# Claudio Attaccalite

*PhD*

## Personal


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|---|---|
| Name | Claudio Attaccalite |
| Sex | Male |
| Date of birth: | 8th July 1977 |
| Place of birth: | Rome (Italy) |
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## 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

2019 **Mercator Fellow of the Research Unit FOR 2824**, Marburg (Germany).

2017 **Habilitation à Diriger des Recherches (arXiv:1609.09639)**, Febraury 2017.

2016 **Prime d'installation chercheur**, Ville de Marseille.

2013 **Abilitazione scientifica nazionale**, professore di seconda fascia 02/B2 (Italy).

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

2021-2024 **Associate Researcher**, *CNR - Montelibretti*, Rome (Italy).

2017-2019 **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-INFM 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, the role of defects on the optical properties of solids and nanostructures and the optical response beyond the linear regime. 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. Then I investigated how correlation effects enhance electron-phonon coupling for particular phonon modes and my predictions were later experimentally verified.
- **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 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 and a new algorithm for ab-initio molecular dynamics.

- **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, resonance valence bonds in molecules, liquid hydrogen at high pressure and metal to Mott-insulator cross-over in one dimensional systems.

## Languages

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|---|---|
| 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

2022 **Ab-initio Many-body methods and simulations with the yambo code**, *ICTP, Trieste (Italy)*.

2021 **Virtual school on electronic excitations in solids and nanostructures using the Yambo code**, *online*.

2020 **Computational School on Electronic Excitations in Novel Materials Using the Yambo Code**, *ICTP, Trieste, (Italy)*.

2018-2019 **Introduction to Statistical Mechanics**, *Tor Vergata University, Rome (Italy)*.

2018 **Theoretical Spectroscopy Lectures**, *Lausanne (Switzerland)*.

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:** 29
**Citations:** 4000
**Number of articles:** 55 (6 PRL, 1 Nanoletters, 2 PRB Rapid-Communication)

## Publications

55. **Tuning the Direct and Indirect Excitonic Transitions of h-BN by Hydrostatic Pressure**
A Segura, R Cuscó, C Attaccalite, T Taniguchi, K Watanabe, L Artús
J. Phys. Chem. C **125**, 23(2021)

54. **Ellipsometry study of hexagonal boron nitride using synchrotron radiation: second gap in the far-UVC**
L. Artús, M. Feneberg, C. Attaccalite, J. H. Edgar, R. Cuscó
Advanced Photonics Research **2** (5), 2000101 (2021)

53. **Strongly Bound Excitons in Metal–Organic Framework MOF-5: A Many-Body Perturbation Theory Study**
AR Kshirsagar, X Blase, C Attaccalite, R Poloni
The Journal of Physical Chemistry Letters **12** (16), 4045-4051(2021)

52. **On-surface chemistry using local high electric fields**
T. Leoni, T. Lelaidier, A. Thomas, A. Ranguis, O. Siri, C. Attaccalite, C. Becker
Nanoscale Advances (2021)

51. **Bethe-Salpeter Study of the Optical Absorption of trans and cis Azobenzene-Functionalized Metal–Organic Frameworks Using Molecular and Periodic Models**
AR Kshirsagar, C Attaccalite, X Blase, J Li, R Poloni
The Journal of Physical Chemistry C **125** (13), 7401-7412 (2021)

50. **TurboRVB: *ab initio* quantum Monte Carlo code implementing Resonating Valence Bond wave function**
K. Nakano, C. Attaccalite et al.
The Journal of Chemical Physics **152** (20), 204121 (2020)

49. **How strong is the Second Harmonic Generation in single-layer monochalcogenides? A response from first-principles real-time simulations**
C. Attaccalite, M. Palummo, E. Cannuccia, M. Gruning
Phys. Rev. Materials **3**, 074003 (2019)

48. **Many-body perturbation theory calculations using the yambo code**
D. Sangalli, A. Ferretti, H. Miranda, C. Attaccalite, I. Marri, E. Cannuccia, et al.
Journal of Physics: Condensed Matter **31** (32), 325902 (2019)

