



# Claudio Attaccalite

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*PhD*

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## Personal

Name **Claudio Attaccalite**  
Sex **Male**  
Date of birth: **8th July 1977**  
Place of birth: **Rome (Italy)**  
Affiliation: **CNRS, CINaM  
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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.

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## Awards and Honors

- 2016 **Prime d'installation chercheur**, Ville de Marseille.
- 2016 **Habilitation à Diriger des Recherches**, submitted June 2016.
- 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).

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## Experience

### Vocational

- 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).

### Miscellaneous

- 1997-2000 **Web developer**, Rome (Italy).

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## 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	<b>Native</b>
English	<b>Fluent</b>
Spanish	<b>Fluent</b>
French	<b>Fluent</b>

## 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

- 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:**19

**Contemporary H-index:** 16 (period 2015-2005 data from ISI web of science)

**Citations:** 1600

**Articles:** 39

## Publications

42. **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  
article in preparation (2016)
41. **On surface synthesis of tetraazapentacene assisted by inelastic electron tunneling**  
T. Leoni, T. Lelaidier, A. Thomas, A. Ranguis, O. Siri, C. Attaccalite, C. Becker  
article in preparation (2016)
40. **Excitonic effects in third harmonic generation: the case of carbon nanotubes and nanoribbons**  
C. Attaccalite, E. Cannuccia and M. Grüning  
article in preparation (2016)
39. **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)
38. **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)
37. **Optical properties of Cu-chalcogenide photovoltaic absorbers from self-consistent GW and the Bethe-Salpeter equation**  
S. Körbel, D. Kammerlander, R. A. Sarmiento-Pérez, C. Attaccalite, M. A. L. Marques, and S. Botti  
Phys. Rev. B **91**, 075134 (2015)
36. **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)
35. **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)
34. **Second Harmonic Generation in h-BN and MoS<sub>2</sub> monolayers: the role of electron-hole interaction**  
M. Grüning, C. Attaccalite  
Phys. Rev. B **89**, 081102(R) (2014)

33. **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)
32. **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)
31. **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)
30. **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)
29. **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)
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 Compounds: 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)

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)
21. **First-principles GW calculations for fullerenes, porphyrins, phthalocyanine, and other molecules of interest for organic photovoltaic applications**  
Xavier Blase, Claudio Attaccalite, Valerio Olevano  
Phys. Rev. B **83**, 115103 (2011)
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)
19. **Strong charge-transfer excitonic effects and Bose-Einstein exciton-condensate in graphene**  
Pierluigi Cudazzo, Claudio Attaccalite, Ilya V. Tokatly, Angel Rubio  
Phys. Rev. Lett. **104**, 226804 (2010)
18. **Electronic structure and electron-phonon coupling of doped graphene layers in KC8**  
A. Grüneis, C. Attaccalite, A. Rubio, D. V. Vyalikh, S. L. Molodtsov, J. Fink, R. Follath, W. Eberhardt, B. Brückner, and T. Pichler  
Phys. Rev. B **79**, 205106 (2009)
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)
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. Attacalite, L. Wirtz and F. Mauri  
Phys. Rev. B Rapid Comm. **78**, 081406(R) (2008).

13. **Angle-resolved photoemission study of the graphite intercalation compound KC8: A key to graphene**  
A. Grüneis and C. Attacalite 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. Attacalite, 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. Attacalite et al.  
Phys. Rev. B **78** 205425 (2008)
10. **The Resonating-Valence-Bond Ground State of Li Nanoclusters**  
L. Spanu, D. Nissenbaum, C. Attacalite, 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. Attacalite et al.  
Phys. Rev. Lett. **100**, 037601 (2008)
8. **Stable liquid Hydrogen at high pressure by a novel *ab-initio* molecular dynamics**  
C. Attacalite and S. Sorella  
Phys. Rev. Lett. **100**, 114501 (2008)
7. **Low energy quasiparticle dispersion of graphite by angle resolved photoemission spectroscopy**  
A. Grüneis, T. Pichler, H. Shiozawa, C. Attacalite, 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. Attacalite, 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 Attacalite, 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. Attacalite, S. Sorella  
Journal of Chem. Phys. **121**, 7110 (2004)

