

Prof. Olivia Pulci Curriculum Vitae

Personal Data:

Name: Pulci, Olivia
Birth: Civitavecchia (Italy), March 3, 1966
Languages: Italian (mother tongue), English (fluent), German (basic knowledge)
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Education:

1986–1992 Physics at the University of Rome “La Sapienza”
Experimental Diploma Thesis
“Light-induced defects in amorphous SiC:H”
Final mark: Summa cum laude
1993–1997 PhD in Physics at the University of Rome ‘Tor Vergata’
Theoretical Thesis: *“Ab initio calculation of the optical properties of Surfaces: Application to the GaAs(110) surface.”*
(Tutor: Prof. R. Del Sole)

Positions:

12/2010 - today Associate Professor at the University of Rome Tor Vergata
09/2005 - 12/2010 Researcher at the University of Rome Tor Vergata
05/2003 -08/2005 INFN Researcher, University of Rome Tor Vergata
09/2001-04/2003 INFN contract (assegno di ricerca), University of Rome Tor Vergata
01/2001-08/2001 contract (assegno di ricerca), University of Rome Tor Vergata
06/2000-12/2000 Researcher, Max Planck Institute “Fritz Haber”,
Berlin (Prof. M. Scheffler)
05/1999-05/2000 DFG contract at the IFTO, Friedrich–Schiller–Universität,
Jena, Germany (Prof. F. Bechstedt)
04/1999-04/1999 Visiting Scientist at Roma Tor Vergata
10/1998-03/1999 Researcher, Ecole Polytechnique, Paris
(Prof. Lucia Reining)
03/1997-09/1998 Researcher, IFTO, Friedrich–Schiller–Universität,
Jena, Germany (Prof. F. Bechstedt)

Summary of my activities:

I am a theoretical physicist with a long-standing experience in the ab-initio computational study of the electronic and optical properties of surfaces. Some highlights are given by publications n.9, 13, 39, 41, and by a chapter in a book (n.64).

In the last few years, my research interests have expanded to the study of nanocrystals and nanodots (see for example n. 77, 61, 58) and, more recently, also to water and biological molecules. In particular, the optical spectrum of liquid water (pure and as a solvent) has been for the first time calculated with the inclusion of excitonic effects (highlights: publications n. 51, 69). *Publication n.51 represents the first many-body calculation on a liquid.*

The inclusion of environment on the optical properties of biological systems is another topic that I am developing. A multiscale approach has been for the first time applied within the Many-Body Perturbation Theory to study the optical spectra of indole in water (highlight: publication n. 69)

I have worked as a researcher in prestigious universities (Friedrich Schiller Universitaet, Jena) and Institutions (Ecole Polytechnique, Paris, and Fritz Haber Institut der Max Plank Gesellschaft, Berlin).

I am co-author of more than 80 publications appearing in peer-reviewed international journals and I have given many invited seminars in research institutions, and invited talks at conferences.

My expertise have been recognized at international level: among other activities and duties, I am beamline responsible scientist at the European Theoretical Spectroscopy Facility (ETSF) for the Optical Beamline.

I have been involved in the education of 10 students (during their diploma Thesis, and/or PhD Thesis, or stage). At the moment, I am responsible scientist of a small group composed of 2 postdocs.

Since 2003 I teach 'Theory of Solid State Physics' for the 'Laurea Specialistica' in Material Science (Scienze e Tecnologia dei Materiali, 6CFU, since 2009 8CFU). Other teaching activities are listed under "teaching classes".

Expertise

- **Surfaces:**

Ground state properties: equilibrium geometry, determination of relaxation and reconstruction, study of the relative stability of surfaces under different growth conditions. Electronic band structure and optical properties of surfaces. Effect of

steps.

- **Nanocrystals, nanodots:**
Absorption and emission spectra of silicon nanocrystals, free standing and embedded.
- **Towards systems of biological interest:**
study of water, and formamide in water; optical spectra within QM/MM+MBPT of indole in water solution; study of the photoisomerization of rhodopsin
- **Functionalizing graphene and other 2-D systems**
study of graphene, silicene and polygermine with adsorbates for opening a gap.

keywords: Ab-initio calculations, computational physics, Density Functional Theory (DFT), Time-Dependent DFT (TDDFT), Many-Body Perturbation Theory, ground state properties, electronic band structure calculations, optical absorption spectra, Reflectance Anisotropy, Surface Differential Reflectivity, GW approximation, excitonic effects.

Teaching experience:

I have given many oral presentations concerning the basics of the theoretical methods in Solid state physics (Density Functional Theory, Many Body Approaches) and concerning my specific research results. The more formal ones are listed under 'Presentations at Conferences, Workshops and Institutions'. In addition, I have been involved in the education of students:

Supervision of students:

- 1999: Supervisor of the theoretical part of the Diploma Thesis of Kathy Lüdge, TU Berlin, Germany, during her stay at the IFTO, Jena
- June -December 2000 Supervisor diploma thesis of Philip Eggert FHI Berlin
- July-October 2002: Supervisor of the student Patrick Hahn (Marie Curie Training site Fellow) during his stay in Rome Tor Vergata
- January 2003-February 2005: Supervisor of the PhD Thesis of Margherita Marsili, Universita' di Roma Tor Vergata, Italy
- September 2003-March 2004: Supervisor of the student Andreas Hoglund (Marie Curie Fellow) during his stage in Rome Tor Vergata
- January 2004-February 2007: Supervisor for the theoretical part of the PhD thesis of Viviana Garbuio

- 2004 Supervisor of the PhD student Eleonora Luppi (University of Modena and Reggio Emilia) during her stage at Roma Tor Vergata
- 2005 Supervisor of the student Ariadna Sanchez (from Mexico) during her stage in Roma Tor Vergata
- September 2006- December 2006: Supervisor of the student Tonatiuh Rangel (from Mexico) during his stage at Roma Tor Vergata
- March 2007-September 2007: tutor of Diploma Thesis of Elena Cannuccia

