

Curriculum Vitae

Personal information

Surname/ First name **Marini Andrea**
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Nationality Italian
Date of birth 09/09/72
Gender Male

Scientific production

h-index 17
48 papers (11 on Phys. Rev. Lett., 2 NanoLetters, 1 review, 2 book chapters)
19 invited talks, 8 invited seminars

Professional experiences

Dates March 2010 - February 2011
Occupation Ikerbasque Fellow
Organization University of the Basque Country, San Sebastian, Spain
Dates 2007 onwards
Occupation Researcher team leader
Organization European Theoretical Spectroscopy Facility (ETSF, www.etsf.eu) core node of Rome "Tor Vergata"
Dates January 2010 onwards
Occupation Researcher
Organization Physics Department, University of Rome "Tor Vergata"
Dates October-December 2009
Occupation HPC researcher
Organization Prof. Angel Rubio, European Theoretical Spectroscopy Facility, University of the Basque Country, San Sebastian, Spain
Dates October 2006-December 2009
Occupation Researcher
Organization CNISM (Consorzio Interuniversitario per la Scienza della Materia), Physics Department, University of Rome "Tor Vergata"
Dates October 2000 onwards
Occupation Coordinator and developer of the *Ab-Initio* code YAMBO (www.yambo-code.org)

[code.org](http://www.yambo-code.org))

Dates 2004 - 2006
Occupation Researcher
Organization CNR (Consiglio Nazionale delle Ricerche), Physics Department, University of Rome "Tor Vergata"

Dates 2002 - 2004
Occupation Post-Doc
Organization Prof. Angel Rubio, *NanoQuanta* Network of Excellence, University of the Basque Country, San Sebastian, Spain

Dates 1999 - 2001
Occupation PhD fellow
Organization Physics Department, University of Rome "Tor Vergata"

Supervised Students

Dates 2009-2010
Student **Davide Sangalli** (PhD): Carbon nanotubes in strong magnetic fields: Aharonov-Bohm effect and Landau oscillations

Dates 2009-2010
Student **Elena Cannuccia** (PhD): Giant polaronic effects in conjugated polymers: breakdown of the band theory

Dates 2008
Student **Julio Fernandez** (Post-Doc): Total energy and Van der Waals forces in graphite from *Ab Initio* Many-Body perturbation theory

Dates 2008
Student **Claudio Attaccalite** (Post-Doc): Collaboration project supported by HPC-Europa Transnational Access Programme (2008). Title: *The role of impurities on the optical properties of BN nanostructure*

Dates 2006-2008
Student **Fabrizio De Fausti** (PhD): Excitons and quasiparticles in collinear and non collinear spin configurations

Participation in Scientific Projects

Dates 2010-2011
Title Electronic dynamics in ultra-intense laser fields (ELISE)
Project Fellowship with the Ikerbasque Science foundation, Spain.
Principal Investigator Andrea Marini

Dates 2008 onwards
Project Host researcher for the HPC++ Europe Programme (www.hpc-europa.org)

Dates 2008
Title *The role of impurities on the optical properties of BN nanostructure*
Project International collaboration with C. Attaccalite, Universidad del Pais Vasco, San Sebastian (Spain), supported by HPC-Europa Transnational Access Programme (2008)
Principal Investigator Claudio Attaccalite

Dates 2008-2010
 Project European Theoretical Spectroscopy Facility (ETSF). A knowledge centre for theoretical spectroscopy, co-funded by the EU under the FP7 Capacities programme
 Coordinator Rex Godby

Dates 2004-2007
 Project Nanoscale Quantum Simulations for Nanostructures and Advanced Materials (Nanoquanta). Network of Excellence under the NMP3 priority of the European Commission's 6th Framework Programme. Contract Number NMP4-CT-2004-500198.
 Coordinator Rex Godby

Dates 2000-2004
 Project Nanophase Research Training Network funded through the European Commission's 5th Framework Improving Human Potential and the Socio-Economic Knowledge Base (IHP) programme
 Coordinator Rex Godby

Teaching

Dates 2004-2006
 Qualification Assistant Professor of *Mathematical methods for Material Science*
 Organization Physics Department, University of Rome "Tor Vergata"

Education and training

Dates 2001
 Qualification Ph.D in Physics
 Organization Physics Department, University of Rome "Tor Vergata"

