, (Italy)

Poster "FIESTA: French Initiative for Electronic Simulations with Thousands of Atoms"

6. *GDR-CORREL Meeting*, 2015 Marseille, (France)
Talk "Nonlinear response of solids within the GW plus Bethe Salpeter approximation: application to second- and third-harmonic generation"
7. *Correlation Meeting*, 2014 Paris, (France)
Talk "GW renormalization of the electron-phonon interaction"
8. *ETSF Meeting*, 2014 Zaragoza, (Spain)
Poster "Real-time approach to nonlinear response in solids: application to second- and third-harmonic generation"
9. *ETSF Meeting*, 2013 Luxemburg (Luxemburg)
Talk "Non-linear optics by means of dynamical Berry phase"
10. *ETSF Meeting*, 2012 Coimbra (Portugal)
Poster "Gate-tunable light-emitting device made of boron nitride nanotubes: from ultraviolet to the visible"
11. *ETSF meeting*, 2011 Turin (Italy)
Poster "Coupling of excitons and defect states in h-BN"
12. *GDR-DFT*, 2011 Obernai (France)
Poster "The time-dependent Bethe-Salpeter equation"
13. *International Winterschool on Electronic Properties of Novel Materials*, 2009 Kirchberg (Austria)
Talk "Electron-phonon coupling in graphene materials"
14. *European Physical Society, Condensed Matter Conference*, 2008 Rome (Italy)
Talk "Electron-electron correlation in graphite and graphene"
15. *Graphene Week 2008*, 2008 Trieste (Italy)
Poster "Electron-electron correlation in graphite and graphene"
16. *The 2007 Quantum Monte Carlo in the Apuan Alps III*, 2007 Vallico Sotto (Italy)
Talk "Ab-initio molecular dynamics for high pressure Hydrogen"
17. *The 2006 Nanoquanta Workshop*, 2006 Houffalize
Poster "Effect of impurities on the optical properties of BN nanotubes"
18. *Paladin Memorial*, 2004 Rome
Poster "Correlated geminal wave function for molecules: an efficient resonating valence bond approach"
19. *Paladin Memorial*, 2001 Rome
Poster "Correlation energy and spin polarization in the 2D electron gas"

Participation in scientific research projects

- 2018-2022 "Towards understanding and modelling intense electronic excitation", COST-Action, coordinator: Antonio Rivera
- 2018-2019 "Opto-electronic properties of 2D Transition Metal Dichalcogenides with DFT and post-DFT simulations", PRACE project, coordinator: M. Palumbo
- 2018-2019 "Optical properties of 2D materials", Graphene FlagShip, coordinator: C. Attaccalite
- 2016-2017 "Optical properties of 2D materials", Graphene FlagShip, coordinator: H. Amara
- 2016 "How we see the world and how the world sees us", EMERGENCE CNRS INP, coordinator: C. Attaccalite
- 2015-2018 "Computational carbon capture", ANR JCJC, coordinator: R. Poloni
- 2011-2014 "Développement de code(s) ab initio pour le photovoltaïque organique", ANR Blanc, coordinator: X. Blase
- 2010-2011 "Development of an ab-initio approach to study inorganic photovoltaic materials", SMINGUE-FMN project of the Rhone-Alpe region (France), coordinator: C. Attaccalite
- 2010 "Ab-initio calculation of out-of-equilibrium quasiparticle self-energies applied to highly excited silicon nanocrystals", collaboration project between Institute Neel, Grenoble (France) and Università di Modena e Reggio Emilia (Italy), supported by HPC-Europe Coordinator: C. Attaccalite
- 2008-2010 Host researcher for the HPC++ Europe Programme (<http://www.hpc-europa.org>)
- 2009 "Quantum Monte Carlo simulation of high temperature superconductor materials" DEISA Extreme Computing Initiative, an EU FP7 Research Infrastructure Project to advance computational sciences in the area of supercomputing in Europe. Coordinators: S. Sorella, M. Casula, C. Attaccalite
- 2009 "Optical Properties of BN Nanotubes and Hexagonal BN", Red Española de Supercomputación, Barcelona Supercomputing Center. Coordinators: C. Attaccalite and A. Rubio
- 2008 "The role of impurities on the optical properties of BN nanostructure", international collaboration with A. Marini, Department of Physics, University of Tor Vergata (Rome), supported by HPC-Europa Transnational Access Programme
- 2008 "Electronic properties of graphite", ETSF project FI-2008-2-003, Universidad del Pais Vasco, San Sebastian (Spain), supported by ETSF Collaboration Programme (<http://etsf.eu>)