- October 2010-May 2011: tutor of the Diploma Thesis of Alessia De Vito
- October 2010-July 2011: tutor of the Diploma Thesis of Daniele Meggiolaro
- February 2011-September 2011: tutor of the Diploma Thesis of Claudia Violante
- Since October 2011: Supervisor of the PhD thesis of Claudia Violante
- January 2011-December 2011: Tutor of the Marie Curie Fellow Lars Matthes
- 2013: tutor of the Diploma Thesis of Luca Retattino

Teaching classes:

- Academic Year 2002-2003:** June 2003: classes for undergraduated and PhD students on modern and advanced methods for Solid State Physics (6 hours).
- Academic Year 2003-2004:** Contract teacher at the University of Rome 'Tor Vergata', for the University course in Material Science (Laurea Specialistica): 'Theory of Solid State Physics' (44 lessons)
- Academic Year 2003-2004:** Contract teacher at the University of Rome 'Tor Vergata', for part of the course 'Advanced mathematical methods' (Metodi Matematici per la Fisica) in Material Science (Laurea Specialistica) (20 lessons)
- June 2004 classes for undergraduated and PhD students on modern and advanced methods for Solid State Physics (6 hours)
- Academic Year 2004-2005:** Contract teacher at the University of Rome 'Tor Vergata', for the University course in Material Science (Laurea Specialistica): 'Theory of Solid State Physics' (44 lessons)
- June 2005 classes for undergraduated and PhD students on modern and advanced methods for Solid State Physics (6 hours)
- Academic Year 2005-2006:** Contract teacher at the University of Rome 'Tor Vergata', for the University course in Material Science (Laurea Specialistica) and for the University course in Engineer: 'Theory of Solid State Physics' (44 lessons)
- May 2006 classes for undergraduated and PhD students on modern and advanced methods for Solid State Physics (4 hours)

-Academic year 2006-2007: Contract teacher at the University of Rome 'Tor Vergata', for the University course in Material Science (Laurea Specialistica) and for the University course in Engineer: 'Theory of Solid State Physics' (40 lessons)
-June 2007 classes for undergraduated and PhD students on modern and advanced methods for Solid State Physics (4 hours)

-Academic year 2007-2008:

Contract teacher at the University of Rome 'Tor Vergata', for the University course in Material Science (Laurea Specialistica) and for the University course in Engineer: 'Theory of Solid State Physics' (6CFU)

-June 2008: classes for undergraduated and PhD students on modern and advanced methods for Solid State Physics (4 hours)

-Academic year 2008-2009:

Contract teacher at the University of Rome 'Tor Vergata', for the University course in Material Science (Laurea Specialistica) and for the University course in Engineer: 'Theory of Solid State Physics' (6CFU)

-June 2009: classes for undergraduated and PhD students on modern and advanced methods for Solid State Physics (4 hours)

-Academic year 2009-2010:

Contract teacher at the University of Rome 'Tor Vergata', for the University course in Material Science (Laurea Specialistica): 'Theory of Solids and Molecular Models' (8CFU)

-March 2010: classes for undergraduated and PhD students on modern and advanced methods for Solid State Physics (6 hours)

-Academic year 2010-2011:

Professor at the University of Rome 'Tor Vergata', for the University course in Material Science (Laurea Specialistica): 'Theory of Solids and Molecular Models' (8CFU)

-Academic year 2011-2012:

Professor at the University of Rome 'Tor Vergata', for the University course in Material Science (Laurea Specialistica): 'Theory of Solids and Molecular Models' (8CFU)

Classes for the PhD school on 'Metodi teorici-computazionali per lo studio di nanostrutture'

-Academic year 2012-2013:

Professor at the University of Rome 'Tor Vergata', for the University course in Physics (Laurea Specialistica): 'Quantum Theory of Solids' (6CFU)

Classes for the PhD school on 'Metodi teorici-computazionali per lo studio di nanos-

trutture' (2CFU)

Module at University course in Material Science (Laurea Specialistica) 'Theory of Solids and Molecular Models' held by Dr.ssa Palummo: DFT and TDDFT (2CFU)

List of Publications :

- 106) M. Marsili et al. *Self-energy effects on the electronic gap of Ge and Si nanocrystals*, submitted October 2012
- 105) Universal infrared absorbance of two-dimensional honeycomb group-IV crystals L. Matthes, P. Gori, O. Pulci, and F. Bechstedt, Phys. Rev. B **87**, 035438 (2013)
- 104) *Photoresponse from noble metal nanoparticles-multi walled carbon nanotube composites* M. Scarselli, L. Camilli, L. Matthes, O. Pulci, P. Castrucci, E. Gatto, M. Venanzi, and M. De Crescenzi, Appl. Phys. Lett. 101, 241113 (2012)
- 103) *Una nuova metodologia d'indagine per la carta antica: applicazione all'Autritratto di Leonardo* M. Missori, L. Teodonio, O. Pulci, A. Mosca Conte, Atti del Seminario Internazionale DIAGNOSTICA CONSERVAZIONE TUTELA. I disegni di Leonardo, ICR-CPAL, Roma, 25-26 giugno, 2012, pag. 67-72, in press.
- 102) A. Mosca Conte, C. Violante, M. Missori, F. Bechstedt, L. Teodonio, E. Ippoliti, P. Carloni, L. Guidoni, O. Pulci Theoretical optical spectroscopy of complex systems, in press on Journal of Electron Spectroscopy and Related Phenomena, available on-line at <http://dx.doi.org/10.1016/j.elspec.2013.02.002>
- 101) Geometric, electronic, and optical properties of the Si(111)21 surface: Positive and negative buckling C. Violante, A. Mosca Conte, F. Bechstedt, and O. Pulci Phys. Rev. B 86, 245313 Published 14 December 2012
- 100) A. Mosca Conte et al., *Experimental and theoretical study of the yellowing of ancient paper* e-Journal of Surface Science and Nanotechnology (in press)
- 99) V. Garbuio, M. Cascella, R. Del Sole, M. Marsili, and O. Pulci *Excited state properties of formamide in water solution: An ab initio study* THE JOURNAL OF CHEMICAL PHYSICS 137, 164317 (2012)