Dates 1998
 Qualification Master degree in Physics
 Organization Physics Department, first University of Rome "La Sapienza"

Personal skills and competences

Mother tongue Italian

Other languages

English

Spanish

Understanding		Speaking		Writing
Listening	Reading	Spoken interaction	Spoken production	
proficient	proficient	proficient	proficient	proficient
good	good	good	good	sufficient

Computer skills and competences Main developer and responsible for the Yambo Project. More informations at www.yambo-code.org

The Yambo Project (general aspects)

The Yambo project represents one of the most important achievement of my scientific career. Yambo is a multi-purpose code with an highly modular structure.

For a complete description of the different code sections please refer to Ref.¹. Thanks to the Yambo project I have been invited to participate in several external collaborations. Presently I have five main international projects that are connected to the Yambo project:

1. In collaboration with Dr. Myrta Grüning (Centre for Computational Physics and Physics Department, University of Coimbra, Portugal) I am developing a real-time approach to High Harmonics Generation in correlated nano-scale materials.
2. In collaboration with Dr. Claudio Attaccalite (Institut Neel, CNRS, Grenoble, France) I am developing a theory of pump-and-probe experiments based on the non-equilibrium many-body theory.
3. In collaboration with Dr. P. Rinke and E. Kioupakis (Materials Research Laboratory, University of California, Santa Barbara, USA) I am studying polaronic effects in oxides.
4. In collaboration with Dr. Gali Ádám and Dr. M. Voros (Research Institute for Solid and Optics, Budapest, Hungary) I will shortly start a collaboration on the electron-phonon coupling in diamondoids.
5. In collaboration with Prof. A. Fortunelli and Dr. L. Sementa (Istituto per i Processi Chimico-Fisici, Pisa, Italy) I am calculating image states on metallic surfaces.

I head up the team of developers of the Yambo project. I have also created and I currently administrate the web-page of the code and a growing user-forum that we use to help the users. Thanks to Yambo my research is supported by an highly efficient code that makes possible to propose novel theoretical and numerical methods. The possibility to test on realistic materials new proposed techniques strongly increases the potential impact of my research.

The Yambo team is currently collaborating with four super-computing centres in Europe to compile, install and test the code on their parallel machines². The code is officially supported by the local support of the CASPUR and of the CINECA centers.

The Yambo Project (schools, hands-on & lectures)

Besides the international collaborations I and the Yambo code were invited to give hands-on and lectures on the code in several schools and departments

- *[Seminar] Highlights from the Yambo Project: Excitonic polarons and non-equilibrium processes.* Scuola Internazionale Superiore di Studi Avanzati (SISSA), September 10th, 2009.
- *[Seminar] Yambo: an ab initio tool for excited state calculations.* ABINIT 2009 - 4th developer workshop, Autrans (France) 24-27th March, 2009.
- *[Seminar] Exploring the Ab-Initio excited-state world with the SELF project.* Department of Physics, University of Rome "Tor Vergata", Rome, April 13, 2007.
- *[Seminar] Talking about my(SELF): theory, applications and challenges.* S³, NanoStructures and bioSystems at Surfaces, Modena, January 23, 2007.
- *[School] São Paulo ICTP/TWAS Advanced School on Computational Materials Science for Energy and Environmental Applications.* 5 - 16 September 2011. (Santo Andre' - Brazil)
- *[Schools] Time dependent Density-Functional Theory: Prospects and*

1 A. Marini, C. Hogan, M. Grüning, D. Varsano, Comp. Phys. Comm. **180**, 1392 (2009).

2 BSC (www.bsc.es), Spain. CASPUR(www.caspur.it) and CINECA(www.cineca.it), Italy. IDRIS (www.idris.fr), France.

Applications. Centro de Ciencias de Benasque Pedro Pascual, Benasque, Spain. 2006, 2008 and 2010 editions.

- [School] Hands-on workshop on excitations in solids and nano-structures from first-principles. SISSA, Trieste, 18-22 October 2010.