47. **Theory of phonon-assisted luminescence in solids: application to hexagonal boron nitride**
E. Cannuccia, B. Monserrat, C. Attaccalite
Physical Review B **99** (8), 081109R (2019)

46. **Influence of halogen substitution on aggregation-induced near infrared emission of boron-difluoride complexes of 2-hydroxychalcones**

Anthony D'Aleo, Andres Saul, Claudio Attaccalite and Frederic Fages
Materials chemistry frontiers **3** (1), 86-92 (2019)

45. **Direct and indirect excitons in boron nitride polymorphs: a story of atomic configuration and electronic correlation**
L. Sponza, H. Amara, C. Attaccalite, S. Latil, T. Galvani, F. Paleari, L. Wirtz, F. Ducastelle
Physical Review B **98** (12), 125206 (2018)

44. **Two-photon absorption in two-dimensional materials: The case of hexagonal boron nitride**
C. Attaccalite, H. Amara, S. Latil, M. Gruning, F. Ducastelle
Phys. Rev. B **98**, 165126 (2018)

43. **Structural, electronic, and optical properties of the CC complex in bulk silicon from first principles**
D. Timerkaeva, C. Attaccalite, G. Brenet, D. Caliste, P. Pochet
Journal of Applied Physics **123** (16), 161421 (2018)

42. **Exciton interference in hexagonal boron nitride**
L. Sponza, H. Amara, C. Attaccalite, F. Ducastelle, A. Loiseau
Phys. Rev. B **97**, 075121 (2018)

41. **Angular resolved electron energy loss spectroscopy in hexagonal boron nitride**
F. Fossard, L. Sponza, L. Schué, C. Attaccalite, et al.
Phys. Rev. B **96**, 115304 (2017)

40. **Optical properties of extended systems within a current-current response formalism: Tricks and Tips**
D. Sangalli, J. A. Berger, C. Attaccalite, M. Grüning, P. Romaniello
Phys. Rev. B, **95**, 155203 (2017)

39. **Excitonic effects in third harmonic generation: the case of carbon nanotubes and nanoribbons**
C. Attaccalite, E. Cannuccia and M. Grüning
Phys. Rev. B **95** (12), 125403 (2017)

38. **Dielectrics in a time-dependent electric field: a real-time approach based on density-polarization functional theory**
M. Grüning, D. Sangalli, C. Attaccalite
Phys. Rev. B **94**, 035149 (2016)

37. **Performance of polarisation functionals for linear and nonlinear optical properties of bulk zinc chalcogenides ZnX (X= S, Se, and Te)**
M. Grüning and C. Attaccalite
Phys. Chem. Chem. Phys. **18**, 21179 (2016)

36. **Optical properties of Cu-chalcogenide photovoltaic absorbers from self-consistent GW and the Bethe-Salpeter equation**
S. Körbel, D. Kammerlander, R. A. Sarmiento-Pèrez, C. Attaccalite, M. A. L. Marques, and S. Botti
Phys. Rev. B **91**, 075134 (2015)

35. **Second harmonic generation in SiC, ZnO, GaN two-dimensional hexagonal crystals: a Green's function perturbation theory study.**
C. Attaccalite, A. Nguerc, E. Cannuccia, and M. Grüning
Phys. Chem. Chem. Phys. **17**, 9533 (2015)

34. **Accurate approximations to the GW self-energy electron-phonon coupling gradients**
C. Faber, P. Boulanger, C. Attaccalite, I. Duchemin, E. Cannuccia, X. Blase
Phys. Rev. B, **91**, 155109 (2015)

33. **Second Harmonic Generation in h-BN and $MoS_2$ monolayers: the role of electron-hole interactio**
M. Grüning, C. Attaccalite
Phys. Rev. B **89**, 081102(R) (2014)

32. **Excited states properties of organic molecules: from density functional theory to the GW and Bethe-Salpeter Green's function formalism**
C. Faber, P. Boulanger, C. Attaccalite, I. Duchemin and X. Blase
Phil. Trans. R. Soc. A, vol. **372** no. 2011 (2014)