- 98) *Infrared absorbance of silicene and germanene* Friedhelm Bechstedt, Lars Matthes, Paola Gori, and Olivia Pulci Appl. Phys. Lett. 100, 261906 (2012)
- 97) A. Mosca Conte, et al. *Role of Cellulose Oxidation in the Yellowing of Ancient Paper*, Phys. Rev. Lett. **108**, 158301 (2012) (selected as Editor's suggestion, and PRL synopsis)
- 96) C. Violante, A. Mosca Conte, O. Pulci, *Structural, electronic and optical properties of the two isomers of Si(111)2x1* Journal of Physics: Conference Series 383, 012015 (2012) doi:10.1088/1742-6596/383/1/012015 . proceedings Young Researcher Meeting in Rome 2012 20 January 2012, University of Rome 'Tor Vergata', Rome, Italy
- 95) P. Gori, O. Pulci, M. Marsili, F. Bechstedt, *Side-dependent electron escape from graphene- and graphane-like SiC layers* Appl. Phys. Lett. 100, 043110 (2012); doi: 10.1063/1.3679175 (selected for the February 6, 2012 issue of Virtual Journal of Nanoscale Science & Technology)
- 94) *Many-body study of the photoisomerization of the minimal model of the retinal protonated Schiff base* Chemical Physics Letters, Volume 515, Issues 4-6, 27 October 2011, Pages 290-295 Adriano Mosca Conte, Leonardo Guidoni, Rodolfo Del Sole, Olivia Pulci
- 93) A.I. Shkrebtii, M. Marsili, E. Heritage, O. Pulci, R. Del Sole and F. Bechstedt *Defect induced modification of the surface gap and optical properties of C(111)21 surface* Phys. Stat. Sol. a Vol. 209, Issue 4/2012, page 669674 (2012)
- 92) 'Strong excitons in novel two-dimensional crystals: silicene and germanene' O. Pulci, P. Gori, M. Marsili, V. Garbuio, R. Del Sole, F. Bechstedt, Europhys. Lett.98 (2012) 37004
- 91) 'Optical properties of flavin mononucleotide: a QM/MM study of protein environment effects' E. Cannuccia, O. Pulci, R. Del Sole, M. Cascella Chemical Physics 389 (2011) 3538
- 90) 'Local-field effects in silicon nanocrystals' R. Guerra, M. Marsili, O. Pulci, and S. Ossicini Phys. Rev. B 84, 075342 (2011)
- 89) G. Bussetti, B. Bonanni, S. Cirilli, A. Violante, M. Russo, C. Goletti, P. Chiaradia, O. Pulci, M. Palummo, R. Del Sole, P. Gargiani, M. G. Betti,

- C. Mariani, R. M. Feenstra, G. Meyer, and K. H. Rieder *Coexistence of Negatively and Positively Buckled Isomers on $n+$ -Doped Si(111)- 2×1* Phys. Rev. Lett. 106, 067601 (2011)
- 88) M. Schwitters, D. S. Martin, P. Unsworth, T. Farrell, J. E. Butler, M. Marsili, O. Pulci, and P. Weightman *The contribution of steps to the optical properties of vicinal Diamond (100):H surfaces* Phys. Rev. **B** 83, 085402 (2011)
 - 87) O. Pulci, A. Marini, M. Palummo, and R. Del Sole, *Test of long-range exchange-correlation kernels of TDDFT at surfaces: application to Si(111) 2×1* , Phys. Rev. **B** 82, 205319 (2010) (selected as Editor's suggestion)
 - 86) Stefano Ossicini, Michele Amato, Roberto Guerra, Maurizia Palummo, and Olivia Pulci, *Silicon and Germanium Nanostructures for Photovoltaic Applications: Ab-Initio Results*, Nanoscale Research Letters 5, 16371649 (2010)
 - 85) M. Marsili, O. Pulci, *The fascinating physics of carbon surfaces: first-principles study of hydrogen on C(001), C(111), and graphene*, invited Review paper in Journ. of Phys. D 43, 374016 (2010)
 - 84) Paola Gori, Munise Rakel, Christoph Cobet, Wolfgang Richter, Norbert Esser, Axel Hoffmann, Rodolfo Del Sole, Antonio Cricenti, and Olivia Pulci, *Optical spectra of ZnO in the far UV: First Principle Calculations and Ellipsometric measurements*, Phys. Rev. **B** 81, 125207 (2010)
 - 83) Adriano Mosca Conte, Emiliano Ippoliti, Rodolfo Del Sole, Paolo Carloni, Olivia Pulci *Many-Body meets QM/MM: Application to indole in water solution* accepted Phys. Stat. Sol. b) Volume 247, Issue 8, August 2010, Pages: 19201924
 - 82) E. Degoli, R. Guerra, M. Marsili, O. Pulci, and S. Ossicini, *Local-fields and disorder effects in free-standing and embedded Si nanocrystallites* accepted Phys. Stat. Sol. (b) Volume 247, Issue 8, August 2010, Pages: 21132117
 - 81) O. Pulci, P. Gori, M. Marsili, V. Garbuio, A. P. Seitsonen, F. Bechstedt, A. Cricenti, and R. Del Sole, *Ab initio calculations of electronic and optical properties of group IV 2-dimensional materials*, Phys. Stat. Sol. (a) **207**, 291 (2010)