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### 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)

### 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. **Preparation and electronic properties of potassium doped graphite single crystals**

A. Grüneis , C. Attaccalite , A. Rubio ,S.L. Molodtsov ,D.V. Vyalikh , J. Fink, R. Follath, T. Pichler  
Physica Status Solidi B **245**, 2072 (2008)

#### 3. **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)

### Patents

#### 1. **Light emitting source and method for emitting light based on boron nitride nanotubes**

A. Rubio, C. Attaccalite, L. Wirtz  
WO/2012/113955

### Conferences and Workshops

#### 1. *Marseille Condensed Matter 2016*, 2016 Marseille, (France)

**Poster** "Dielectrics in a time-dependent electric field: a density-polarization functional theory approach"

#### 2. *Excited States Bridging Scale*, 2016 Marseille, (France)

**Invited Talk** "Electronic and optical excitations in molecules by means of Green's function theory"

#### 3. *Korean-Physical Society*, 2016 Daejeon, (Korea)

**Invited Talk** "Non-linear response of bulk materials"

#### 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)

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

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. *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"
8. *Correlation Meeting*, 2014 Paris, (France)  
**Talk** "GW renormalization of the electron-phonon interaction"
9. *ETSF Meeting*, 2014 Zaragoza, (Spain)  
**Poster** "Real-time approach to nonlinear response in solids: application to second- and third-harmonic generation"
10. *ETSF Meeting*, 2013 Luxemburg (Luxemburg)  
**Talk** "Non-linear optics by means of dynamical Berry phase"
11. *PRACE Second Face to Face Meeting*, 2012 Paris (France)  
**Invited talk** "Yambo: present, past and future"
12. *ETSF Meeting*, 2012 Coimbra (Portugal)  
**Poster** "Gate-tunable light-emitting device made of boron nitride nanotubes: from ultraviolet to the visible"
13. *ETSF meeting*, 2011 Turin (Italy)  
**Poster** "Coupling of excitons and defect states in boron nitride nanostructures"
14. *GDR-DFT*, 2011 Obernai (France)  
**Poster** "The time-dependent Bethe-Salpeter equation"
15. *PSI-K Conference*, 2010 Berlin (Germany)  
**Invited talk** "Tunable electron-phonon coupling in doped graphene"
16. *International Winterschool on Electronic Properties of Novel Materials*, 2009 Kirchberg (Austria)  
**Talk** "Electron-phonon coupling in graphene materials"
17. *Total Energy*, 2009 Trieste (Italy)  
**Invited talk** "Electron-phonon coupling in graphene"
18. *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"
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"

## Participation in scientific research projects

- 2016 "Optical properties of 2D materials", Graphene FlagShip, coordinator: F. Ducastelle
- 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 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
- 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

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- 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

- **Dr. Lorenzo Sponza**, Postdoc (2016-2017)  
*Optical properties of 2D materials*
- **Alassane Nguer**, Master 2(M2) student (2013)  
*Optical properties of two-dimensional crystals*
- **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*
- **Dr. David Kammerlander**, Postdoc (2010-2011)  
*Development of an ab-initio approach to study inorganique photovoltaic materials*
- **Carina Faber**, Phd student, co-supervised with X. Blase (2011-2014)  
*Développement de code(s) ab initio pour le photovoltaïque organique*

## Conference and Seminar Organisation

- 2015-present, 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)

## Software Development

- **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.
- **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

## Miscellaneous

- Referee for Phys. Rev. B, Phys. Rev. Lett., Nature Communication, Phys. Status Solidi
- Member of the GDR (Scientific Research Group) REST: <http://gdr-rest.polytechnique.fr/>
- Member of the GDR (Scientific Research Group) UltraFast Phenomena: <http://gdrupilm.univ->

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