Details of student/postdoc supervision

- **Stella Prete**, PhD student (2016-2019)
Two dimensional topological materials

- **Ayoub Riani**, Master 2(M2) student (2017)
Optical properties of molecules on surfaces
- **Dr. Lorenzo Sponza**, Postdoc (2016-2018)
Electron-loss spectroscopy in layered materials
- **Alassane Nguer**, Master 2(M2) student (2013)
Optical properties of two-dimensional crystals
- **Dr. David Kammerlander**, Postdoc (2010-2011)
Development of an ab-initio approach to study inorganique photovoltaic materials
- **Dr. Marco Govoni**, internship student supported by the HPC-Europe programme (2010)
Ab-initio calculation of out-of-equilibrium quasiparticle self-energies applied to highly excited silicon nanocrystals

Conference and Seminar Organisation

- 2018, GDR-Rest general meeting, Porquerolles (France)
- 2015-2017, Weekly Seminar organiser at CINaM, Marseille (France)
- 2016, Marseille Condensed Matter Workshop: optics and magnetism, Marseille (France)
- 2015, Computer Simulations for condensed phase systems, Roma (Italie)
- 2015, NonLinear Optics and Nanoplasmonics Symposia, Psi-k conference, San Sebastian (Spain)
- 2014, Workshop on Gutzwiller Wave Functions and Related Methods, Valence (France)
- 2011-2014, ETSF Workshop on Electronic Excitations (Italy, Portugal, Luxembourg, Spain)

Administrative tasks

- Editor Fellow for SciPost: <https://scipost.org>
- Referee for Phys. Rev. B, Phys. Rev. Lett., Nature Communication, Phys. Status Solidi
- Management board of GDR (Scientific Research Group) REST: <http://gdr-rest.polytechnique.fr/>
- Management board of European COST action CA17126 (European research network funded by EC)
- Member of the GDR (Scientific Research Group) UltraFast Phenomena: <http://gdrupilm.univ-lyon1.fr>
- Rapporteur pour different theèse:
 - Leonardo Espinoza, 2012 San Sebastian (Spain)
 - Gabriel Antonius, 2013, Montreal (Canada)
 - Nathaniel Raimbault, 2016, Toulouse (France)
 - Lucie Prussel, 2017, Ecole polytechnique, Paris (France)

Software Development

- **QEPlayground**(<https://github.com/attacc/QEplayground>): a python wrapper for electron-phonon coupling in solids with QuantumEspresso.

- **TurboRVB**(<http://people.sissa.it/~sorella/web/index.html>): a fortran90 Quantum Monte Carlo code for solids and molecules.
- **Qumax**(<http://sourceforge.net/projects/qumax/>): a C++ Quantum Monte Carlo code for solids and molecules.
- **Lumen**(<http://attacalite.com/lumen>): A many-body code for non-linear spectroscopy derived from Yambo.
- **Yambo**(<http://yambo-code.org>): FORTRAN/C code for Many-Body calculations in solid state and molecular physics.
- **Fiesta**(<http://perso.neel.cnrs.fr/xavier.blase/fiesta/>): a many-body perturbation theory GW and Bethe-Salpeter code using auxiliary Gaussian basis and contour deformation techniques.
- **freeScience.info**, one of the largest free scientific library of the net, with more than 1000 visitors per day

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Clouder Attacalite