- 80) O. Pulci, E. Degoli, F. Iori, M. Marsili, M. Palummo, R. Del Sole, S. Ossicini, *Electronic and optical properties of Si and Ge nanocrystals: an ab-initio study*, Superlattices and Microstructures **47**, 178 (2010)
- 79) *Excited state properties calculations: applications to biological systems* A. Mosca Conte, V. Garbuio, M. Marsili, E. Ippoliti, R. Del Sole, P. Carloni, O. Pulci Proceedings CSFI08, in 'Nuovo Cimento C' **32**, 73 (2009)
- 78) *Excited state properties calculations: applications to biological systems* Adriano Mosca Conte, Elena Cannuccia, Viviana Garbuio, Emiliano Ippoliti, Rodolfo Del Sole, Paolo Carloni, Olivia Pulci proceedings of the school EPIOPTICS-10, Erice 2008 World Scientific, ed. A. Cricenti (accepted)
- 77) *Silicon Nanocrystallites in SiO₂ Matrix: The Role of Disorder and Size* R. Guerra, I. Marri, R. Magri, L. Martin-Samos, O. Pulci, E. Degoli, and S. Ossicini, Phys. Rev. **B** 79, 155320 (2009)
- 76) M. Marsili, O. Pulci, M. Palummo, P.L. Silvestrelli, and R. Del Sole, *Electronic and optical properties of acetylene and ethylene on Si(001)*, "Superlattices and Microstructures" **46**, 240 (2009)
- 75) O. Pulci, V. Garbuio, R. Del Sole, *Optical and electron energy loss spectra of liquid water: an ab-initio study* paper in the book *Synchrotron Radiation and Nanostructures*, in honour of Paolo Perfetti, World Scientific, / /Ed. Cricenti, Margaritondo, pag. 90 (2009)
- 74) *Ab-initio study of Ethylene on Si(001)*, M. Marsili, O. Pulci, R. Del Sole (submitted) proceedings of the school EPIOPTICS-10, Erice 2008 World Scientific, ed. A. Cricenti
- 73) *First-principles calculations and bias-dependent STM measurements at the α -Sn/Ge(111) surface: A clear indication for the 1U2D configuration* P. Gori, F. Ronci, S. Colonna, A. Cricenti, O. Pulci, G. Le Lay, Europhys. Letters **85**, 66001 (2009)
- 72) *Optical Properties of Silicon Nanocrystallites in SiO₂ Matrix: Crystalline vs. Amorphous Case*, R. Guerra, I. Marri, R. Magri, L. Martin-Samos, O. Pulci, E. Degoli, and S. Ossicini "Superlattices and Microstructures" **46**, 246 (2009)

- 71) *Tight Binding calculations of quasiparticle wavefunctions for C(111)2×1* M. Marsili, O. Pulci, F. Bechstedt, and R. Del Sole Phys. Rev. **B 78**, 205414 (2008)
- 70) *Ab-initio calculation of luminescence and optical gain properties in silicon nanostructures* Elena Degoli, Roberto Guerra, Federico Iori, Rita Magri, Ivan Marri, Olivia Pulci, Olmes Bisi, and Stefano Ossicini in special volume "Theoretical Spectroscopy", CR de Physique de l'Academie des Sciences, Elsevier doi:10.1016/j.crhy.2008.09.003 C. R. Physique 10 (2009) 575586
- 69) *Many-Body Theory meets QM/MM: application to indole in water solution* A. Mosca Conte, E. Ippoliti, R. Del Sole, P. Carloni, O. Pulci J. Chem. Theory Comput., 5, 1822 (2009)
- 68) *Excited state properties of Liquid Water*, V. Garbuio, M. Cascella, O. Pulci, invited topical Review Article at J. Phys.: Condens. Matter **21**, 033101 (2009)
- 67) *Ab-initio absorption spectra of 3-tert-butylcyclohexene* Katalin Gaal-Nagy, Olivia Pulci, and Giovanni Onida, accepted in special volume "Theoretical Spectroscopy", CR de Physique de l'Academie des Sciences, Elsevier doi:10.1016/j.crhy.2008.08.002 C. R. Physique 10 (2009) 491503 o
- 66) *Codoping goes Nano: Structural and Optical properties of Boron and Phosphorus codoped Silicon Nanocrystals*, R. Magri, F. Iori, E. Degoli, O. Pulci, S. Ossicini, AIP Conf. Proc. **963**, 359 (2007)
- 65) *Role of Surface passivation and doping in silicon nanocrystals*, R. Magri, E. Degoli, F. Iori, E. Luppi, O. Pulci, S. Ossicini, G. Cantele, F. Trani, D. Ninno, Journal of Computational Methods in Science and Engineering, **7**, 219-232 (2007)
- 64) *Quantum mechanical calculations of electronic and optical properties of surfaces* Cecilia Noguez and Olivia Pulci, 'Quantum Mechanical Calculations of Electronic and Optical Properties of Semiconductor Surfaces', chap. 12 in the book 'Quantum Chemical Calculations of Surfaces and Interfaces of Materials', ISBN: 1-58883-138-8, American Scientific Publishers, Vladimir A. Basiuk and Piero Ugliengo Eds., Pages: 217-248 (2009)

- 63) *Adsorption of small hydrocarbon molecules on Silicon surfaces: ethylene on Si(001)* M. Marsili, N. Witkowski, O. Pulci, O. Pluchery, P. L. Silvestrelli, R. Del Sole, Y. Borenzstein, Phys. Rev. **B 77**, 125337 (2008)
- 62) *Ab-initio optical spectra of complex system* E. Cannuccia, O. Pulci, M. Palummo, V. Garbuio, R. Del Sole, Phys. Stat. Solidi C **5** 2543 (2008)
- 61) *Engineering Silicon Nanocrystals: Effect of Codoping with Boron and Phosphorus* F. Iori, E. Degoli, R. Magri, I. Marri, G. Cantele, D. Ninno, F. Trani, O. Pulci, S. Ossicini, Phys. Rev. B **76**, 085302 (2007)
- 60) *Electronic and optical properties of ZnO between 3 and 32 eV* M. Rakel, C. Cobet, N. Esser, P. Gori, O. Pulci, A. Seitsonen, A. Cricenti, N.H. Nickel, W. Richter proceedings of the school EPIOPTICS-9, Erice 2006 p.115 World Scientific, ed. A. Cricenti
- 59) M. Marsili, V. Garbuio, M. Bruno, O. Pulci M. Palummo, E. Degoli, E. Luppi, R. Del Sole *Excited state properties calculations: from 0 to 3 dimensional systems* proceedings of the school EPIOPTICS-9, Erice 2006 p.41 World Scientific, ed. A. Cricenti
- 58) E. Luppi, F. Iori, R. Magri, O. Pulci, S. Ossicini, E. Degoli, V. Olevano, *Excitons in Silicon Nanocrystallites: the Nature of Luminescence* Phys. Rev. **B 75**, 033303 (2007)
- 57) M. Palummo, M. Bruno, O. Pulci, E. Luppi, E. Degoli, S. Ossicini, R. Del Sole *Ab-initio electronic and optical properties of low dimensional systems: from single particle to many-body approaches* Surf. Sci. **601** (13), p.2696-2701, Jul 2007
- 56) M. Marsili, O. Pulci, F. Fuchs, F. Bechstedt, R. Del Sole, *Many body effects in the electronic and optical properties of the (111) surface of diamond.* Surf. Sci. **601** (18), p.4097-4101, Sep 2007
- 55) P. Gori, O. Pulci, S. Colonna, F. Ronci, A. Cricenti *Structure and phase transitions of the Sn/Ge(111) surface* Surf. Sci. **601** (18), p.4381-4385, Sep 2007
- 54) M. Palummo, O. Pulci, A. Marini, L. Reining, R. Del sole *Many-body effects on the EEL spectrum of the C(100) surface* Phys. Rev. **B 74**, 235431 (2006)