31. **Nonlinear optics from an ab initio approach by means of the dynamical Berry phase: Application to second- and third-harmonic generation in semiconductors**
C. Attaccalite, M. Grüning
Phys. Rev. B, **88**, 235113 (2013)

30. **Many-body Green's function GW and Bethe-Salpeter study of the optical excitations in a paradigmatic model dipeptide**
C. Faber, I. Duchemin, C. Attaccalite, T. Deutsch, X. Blase
J. Chem. Phys. **139**, 194308 (2013)

29. **Efficient Gate-tunable light-emitting device made of defective boron nitride nanotubes: from ultraviolet to the visible**
C. Attaccalite, L. Wirtz, A. Marini, A. Rubio
Nature Scientific Reports **3**, Article number: 2698 (2013)

28. **Speeding up the solution of the Bethe-Salpeter equation by a double-grid method and Wannier interpolation**
David Kammerlander, Silvana Botti, Miguel A. L Marques, Andrea Marini, C. Attaccalite
Phys. Rev. B **86**, 125203 (2012)

27. **Comment on "Electronic Structure of Superconducting KC8 and Nanosuperconducting**

**LiC6 Graphite Intercalation Com-ounds: Evidence for a Graphene-Sheet-Driven Superconducting State from electron-phonon interaction."**
M. Calandra, C. Attaccalite, G. Profeta and F. Mauri
Phys. Rev. Lett. **108**, 149701 (2012)

26. **Electron-phonon coupling and charge-transfer excitations in organic systems from many-body perturbation theory**
C. Faber, I. Duchemin, T. Deutsch, C. Attaccalite, V. Olevano and X. Blase
Journal of Materials Science, Volume **47**, Number 21, Pages 7472-7481 (2012)

25. **A real-time approach to the optical properties of solids and nano-structures: the time-dependent Bethe-Salpeter equation**
Claudio Attaccalite, Myrta Grüning and Andrea Marini
Phys. Rev. B **84**, 245110 (2011)

24. **Charge-transfer excitations in molecular donor-acceptor complexes within the many-body Bethe-Salpeter approach**
Xavier Blase and Claudio Attaccalite
Appl. Phys. Lett. **99**, 171909 (2011) [More than 100 citations]

23. **Strong electronic correlation in hydrogen chains: a Variational Monte Carlo study**
Lorenzo Stella, Claudio Attaccalite, Sandro Sorella and Angel Rubio
Phys. Rev. B **84**, 245117 (2011)

22. **First-principles GW calculations for DNA and RNA nucleobases**
Carina Faber, Claudio Attaccalite, Valerio Olevano, Erich Runge and Xavier Blase
Phys. Rev. B **83**, 115123 (2011) [More than 100 citations]

21. **First-principles GW calculations for fullerenes, porphyrins, phtalocyanine, and other molecules of interest for organic photovoltaic applications**
Xavier Blase, Claudio Attaccalite, Valerio Olevano
Phys. Rev. B **83**, 115103 (2011) [More than 300 citations]

20. **Coupling of excitons and defect states in BN nanostructures**
C. Attaccalite, M. Bockstedte, A. Marini, A. Rubio and L. Wirtz
Phys. Rev. B **83**, 144115 (2011) [More than 100 citations]

19. **Strong charge-transfer excitonic effects and Bose-Einstein exciton-condensate in graphane**
Pierluigi Cudazzo, Claudio Attaccalite, Ilya V. Tokatly, Angel Rubio
Phys. Rev. Lett. **104**, 226804 (2010) [More than 100 citations]

18. **Electronic structure and electron-phonon coupling of doped graphene layers in KC8**
A. Grüneis, C. Attaccalite, et al.
Phys. Rev. B **79**, 205106 (2009) [More than 100 citations]

17. **Fermi velocity renormalization in doped graphene**
C. Attaccalite and A. Rubio
Physica Status Solidi B, **246**(11) 2523 (2009)

16. **Phonon surface mapping of graphite: disentangling quasi-degenerate phonon dispersions**
A. Grüneis, J. Serrano, A. Bosak, M. Lazzeri, S.L. Molodtsov, L. Wirtz, C. Attaccalite, M. Krisch, A. Rubio, F. Mauri, T. Pichler
Phys. Rev. B **80**,085423 (2009) [More than 100 citations]