**The ELISE Project
(Electronic
dynamics in ultra-
intense laser fields)**

In 2010 I won a fellowship with the Ikerbasque Science Foundation to study the electronic dynamics induced by ultra-intense laser fields (ELISE project). The motivation of the project was given by the many experiments that have disclosed the existence of a paradigmatic new state of the matter created by the excitation by means of an ultra-intense laser field. In this state electrons and complex multi-particle excitations coexist in a dynamical equilibrium. The main objective of the ELISE project is to devise a parameter-free approach to the study of the dynamics of electrons and multi-particle excitations subject to ultra-intense laser fields. The aim is to develop a coherent theoretical and numerical approach based on the Non-equilibrium Green's function theory and Density Functional Theory. Thanks to this research contract I am currently studying intriguing non-linear phenomena like the excitonic Mott transition and the photo-induced transparency of simple metals. The objectives of the ELISE project are relevant to predict the physics that will be studied in the next generation laser resources, like the European XFEL (www.xfel.eu).

Invited Talks	Event	Title
	"Graphene roadmap consultation workshop: First principles computational methodologies for 2D materials ", Lancaster University, UK, September 14, 2011 to June 16, 2011	<i>Carbon nanotubes in confined magnetic fields: the anomalous Aharonov-Bohm effect</i>
	"Challenges and Solutions in GW Calculations for Complex System", CECAM-HQ-EPFL, Lausanne, Switzerland June 7, 2011 to June 10, 2011	<i>Giant zero-point-motion effects in carbon-based nanostructures</i>
	I Workshop su Fisica della Materia e Scienza dei Materiali Computazionali al Dipartimento Materiali e Dispositivi del CNR DMD-TeoC 2011	<i>Anomalous Aharonov-Bohm gap oscillations in carbon nanotubes</i>
	"Theoretical Spectroscopy: density functional theory and beyond for real materials". DPG Spring Meeting in Regensburg, Germany, 21-26 March 2010	<i>Giant polaronic effects in solids and nanstructure</i>
	Società Italiana di Fisica XCV Congresso Nazionale, Bari, 28 Sept. - 3 Oct. 2009	<i>Electronic excitations and atomic vibrations: a many-body approach</i>
	"ABINIT 2009 - 4 th developer workshop" Autrans (France) 24-27 th March.	<i>Yambo: an ab initio tool for excited state calculations</i>
	Italo-Russian workshop, April 10th, 2009	<i>Exciton-Phonon coupling and finite temperature optics</i>
	"Meeting on Optical Response in Extended Systems" (MORE) 2008. November 19-21, 2008, Vienna, Austria.	<i>Breakdown of the electronic picture of the excitonic states: evidence of phonon mediated bright to dark (and vice-versa) transitions</i>

44th Workshop: Dynamical Phenomena in low Dimensional Systems 20-26 July, 2008. Erice.	<i>Breakdown of the electronic picture of the excitonic states: evidence of phonon mediated bright to dark transition</i>
Progress in Computational Electronic Structure Theory, Gustav Stresemann-Institut, Bonn, Germany. 10-12/1/2008	Ab-Initio finite temperature excitons
Nanoquanta Workshop on Electronic Excitations. Aussois, France. 21/9/2007	Exciton-Phonon coupling in the finite temperature optical absorption of semiconductors
Young Researcher's Meeting, Rome. 3-5/5/2006	The curse of linear response island: secrets and pioneers
Ψ_k^{2005} Conference, Schwäbisch Gmünd, Germany. 17-21/9/2005	Optical properties of interacting electronic systems: many-body versus time-dependent density-functional approach
NANOEXC2004 workshop on <i>Theory and Modeling of Electronic Excitations in Nanoscience</i> , Hotel Villa del Mare, Acquafredda di Maratea (PZ), Italy. 19-23 September 2004	A three-point Many-Body vertex function from Time-Dependent Density-Functional-Theory
Workshop on "Ab-initio Methods for Correlated Spintronics Materials: Theories and Applications", Monastery of Mont Sainte Odile, Strasbourg, France. 4-7/9/2004	Quasiparticles and excitons in extended systems: Many-Body versus Time-Dependent Density-Functional-Theory
3 rd International conference "Computational Modeling and Simulation of Materials". Acireale, Italy. 29/5-4/6/2004	New theoretical tools to describe electron-hole effects in the spectra of solids and nanostructures
The 20 th General Conference of the Condensed Matter Division of the European Physical Society, Prague. 19-23/7/2004	Bound excitons in time-dependent density-functional-theory: a Many-Body approach to the exchange-correlation Kernel
Coincidence Studies of Surfaces, Thin Films and Nanostructures, Ringberg-castle, Germany. 7-10/9/2003	Quasiparticles, plasmons and excitonic effects in metals: a Many-Body approach to the electronic and optical properties of copper and silver
XXI Convegno di fisica teorica e struttura della materia}, Fai della Paganella. 21-24/4/2002	Proprieta' ottiche ed elettroniche di rame ed argento nell'approssimazione GW
5th International Workshop on Auger Spectroscopy and Electronic Structure (IWASES-5), Cortona. 2-6/7/2001	One, two and three-body channels of the Core-Valence-Valence Auger Photoelectron Coincidence Spectra of early transition metal