- 53) S. Ossicini et al., *First Principle Study of Silicon Nanocrystals: Structural and Electronic Properties, Absorption, Emission and Doping*, Journal of Nanoscience and Nanotechnology 8, 479- 492 (2008)
- 52) S. Ossicini, E. Degoli, F. Iori, O. Pulci, G. Cantele, R. Magri, O. Bisi, F. Trani, D. Ninno, *Doping in Silicon Nanocrystals*, Surf. Sci. **601**, 2724 (2007)
- 51) V. Garbuio, M. Cascella, L. Reining, R. Del Sole, and O. Pulci, *Ab-initio calculations of Many-Body effects in liquids: the electronic excitations of water*, Phys. Rev. Lett. **97**, 137402 (2006)
- 50) O. Pulci, M. Marsili, P. Gori, M. Palummo, R. Del Sole, A. Cricenti, F. Bechstedt, *Geometry and electronic band structure of surfaces: the case of Ge(111):Sn and C(111)* Appl. Phys. A 85, 361 (2006)
- 49) P. Gori, O. Pulci, and A. Cricenti, *Surface structure and energy bands of 1/3ML Sn/Ge(111)*, Jpn. J. Appl. Phys., **45**, 2140 (2006)
- 48) P. Gori, O. Pulci, and A. Cricenti, *Surface Structure and energy bands of 1/3 ML Sn/Ge(111)* J. Phys. IV **132**, 91-94 (2006), Editions de Physique, Les Ulis, France
- 47) E. Degoli, G. Cantele, E. Luppi, R. Magri, S. Ossicini, D. Ninno, O. Bisi, G. Onida, M. Gatti, A. Incze, O. Pulci, R. Del Sole, *Ab-initio Calculations Of The Electronic Properties of Silicon Nanocrystals: Absorption, Emission, Stokes Shift*, AIP Conf. Proc. 772, 859 (2005)
- 46) O. Pulci, M. Marsili, E. Luppi, C. Hogan, V. Garbuio, F. Sottile, R. Magri, and R. Del Sole *Electronic excitations in solids: Density Functional and Green's function Theory* , Phys. Stat. Sol. (b) 242, 2737 (2005)
- 45) *Ab-initio Theories for the calculation of electronic excited states properties* O. Pulci, M. Marsili, E. Luppi, C. Hogan, E. Degoli and R. Del Sole, in 'Epioptics-8', p.1, World Scientific, ed. A. Cricenti (Erice 2004).
- 44) R. Del Sole, O. Pulci, V. Olevano, A. Marini, *Many-body Perturbation Theory combined with Time Dependent DFT: a new method for the calculation of the dielectric function of solids* , Phys. Stat. Solidi (b) 242, 2729 (2005)
- 43) P. Gori, O. Pulci, A. Cricenti, *Ab initio study of the Ge(111):Sn surface* in 'Epioptics-8', p. 62 World Scientific, ed. A. Cricenti (Erice 2004 Proceedings)

- 42) O. Pulci, M. Palummo, M. Marsili, R. Del Sole, *Theory of Surface Optical Properties* Adv. in Solid State Phys. Vol. 45, 161-172 (2005)
- 41) M. Marsili, O. Pulci, F. Bechstedt, R. Del Sole, *The electronic structure of C(111) surface: solution by ab-initio calculation*, Phys. Rev. **B 72**, 115415 (2005)
- 40) X. López-Lozano, O. Pulci, C. Noguez, K. Fleischer, R. Del Sole, W. Richter, *Electronic structure and Reflectance Anisotropy spectrum of InAs(110)* Phys. Rev. **B 71**, 125337 (2005)
- 39) M. Palummo, O. Pulci, R. Del Sole, et al. 'Reflectance Anisotropy spectra of the diamond (100) 2x1 surface: evidence of strongly bound surface state excitons' Phys. Rev. Lett. **94**, 087404 (2005)
- 38) Eleonora Luppi, Elena Degoli, G. Cantele, Stefano Ossicini, Rita Magri, D. Ninno, O. Bisi, O. Pulci, G. Onida, M. Gatti, A. Incze, R. Del Sole, *The Electronic and Optical Properties of Silicon Nanoclusters: Absorption and Emission*, Optical Materials 27, 1008 (2005)
- 37) O. Pulci, K. Fleischer, M. Pristovsek S. Tsukamoto, R. Del Sole, W. Richter *Structural Analysis by Reflectance Anisotropy Spectroscopy: As and Sb on GaAs(110)* Journal of Physics Condensed Matter **16**, S4367-S4374 (2004)
- 36) M. Palummo, O. Pulci, R. Del Sole, A. Marini, P. Hahn, G. Schmidt, F. Bechstedt *The Bethe-Salpter equation: a first-principle approach to calculate the surface optical spectra*, Journal of Physics C **16**, S4313-S4322 (2004)
- 35) O. Pulci, P.L. Silvestrelli, M. Palummo, F. Ancelotto, R. Del Sole, *Ab-initio study of the adsorption of Acetylene on Si(001) surface* Phys. Stat. Solidi (c) 0, 2997 (2003)
- 34) F. Bechstedt, R. Del Sole, S. Glutsch, P.H. Hahn, O. Pulci, W.G. Schmidt, *Many body and overlayer effects on surface optical properties* Phys. Stat. Solidi (b) 240, 469 (2003)
- 33) P.H. Hahn, W.G. Schmidt, F. Bechstedt, O. Pulci, R. Del Sole, *P-rich GaP(001)(2x1)/(2x2) Surface - A Hydrogen-Adsorbate Structure*, Phys. Rev. B 68, 033311 (2003)