15. **Doped Graphene as Tunable Electron-Phonon Coupling Material**
C. Attaccalite, M. Lazzeri, L. Wirtz , A. Rubio and F. Mauri
Nano Letters, **10**(2) 1172 (2010)

14. **Impact of the electron-electron correlation on phonon dispersions: failure of LDA and GGA functionals in graphene and graphite**
M. Lazzeri, C. Attaccalite, L. Wirtz and F. Mauri
Phys. Rev. B Rapid Comm. **78**, 081406(R) (2008). [More than 300 citations]

13. **Angle-resolved photoemission study of the graphite intercalation compound KC8: A key to graphene**
A. Grüneis and C. Attaccalite et al.
Phys. Rev. B **80**,075431 (2009)

12. **Comment on "Huge Excitonic Effects in Layered Hexagonal Boron Nitride"**
L. Wirtz, A. Marini, M. Grüning, C. Attaccalite, G. Kresse and A. Rubio
Phys. Rev. Lett. **100**, 189701 (2008)

11. **Tight-binding description of the quasiparticle dispersion of graphite and few-layer graphene**
A. Grünis, C. Attaccalite et al.
Phys. Rev. B **78** 205425 (2008) [More than 200 citations]

10. **The Resonating-Valence-Bond Ground State of Li Nanoclusters**
L. Spanu, D. Nissenbaum, C. Attaccalite, B. Barbiellini and A. Bansil
Phys. Rev. B **79**, 035416 (2009)

9. **Electron-Electron Correlation in Graphite: A Combined Angle-Resolved Photoemission and First-Principles Study**
A. Grünis, C. Attaccalite et al.
Phys. Rev. Lett. **100**, 037601 (2008) [More than 100 citations]

8. **Stable liquid Hydrogen at high pressure by a novel *ab-initio* molecular dynamics**
C. Attaccalite and S. Sorella
Phys. Rev. Lett. **100**, 114501 (2008) [More than 100 citations]

7. **Low energy quasiparticle dispersion of graphite by angle resolved photoemission spectroscopy**

A. Grüneis, T. Pichler, H. Shiozawa, C. Attaccalite, L. Wirtz, and A. Rubio
Physica Status Solidi B, **244**, 4219, (2007)

6. **Absorption of BN nanotubes under the influence of a perpendicular electric field**
   C. Attaccalite, L. Wirtz, A. Marini and A. Rubio
   Physica Status Solidi B, **244**, 4288 (2007)

5. **Resonating Valence Bond wave function: from lattice models to realistic systems**
   Michele Casula, Seiji Yunoki, Claudio Attaccalite, Sandro Sorella
   Computer Physics Communications **169** (1-3): 386-393 (2005)

4. **Correlated geminal wave function for molecules: an efficient resonating valence bond approach**
   M. Casula, C. Attaccalite, S. Sorella
   Journal of Chem. Phys. **121**, 7110 (2004) [More than 200 citations]

3. **Properties of Gutzwiller wave functions for multiband models**
   C. Attaccalite, M. Fabrizio
   Phys. Rev. B **68**, 155117 (2003)

2. **Two-Dimensional electron gas: correlation energy versus density and spin polarization.**
   C. Attaccalite, P. Gori Giorgi, S. Moroni, G. B. Bachelet
   Phys. Rev. Lett. **88**, 256601 (2002) [More than 500 citations]

1. **Energy and spin polarization in the 2D electron gas**
   P. Gori Giorgi, C. Attaccalite, S. Moroni, G. B. Bachelet
   Intern. Journ. of Quantum Chemistry **91**,126 (2002)

## Conference proceeding and other publications

1. ***Ab-initio* band structure of doped graphene**
   C. Attaccalite, A. Grüneis, T. Pichler and A. Rubio
   http://arxiv.org/abs/0808.0786

2. **Trends in condensed matter physics: is research going faster and faster?**
   C. Attaccalite and S. Barland
   Journal of Unsolved Questions, **3**, 1, Articles 1-4, (2013)