Invited Seminars	Location	Title
	Centre for Computational Physics and Physics Department, University of Coimbra (Portugal), September 24 th , 2010	Carbon nanotubes in confined magnetic fields: gap oscillations and persistent currents from a new perspective
	Scuola Internazionale Superiore di Studi Avanzati (SISSA), September 10 th , 2009	Highlights from the Yambo Project: Excitonic polarons and non-equilibrium processes.
	Unite' de Physico-Chimie et de Physique des Materiaux (PCPM) Louvain-la-Neuve, Belgium. 6/8/2007	Exciton-Phonon coupling in the finite temperature optical absorption of semiconductors

Department of Physics, University of Rome "Tor Vergata", Rome. 13/3/2007	Exploring the Ab-Initio excited-state world with the SELF project
S ³ , NanoStructures and bioSystems at Surfaces, Modena. 23/1/2007	Talking about my(SELF): theory, applications and challenges
Dipartimento di Fisica, Universita' di Cagliari Cittadella Universitaria. 19/10/2005	From quasiparticles to quasiexcitons: the many-body quasi-life in noble d-metals.
Institut d'Electronique de Microelectronique et de Nanotechnologie -- Dept. ISEN, Lille, France. 25/1/2005	Solids beyond the single-particle approximation: an introduction to Ab-Initio Many-Body perturbation theory
Dipartimento di Fisica, Universita' degli Studi di "Roma Tre". 4/10/2002	Proprieta' ottiche ed elettroniche di rame ed argento: teoria del funzionale densita', quasiparticelle ed eccitoni in sistemi metallici

Publications

Reviews

	Title	Authors and Journal
47	Optical properties of solids and nanostructures from a many-body xc-kernel.	Andrea Marini, Rodolfo Del Sole, and Angel Rubio, Lect. Notes Phys. 706 , 301 (2006)
46	Approximate functionals from many-body perturbation theory	Andrea Marini, Rodolfo Del Sole, and Angel Rubio, Lect. Notes Phys. 706 , 161 (2006)
45	Auger spectroscopy of strongly correlated systems: present status and future trends	Verdozzi, M. Cini e A. Marini, J. Electron Spectrosc. and Rel. Phenomena 117-118 , 41--55 (2001).

Referred

44	Anomalous Aharonov-Bohm Gap Oscillations in Carbon Nanotubes	D. Sangalli and A. Marini, Nano Letters, in press (2011).
43	Anisotropic excitonic effects in the energy loss function of hexagonal boron nitride	S. Galambosi, L. Wirtz, J. A. Soininen, J. Serrano, A. Marini, S. Huotari, A. Rubio, K. Hämäläinen, Phys. Rev. B 83 , 081413(R) (2011).
42	Coupling of excitons and defect states in boron-nitride nanostructures	C. Attaccalite, M. Bockstedte, A. Marini, A. Rubio, L. Wirtz, Phys. Rev. B 83 , 144115 (2011).
41	Implementation and testing of Lanczos-based algorithms for Random-Phase Approximation eigenproblems	M. Gruning, X. Gonze and A. Marini, Computational Materials Science 50 2148 (2011).
40	Double excitations in correlated systems: A many-body approach	D. Sangalli, P. Romaniello, G. Onida, and A. Marini, J. Chem. Phys., 134 034115 (2011).
39	Test of long-range exchange-correlation kernels of TDDFT at surfaces: Application to Si(111)2X1	O. Pulci, A. Marini, M. Palumbo and R. Del Sole, Phys. Rev. B 82 , 205319 (2010).
38	Many body effects in the excitation spectrum of a defect in SiC	M. Bockstedte, A. Marini, O. Pankratov, A. Rubio, Phys. Rev. Lett. 105 , 026401 (2010)
37	Exciton-Plasmon States in Nanoscale Materials: Breakdown of the	M. Gruning, A. Marini, and X. Gonze, Nano Lett. 9 , 2820 (2009)