- 32) P.L. Silvestrelli, O. Pulci, M. Palummo, R. Del Sole, and F. Ancelotto, *Acetylene on Si(100) from first principles: the “end bridge” structure* Phys. Rev. B **68** (23) 235306 (2003).
- 31) O. Pulci, J. Power, A. I. Shkrebtii, W. Richter, R. Del Sole, *GW calculations on surfaces: an application to the study of clean and Sb-covered Si(001)* Comp. Mat. Sci. Vol 30/1-2, 98-103 (2004)
- 30) J. Power, O. Pulci, A. I. Shkrebtii, S. Galata, A. Astropkakis, K. Hinrichs, N. Esser, R. Del Sole, W. Richter, *The Sb-induced (1×1) reconstruction on Si(001)* Phys. Rev. **B 67**, 115315 (2003)
- 29) R. Del Sole, M. Palummo, O. Pulci, *Theory of surface optical properties*, in 'Epioptics-7', pag. 1-20, World Scientific, ed. A. Cricenti.
- 28) M. Palummo, O. Pulci, R. Del Sole, *First-principles optical spectra of semiconductor surfaces: from one-particle to many-body approach* in 'Epioptics-7', pag. 29-43, World Scientific, ed. A. Cricenti.
- 27) R. Di Felice, C.A. Pignedoli, C.M. Bertoni, A. Catellani, P.L. Silvestrelli, C. Sbraccia, F. Ancilotto, M. Palummo, O. Pulci, *Ab-initio investigation of the Adsorption of Organic Molecules at Si(111) and Si(100) surfaces*, Surf. Sci. 532-535, 982 (2003)
- 26) D. Paget, O. Pulci, M. Sauvage, Y. Garreau, Lucia Reining, P. Chiaradia, F. Bechstedt, R. Pinchaux
Do we understand the structure of the Gallium-rich surface of GaAs(001)? Experimental and Theoretical approaches Surface Review and Letters, **9**, 1497 (2002)
- 25) O. Pulci, M. Palummo, V. Olevano, G. Onida, L. Reining, R. Del Sole
Many-Body Effects on the Electronic and Optical Properties of bulk GaP Phys. Stat. Sol. (a) **88**, 1261 (2001)
- 24) G. Onida, W.G. Schmidt, O. Pulci, M. Palummo, A. Marini, C. Hogan, R. Del Sole
Theory for Modeling the Optical Properties of Surfaces Phys. Stat. Sol. (a) **88**, 1233 (2001).
- 23) O. Pulci, K. Lüdge, P. Vogt, N. Esser, W. G. Schmidt, W. Richter, F. Bechstedt

First-principles study of InP and GaP(001) surfaces
Computational Materials Science **22**, 32 (2001).

- 22) O. Pulci, W.G. Schmidt, F. Bechstedt
Structure and energetics of P-rich GaP(001) surfaces,
Phys. Stat. Sol. (a) **184**, 105 (2001)
- 21) O. Pulci, L. Reining, G. Onida, R. Del Sole, F. Bechstedt,
Many-body effects on one-electron energies and wavefunctions in low dimensional systems,
Computational Materials Science **20**, 300 (2001)
- 20) K. Lüdge, P. Vogt, O. Pulci, N. Esser, F. Bechstedt, W. Richter
Atomic structure of GaP(001) and InP(001) reconstructions: Scanning Tunneling Microscopy and ab initio Theory
Proc. 25th Int. Conf. Phys. Semicond., Osaka 2000 (Eds. N. Miura and T. Ando), p. 445
- 19) O. Pulci, K. Lüdge, W.G. Schmidt, F. Bechstedt,
First-principles study of (2×1) and (2×2) phosphorus-rich InP(001) surfaces.,
Surf. Sci. **464**, 272 (2000)
- 18) K. Lüdge, P. Vogt, O. Pulci, N. Esser, F. Bechstedt, W. Richter
Clarification of the GaP(001)(2×4) Ga-rich Reconstruction by Scanning Tunneling Microscopy and ab initio Theory,
Phys. Rev. **B 62**, 11046 (2000)
- 17) L. Reining, O. Pulci, M. Palummo, G. Onida, *First-principles calculations of electronic excitations in clusters*,
Intern. Journ. of Quantum Chem. **77**, 951 (2000).
- 16) O. Pulci, F. Bechstedt, G. Onida, R. Del Sole, L. Reining
State mixing for quasiparticles at surfaces: Non-perturbative GW approximation
Phys. Rev. **B 60**, 16758 (1999)
- 15) F. Bechstedt, O. Pulci, W.G. Schmidt
Theoretical Aspects of the Optical Response of Semiconductor Surfaces
Phys. Stat. Sol. (a) **175**, 5 (1999)