3. **Doped Graphene as Tunable Electron-Phonon Coupling Material(errata)**
   C. Attaccalite, L. Wirtz, M. Lazzeri, F. Mauri, A. Rubio,
   Nano Letters **11**, 914-914 (2011)

4. **Preparation and electronic properties of potassium doped graphite single crystals**
   A. Grüneis , C. Attaccalite, et al.
   Physica Status Solidi B **245**, 2072 (2008)

5. **Tight-binding description of the quasiparticle dispersion of graphite and few-layer graphene**

A. Grüneis, C. Attaccalite, L. Wirtz, H. Shiozawa, R. Saito, T. Pichler, and A. Rubio
Virtual Journal of Nanoscale Science & Technology Vol. **18**, Issue 22 (2008)

6. **Correlation energy and spin polarization in the 2D electron gas (errata)**
   C. Attaccalite, P. Gori Giorgi, S. Moroni, G. B. Bachelet
   Phys. Rev. Lett. **91**, 109902 (2003)

## Patents

1. **Light emitting source and method for emitting light based on boron nitride nanotubes**
   A. Rubio, C. Attaccalite, L. Wirtz
   WO/2012/113955

## Invited Seminars

1. *"TUMIEE meeting"*, 2021 Marseille, (France)
   **Invited Talk** "to be annonced"

2. *"Recent developments in QMC"*, 2021 Rome, (Italie)
   **Invited Talk** "to be annonced"

3. *"Berkeley Excited States Conference"*, 2021 Berkeley, (USA) [online]
   **Invited Talk** "Exciton-phonon coupling and luminescence in hexagonal boron nitride"

4. *"Amorphous Molecular Materials with Extreme Non-Linear Optical Properties"*, 2019 Marburg, (Germany)
   **Invited Talk** "Non-linear response in extended systems: a real-time approach"

5. *"MIFP March Meeting 2019"*, 2019 Rome, (Italy)
   **Invited Talk** "Non-linear response of two dimensional crystals and layered materials"

6. *"CECAM workshop: Green's function methods"*, 2019 Lausanne, (Switzerland)
   **Invited Talk** "Theory of phonon-assisted luminescence: the case of hexagonal-BN"

7. *"MIFP March Meeting 2018"*, 2018 Rome, (Italy)
   **Invited Talk** "Invisible excitations in hexagonal boron nitride"

8. *"2D layered materials for opto-electronics workshop"*, 2017 Rome, (Italy)
   **Invited Talk** "Invisible excitations in hexagonal boron nitride"

9. *SFB/TRR 142 "Tailored Nonlinear Photonics"*, 2017 Paderborn, (Germany)
   **Invited Talk** "Non-linear response in extended systems: a real-time approach"

10. *Korean-Physical Society*, 2016 Daejeon, (Korea)
    **Invited Talk** "Non-linear response of bulk materials"

11. *Excited States Bridging Scale*, 2016 Marseille, (France)
    **Invited Talk** "Electronic and optical excitations in molecules by means of Green's function theory"

12. *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"

13. *PSI-K Conference*, 2010 Berlin (Germany)
    **Invited talk** "Tunable electron-phonon coupling in doped graphene"

14. *PRACE Second Face to Face Meeting*, 2012 Paris (France)
    **Invited talk** "Yambo: present, past and future"

15. *Total Energy*, 2009 Trieste (Italy)
    **Invited talk** "Electron-phonon coupling in graphene"

16. *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. *"GDR-HOWDI kick-off meeting"*, 2021, (France) [online]
   **Talk** "Recent theoretical developments for 2D heterostructures"

2. *"Yambo Fridays in December"*, 2020 Milan, (Italy) [online]
   **Talk** "Implementation of exciton-phonon coupling"

3. *Lavoisier Discussions - GRAPHENE*, 2018 Montpellier, (France)
   **Talk** "Non-linear response of low dimensional crystals"

4. *GDR-REST general meeting*, 2018 Porquerolles, (France)
   **Talk** "Invisible excitations in hexagonal boron nitride"