	Tamm–Dancoff Approximation	
36	yambo: An ab initio tool for excited state calculations	A. Marini, C. Hogan, M. Gruning, D. Varsano Computer Physics Communications 180 , 1392 (2009).
35	Defects Identified in SiC and Their Implications	M Bockstedte, A. Marini, A. Gali, O. Pankratov and A. Rubio. Materials Science Forum 600, 285 - 290 (2009)
34	Ab-Initio finite temperature excitons	Andrea Marini, Phys. Rev. Lett. 101 , 106405 (2008)
33	Comment on "Huge Excitonic Effects in Layered Hexagonal Boron Nitride"	L. Wirtz, A. Marini, M. Gruning, C. Attaccalite, G. Kresse, and A. Rubio, Phys. Rev. Lett. 100 , 189701 (2008)
32	Optical saturation driven by exciton confinement in molecular-chains: a TDDFT study	D. Varsano, A. Marini, and A. Rubio. Phys. Rev. Lett. 101 , 133002 (2008)
31	Advanced Correlation Functionals: Application to Bulk Materials and Localized Systems	P. Garcia-Gonzalez, J. J. Fernandez, A. Marini, and A. Rubio. J. Phys. Chem. A., 111 12458 (2007).
30	Many-body corrections and optical properties of graphene nanoribbons	D. Prezzi, D. Varsano, A. Ruini, A. Marini, and E. Molinari, Phys. Rev. B 77 , 041404(R) (2008).
29	From Si nanowires to porous silicon: The role of excitonic effects	M. Bruno, M. Palummo, A. Marini, R. Del Sole, S. Ossicini Phys. Rev. Lett. 98 , 036807 (2007).
28	Anisotropic gap of superconducting CaC ₆ : A first-principles density functional calculation	A. Sanna, G. Profeta, A. Floris, A. Marini, E.K.U. Gross, S. Massidda, Phys. Rev. B 75 , 020511(R) (2007)
27	Ab initio calculation of many-body effects on the EEL spectrum of the C(100) surface	M. Palummo, O. Pulci, A. Marini, L. Reining, R. Del Sole, Phys. Rev. B 74 , 235431 (2006)
26	Effect of spatial nonlocality on the density functional band gap	M. Gruning, A. Marini, and A. Rubio, Phys. Rev. B 74 , 161103(R) (2006)
25	Density functionals from many-body perturbation theory: the bandgap for semiconductors and insulators	M. Gruning, A. Marini, and A. Rubio, J. Chem. Phys. 124 , 154108 (2006)
24	First-Principles Description of Correlation Effects in Layered Materials	A. Marini, P. Garcia-Gonzalez, and A. Rubio. Phys. Rev. Lett. 96 , 136404 (2006).
23	Excitons in boron nitride nanotubes: dimensionality effects	L. Wirtz, A. Marini, and A. Rubio. Phys. Rev. Lett. 96 , 126104 (2006).
22	An exact Coulomb cutoff technique for supercell calculations	C. A. Rozzi, D. Varsano, A. Marini, E. K. U. Gross, and A. Rubio, Phys. Rev. B 73 , 205119 (2006).
21	Excitons in germanium nanowires: Quantum confinement, orientation, and anisotropy effects within a first-principles approach	M. Bruno, M. Palummo, A. Marini, R. Del Sole, V. Olevano, A. N. Kholod, and S. Ossicini, Phys. Rev. B 72 , 153310 (2005).
20	Reflectance anisotropy spectra of the diamond (100)-(2x1) surface: Evidence of strongly bound surface state excitons	M. Palummo, O. Pulci, R. Del Sole, A. Marini, M. Schwitters, S.R. Haines, K.H. Williams, D.S. Martin, P. Weightman. J.E. Butler, Phys. Rev. Lett., 94 , 087404 (2005).
19	Electron linewidths of wide gap insulators: excitonic effects in LiF	A. Marini, A. Rubio, Physical Review B 70 , 081103(R) (2004).