- 14) O. Pulci, M. Palummo, A.I. Shkrebtii, G. Onida, R. Del Sole,
Theoretical Study of the surface optical properties of clean and hydrogenated GaAs(110)
Phys. Stat. Sol. (a) **175**, 71 (1999)
- 13) O. Pulci, G. Onida, R. Del Sole, L. Reining,
Ab-initio calculation of Self-Energy effects on surface bandstructure and optical properties of GaAs(110)
Physical Rev. Letters **81**, 5374 (1998)
- 12) O. Pulci, B. Adolph, and F. Bechstedt,
The triangle method: Reflectance anisotropy of As-covered InP(110) surfaces,
Physica Status Solidi (a) **170**, 423 (1998)
- 11) J. Sipe, A. Shkrebtii, O. Pulci,
Issues Concerning the Calculation of the Optical Response of Semiconductors
Physica Status Solidi (a) **170**, 431 (1998)
- 10) G. Onida, R. Del Sole, M. Palummo, O. Pulci, L. Reining,
Ab initio calculation of the optical properties of surfaces,
Physica Status Solidi (a) **170**, 365 (1998)
- 9) O. Pulci, U. Grossner, F. Bechstedt
Theoretical study of As overlayers on InP(110) surface: optical properties
Surface Science Letters **417** L1133-L1138, (1998)
- 8) O. Pulci, B. Adolph, U. Grossner, F. Bechstedt
"Ab initio" calculation of the reflectance anisotropy of surfaces: the triangle method
Phys. Rev. **B 58**, 4721 (1998)
- 7) O. Pulci, G. Onida, R. Del Sole, A. I. Shkrebtii,
Ab initio calculation of the Reflectance Anisotropy of GaAs(110),
Physical Review **B 58**, 1922 (1998).
- 6) V. M. Akulin, E. Borsella, G. Onida, O. Pulci, and A. Sarfati
Optical Spectra of Silicon Nano-Structures from the Random Matrix Model
Phys. Rev. **B 57**, 6514 (1998).
- 5) A.I. Shkrebtii, J.L.P. Hughes, J.E. Sipe, O. Pulci,
Linear and Nonlinear Spectroscopy of GaAs and GaP: Theory versus Exper-

iment ,

Thin Solid Films **313-314**, 574 (1998).

- 4) O.Pulci, G.Onida, A.I. Shkrebtii, R. Del Sole and B. Adolph,
Plane wave pseudopotential calculation of the optical properties of GaAs,
Phys. Rev. **B 55**, 6685 (1997)
- 3) O. Pulci, G. Onida, C. Kress, A. Shkrebtii, and R. Del Sole,
Surface optical properties from first principle calculations: GaAs(110), Si(100)2×1, C(100)2×1.
Proc. ICPS 23, Berlin, (1996)
World Scientific, Eds. M. Scheffler, R. Zimmermann, p.815
- 2) O. Pulci, G. Onida, A. Shkrebtii, C. Kress and R. Del Sole,
“Ab initio” calculation of optical properties of GaAs(110)
”Il Vuoto, Scienza e Tecnologie” **4**, 56 (1996).
- 1) M. Sebastiani, F. Pozzilli, F. Alvarez, P. Fiorini, O. Pulci e F. Evangelisti,
Metastability of light-induced defects in very low density of gap states a-SiC:H alloys,
Proc. MRS Symposium, Vol.258, 601 (1992). Spring Meeting (1992)

REPORTS

- ”Many-Body effects on silicon-based 2D systems” P. Gori, M. Marsili, V. Garbuio, A. Mosca Conte, C. Violante, O. Pulci (report in ”High Performance Computing on CRESCO infrastructure: research activities and results 2010-2011”, page 77) (ISBN 978-88-8282-268-8)
- ”Ab-initio calculations of excited state properties of Complex Systems” M. Marsili, P. Gori, O. Pulci (report in ”High Performance Computing on CRESCO infrastructure: research activities and results 2009-2010”, page 145) (ISBN 978-88-8282-242-8)

Invited talks and lectures

1. XVIII Meeting of Theoretical Solid State Physics, Fai della Paganella (Trento), 30 March 1999 (invited).
2. *17th Heimbach Meeting*, Isola Polvese, Italy 29September -3 October 2003 (2 invited lectures)
3. EPIOPTIC-8 School, Erice 20th-26th July 2004 (2 Invited Lectures, 4 hours)
4. Deutsche Physikalische Gesellschaft Spring Meeting 2005: Invited Talk (8 March 2005 Berlin, Germany)
5. Invited talk at the EPS 2006 Meeting (DPG, Dresden, Germany, 27-31March 2006) 'Ab-initio calculations of excitations at surfaces'
6. Invited Lecture at EPIOPTICS-9 (38th school, Erice 20-26 July 2006), "The optical properties of surfaces: ab-initio calculations within two-particle schemes"
7. Invited talk at the 11th Nanoquanta Workshop on Electronic Excitations: 'A decade of applications of the Bethe-Salpeter Equation', 19-22 September 2006 Houffalize (Belgium). Title of the talk: *Electronic and Optical properties of Surfaces: ab-initio calculations within MBPT and TDDFT approaches*
8. Invitation to give a talk at the APS March meeting (March 2007) (I could not travel for health reasons)
9. Invited talk at the conference SIMBIOMA "Progress in ab initio modelling of biomolecules : towards computational spectroscopy", Rome 2-4 April 2007
10. Invited talk at the 'PhD school for Nano and Bio Technologies', 21-31 May 2007, Rome Tor Vergata. Title of the Talk: 'Ab-initio calculations of optical properties of Silicon nanocrystals'
11. Invited talk at the International workshop on computational physics and Materials "Progress in Computational Electronic Structure Theory" Bonn 10-12 January 2008 ' Optical spectrum of water: many-body perturbation theory meets molecular dynamics'
12. Invited talk at the russian-italian mini-workshop 14 March 2008 Castel Gandolfo, Rome 'Ab-initio calculations of Silicon nanocrystals'
13. Two Invited Lectures at EPIOPTICS-X (Erice 20-27 June 2008)