5. *GDR-REST general meeting*, 2018 Porquerolles, (France)
   **Poster** "Chemical reactions by STM: a new way to synthetize tetra-aza-pentacene(TAP)"

6. *ETSF meeting*, 2017 Rome, (Italy)
   **Talk** "Lumen: an ab-initio code for non-linear response in solids"

7. *ETSF meeting*, 2017 Rome, (Italy)
   **Talk** "Green Open Access Journals and SciPost"

8. *Marseille Condensed Matter 2016*, 2016 Marseille, (France)
   **Poster** "Dielectrics in a time-dependent electric field: a density-polarization functional theory approach"

9. *PSI-k conference*, 2015 San-Sebastian, (Spain)
   **Talk** "Nonlinear response of solids within the GW plus Bethe-Salpeter approximation "

10. *Computer Simulations for Condensed Matter Systems*, 2015 Rome, (Italy)
    **Poster** "FIESTA: French Initiative for Electronic Simulations with Thousands of Atoms"

11. *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"

12. *Correlation Meeting*, 2014 Paris, (France)
    **Talk** "GW renormalization of the electron-phonon interaction"

13. *ETSF Meeting*, 2014 Zaragoza, (Spain)
    **Poster** "Real-time approach to nonlinear response in solids: application to second- and third-harmonic generation"

14. *ETSF Meeting*, 2013 Luxemburg (Luxemburg)
    **Talk** "Non-linear optics by means of dynamical Berry phase"

15. *ETSF Meeting*, 2012 Coimbra (Portugal)
    **Poster** "Gate-tunable light-emitting device made of boron nitride nanotubes: from ultraviolet to the visible"

16. *ETSF meeting*, 2011 Turin (Italy)
    **Poster** "Coupling of excitons and defect states in h-BN"

17. *GDR-DFT*, 2011 Obernai (France)
    **Poster** "The time-dependent Bethe-Salpeter equation"

18. *International Winterschool on Electronic Properties of Novel Materials*, 2009 Kirchberg (Austria)
    **Talk** "Electron-phonon coupling in graphene materials"

19. *European Physical Society, Condensed Matter Conference*, 2008 Rome (Italy)
    **Talk** "Electron-electron correlation in graphite and graphene"

20. *Graphene Week 2008*, 2008 Trieste (Italy)
    **Poster** "Electron-electron correlation in graphite and graphene"

21. *The 2007 Quantum Monte Carlo in the Apuan Alps III*, 2007 Vallico Sotto (Italy)
    **Talk** "*Ab-initio* molecular dynamics for high pressure Hydrogen"

22. *The 2006 Nanoquanta Workshop*, 2006 Houffalize
    **Poster** "Effect of impurities on the optical properties of BN nanotubes"

23. *Paladin Memorial*, 2004 Rome
    **Poster** "Correlated geminal wave function for molecules: an efficient resonating valence bond approach"

24. *Paladin Memorial*, 2001 Rome
    **Poster** "Correlation energy and spin polarization in the 2D electron gas"

## Popular science activity

- *"CINaM: journée du labo"*, 2021 Cassis, (France)
  **Talk** "La science ouverte: boîte à outils"

- *"10th Young Research Meeting"*, 2019 Rome, (Italy)
  **Invited Talk** "The story of Academic Publishing: from Galileo to Nature"

## Participation in scientific research projects

- 2020-2023 "Exciton-phononn coupling in layered materials", PhD scholarship funded by Aix-Marseille Universite, coordinator: C. Attaccalite

- 2018-2022 "Towards understading 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. Palummo

- 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 approch to study inorganique 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 Universita' di Modena e Reggio Emilia (Italy), supported by HPC-Europe Coordinator: C. Attaccalite
- 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

- **Ilan Boulet**, Directeur: C. Attaccalite, Co-directeur: R. Parret, PhD student (2020-2023)
  *Propriétés physiques de dispositifs optoélectroniques hybrides molécules/matériaux 2D*
- **Pierre Lechifflard**, Phd student (2020-2023)
  *Exciton-phonon coupling in low dimensional systems*
- **Wei Yadong**, intership student (2020), supported by Harbin Institute of Technology
  *Non-linear response of low-dimensional systems (cancelled due to COVID19)*
- **Pierre Lechifflard**, Master 2(M2) student (2020)
  *Electron-phonon coupling in low dimensional systems*