18	Accurate band mapping via photoemission from thin films	A. Mugarza, A. Marini, T. Strasser, W. Schattke, A. Rubio, F.J. Garcia de Abajo, J. Lobo, E.G. Michel, J. Kuntze, J.E. Ortega, Phys. Rev. B, 69 115422 (2004).
17	Optical absorption and electron energy loss spectra of carbon and boron nitride nanotubes: a first principles approach	A.G. Marinopoulos, L. Wirtz, A. Marini, V. Olevano, A. Rubio, and L. Reining, Appl. Phys. A, 78 , 1157 (2004)
16	Bound excitons in time dependent density-functional theory: Optical and energy-loss spectra	A. Marini, R. Del Sole, and A. Rubio, Phys. Rev. Lett. 91 , 256402 (2003).
15	Ab-initio calculation of the exchange-correlation kernel in extended systems	G. Adragna, R. Del Sole and A. Marini, Phys. Rev. B 68 , 165108 (2003).
14	Dynamical excitonic effects in metals and semiconductors	A. Marini, R. Del Sole, Phys. Rev. Lett. 91 , 176402 (2003).
13	Quasiparticle bandstructure effects on the d-hole lifetimes of copper within the GW approximation	A. Marini, R. Del Sole, A. Rubio e G. Onida, Phys. Rev. B 66 , 161104(R) (2002).
12	First-principles calculation of the plasmon resonance and of the reflectance spectrum of Silver in the GW approximation	A. Marini, R. Del Sole e G. Onida, Phys. Rev. B 66 , 115101 (2002).
11	Quasiparticle electronic structure of Copper in the GW approximation	A. Marini, G. Onida e R. Del Sole, Phys. Rev. Lett. 88 , 016403 (2002).
10	Plane-wave DFT-LDA calculation of the electronic structure and absorption spectrum of copper	A. Marini, G. Onida e R. Del Sole, Phys. Rev. B 64 , 195125 (2001).
9	Three-body and one-body channels of the Auger core valence-valence decay: A simplified approach	A. Marini e M. Cini, Phys. Rev. B 60 , 11391 (1999).
Proceedings		
8	Absorption of BN nanotubes under the influence of a perpendicular electric field	C. Attacalite, L. Wirtz, A. Marini and A. Rubio, Phys. Stat. Sol. (b) 244 , 4288 (2007).
7	Optical properties of one dimensional pgraphene polymers: the case of polyphenanthrene	D. Prezzi, D. Varsano, A. Ruini, A. Marini, and E. Molinari, Phys. Stat. Sol. (b) 244 , 4124 (2007).
6	Many body pertubation theory combined with time dependent DFT: A new method for the calculation of dielectric properties of solids	R. Del Sole, O. Pulci, V. Olevano, and A. Marini, Phys. Stat. Sol. (b) 242 , 2729 (2005).
5	The Bethe-Salpeter equation: a first-principles approach for calculating surface optical spectra	M. Palummo, O. Pulci, R. Del Sole, A. Marini, P. Hahn, W. G. Schmidt and F. Bechstedt, J. Phys.: Condens. Matter 16 (2004) S4313-S4322.
4	Many-Body approach to the electronic and optical properties of copper and silver	A. Marini on <i>Correlation Spectroscopy of Surfaces, Thin Films and Nanostructures</i> , page 17, Edited by Jamal Berakdar and Jurgen Kirschner, Wiley-Vch Verlag, (2004)
3	One, two and three-body channels of the Core-Valence Valence Auger Photoelectron Coincidence Spectra of early transition metals	A. Marini e M. Cini, J. Electron Spectrosc. and Rel. Phenomena, 127/1-2 , 17-28 (2002)
2	Theory for Modeling the Optical Properties of Surfaces	G. Onida, W. G. Schmidt, O. Pulci, M. Palummo, A. Marini, C. Hogan and R. Del Sole, Phys. Stat. Sol. (a) 188 , No. 4, 1233-1242 (2001).
1	All-electron versus Pseudopotential	P. Monachesi, A. Marini, G. Onida, M.