- **Stella Prete**, PhD student (2016-2019), *Two dimensional topological materials*
- **Dr. Lorenzo Sponza**, Postdoc (2016-2018), *Electron-loss spectroscopy in layered materials* (now CNRS researcher at ONERA-Paris)
- **Ayoub Riani**, Master 2(M2) student (2017), *Optical properties of molecules on surfaces*
- **Alassane Nguer**, Master 2(M2) student (2013), *Optical properties of two-dimensional crystals*
- **Dr. David Kammerlander**, Postdoc (2010-2011), *Development of an ab-initio approch to study inorganique photovoltaic*
  (now Technology Development Engineer at Infineon Technologies)
- **Dr. Marco Govoni**, internship student supported by the HPC-Europe programme (2010)
  *Out-of-equilibrium quasiparticle in highly excited silicon nanocrystals*
  (now Assistant Scientist at Argonne National Laboratory)
- **Dr. Lorenzo Stella**, internship student supported by the HPC-Europe programme (2009)
  *Strong correlation in the hydrogen chain: a Quantum Monte Carlo study*
  (now Assistant Professor at Queen's University Belfast, UK)

## Conference and Workshop Organisation

- 2022, School, "Ab-initio Many-body methods and simulations with the yambo code", ICTP, Trieste (Italy)
- 2021, Symposium "New developments in Quantum Monte Carlo" at Psi-k 2021 conference
- 2021, Symposium "Extreme non-linear optics" at the Psi-k 2021 conference
- 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)
- 2013, Yambo hands-on tutorial on electronic and optical excitations, Lausanne (Switzerland)
- 2011-2014, ETSF Workshop on Electronic Excitations (Italy, Portugal, Luxembourg, Spain)

## Administrative tasks

- Member of the Scientific Commitee of the GDR-HOWDI (2021-present)
- Correspondant science ouverte du CINaM
- Editor Fellow for SciPost: https://scipost.org (2018-present)
- Referee for Phys. Rev. B, Phys. Rev. Lett., Nature Communication, Nanoletters
- Member of the management board of GDR-IRN HOWDI (2021-presnet)
- Member of the management board of GDR (Scientific Research Group) REST: http://gdr-rest.polytechnique.fr/ (2016-present)

- Member of the management board of the European Theoretical Spectroscopy Facility(http://etsf.eu/) (2016-2020)

- Member of the management board of European COST action CA17126 (European research network funded by EC)

- Rapporteur pour different thèse:
  Davide Grassano, 2019, Universitá Tor Vergata, Rome (Italy)
  Davide Grassano, 2019, Universitá Tor Vergata, Rome (Italy)
  Anna Tararan, 2018, Université Paris Saclay, Paris (France)
  Lucie Prussel, 2017, Ecole polytechnique, Paris (France)
  Nathaniel Raimbault, 2016, Toulouse (France)
  Gabriel Antonius, 2013, Montreal (Canada)
  Leonardo Espinoza, 2012 San Sebastian (Spain)

- Host researcher for the HPC++ Europe Programme (http://www.hpc-europa.org) (2008-2010)

## Software Development

- **Yambo**(http://yambo-code.org): FORTRAN/C code for Many-Body calculations in solid state and molecular physics.
- **TurboRVB**(http://people.sissa.it/ sorella/web/index.html): a fortran90 Quantum Monte Carlo code for solids and molecules.
- **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.
- **QEPlayground**(https://github.com/attacc/QEplayground): a python wrapper for electron-phonon coupling in solids with QuantumEspresso.
- **Qumax**(http://sourceforge.net/projects/qumax/): a C++ Quantum Monte Carlo code for solids and molecules.
- **Lumen**(http://attaccalite.com/lumen): A many-body code for non-linear spectroscopy derived from Yambo.
- **freeScience.info**, one of the largest free scientific library of the net, with more than 1000 visitors per day

Date: September 28, 2021