14. Invited talk at the conference School of Nanophotonic and Photovoltaics *Ab initio theory and calculation of the optical properties of nanostructures* Santiago de Cuba 7-14 January 2009
15. invited talk at the NAST-ISM(CNR) meeting Rome (Italy) (22 June 2009) *Theoretical Approaches to the Ab-initio study of complex systems*
16. invited talk at ICFSI-12 Weimar (Germany) 5-10 July 2009
17. invited talk at OSI-8 Ischia (Italy) 6-11 September 2009
18. invited talk at ICCMSE 2009 Rhodes (Crete, Greece) 29-September- 4 October 2009
19. invited talk at the conference 'PhysCompTech' Natal, Brasil 1-5 March 2010
20. invited talk at the international School on optical properties of surfaces EPIOTICS-XI (Erice July 2010)
21. invitation to ECOSS27 (29 August- 3 September 2010) (could not attend for family reasons)
22. invited talk at the international conference NANO 2010 (Rome La Sapienza 13-17 September 2010)
23. invited talk at the 2nd International School on Nanophotonics and Photovoltaic, Tsakhadzor, Armenia (16-22 September 2010)
24. Invited talk at ICSFS15 (Beijing, China 5-10 October 2010)
25. Invited talk at the first meeting of the Mediterranean Institute of Fundamental Physics (MIFP) Marino, ROME 16-19 March 2011
26. Invitation to give a talk at CECAM workshop "Spectroscopic characterisation of liquid water from the electronic structure" July 2011 Lausanne (I could not participate)
27. Invited talk at the School of Nanophotonics Maratea (September 2011)
28. Invitation to Nano-S&T 2011, Dalian, China 23-26 October 2011 (could not participate)
29. invited talk at the workshop CMCSN on water, Seattle 10-12 February 2012
30. invited talk at the ESF Polaronic workshop, Marino March 20-23, 2012
31. invitation to give a talk 12th International Conference on Electronic Spectroscopy and Structure (ICESS12), to be held in Saint-Malo, Bretagne, France, September 16-21, 2012 (I could not participate for family reasons)

32. invitation to give a key-note lecture at the International School on New Materials for Renewable Energies (Tbilisi, Georgia, 19-23 September 2012) (I could not participate for family reasons)
33. Invitation to give a talk at OSI10 (September 2013 Chemnitz)

Invited seminars at Universities and Research Centers

1. Invited seminar at the Hahn-Meitner-Institut, Berlin, Germany (November 4, 1996).
2. Invited seminar at the Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany (7 July 1998)
3. Invited seminar at the Laboratoire CEA, Saclay, France (16 December 1998)
4. Invited seminar at the Laboratoire de Physique des Solides Université Paris-Sud, Orsay, France (18 March 1999)
5. Invited seminar at the Fritz-Haber Institut, Berlin (Germany), (24 June 1999)
6. Invited seminar at the University of Modena (20 February 2002)
7. Invited seminar at ENEA (Casaccia, Rome) (27 February 2002)
8. Invited seminar at SISSA, Trieste (12/12/2002)
9. 'Ab-initio calculations of electronic and optical properties of surfaces', invited seminar at CNR ISM (Rome), 18 November 2004
10. Invited seminar at the Universidad Nacional Autonoma del Mexico (UNAM) 26 January 2005
11. Invited seminar at the Friedrich Schiller Universitaet Jena (Germany) "Computational solid state physics: theoretical approaches and challenges for the description of the electronic and optical properties of complex systems" November 2010
12. Invited seminar at CNR Montelibretti 7 May 2012 'Strong excitonic effects in graphene-like 2D hoenycomb systems'

Presentations at Conferences

1. XX Annual Meeting "*Advances in Surface and Interface Physics*", Modena, Italy (December 1995) (oral contribution)

2. European Physical Society: *15th General Conference of the Condensed Matter Division* Baveno-Stresa, Italy (April 1996) (poster)
3. *International School of Solid State Physics, 9th workshop: EPIOPTCS4* Erice, Italy (June 1996) (oral contribution)
4. *EXCAM Workshop: Electronic Exchange and Correlation in Advanced Materials* Ecole Polytechnique, Palaiseau, Paris, France (September 1996) (poster)
5. Seminar at the University of Rome Tor Vergata, Italy (May 20, 1997)
6. *Surface and Interface Optics 1997 (SIO97)*, Aalesund, Norway (June 1997) (oral)
7. EXCAM workshop 1997: Electronic Exchange and Correlation in Advanced Materials; CECAM, Lyon, France (September 1997) (oral)
8. Seminar at the University of Rome Tor Vergata, Italy (5 June 1998)
9. *EPIOPTICS 5 (international school of Solid state physics, 14th Workshop)*, Erice, Italy (June 1998) (poster)
10. *INFM Meeting* (Italian Institute Material Science workshop) Rimini, Italy (June 1998) (poster)
11. IX Workshop on Computational Material Science, Cagliari (Italy), (10-13 September 1999) (poster)
12. SEMAT 99 (Structure Electronique et Materiaux) Strasbourg 12-13 October 1999 (oral)
13. X Workshop on Computational Material Science, Cagliari (Italy), (7-12 September 2000) (poster)
14. Optical Spectroscopy at Interfaces (OSI2001), Bad Honnef, Germany (21-23 May 2001) (poster)
15. INFM Meeting 2001 (Annual workshop of the Italian Material Science Society), Rome, Italy (18-22 June 2001) (poster)
16. CMS2001 (XI Computational Material Science Workshop), Villasimius, Cagliari (Italy) (17-23 September 2001) (poster)
17. XXI Workshop of Theoretical Physics and Solid State Matter, Fai della Paganella, (21-24 March 2002) (poster)
18. INFM Meeting 2002 (Annual workshop of the Italian Material Science Society), Bari, Italy (24-28 June 2002) (poster)

19. Ab initio Theoretical approaches to the electronic and optical spectra of materials (CECAM/Psi-k workshop), Lyon, France (23-25 September 2002) (poster)
20. CMS2002 (XII Computational Material Science Workshop), Villasimius, Cagliari (Italy) (23-29 September 2002) (oral)
21. XI International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, ICTP, Trieste (16-18/1/2003) (poster)
22. OSI5: Optics of Surfaces and Interfaces, 26-30 May 2003 Leon, Mexico (oral presentation + poster presentation)
23. INFMeeting 23-25 June 2003, Genova, Italy (poster)
24. *CMS2003* 13-18 September 2003, Cagliari, Italy (poster)
25. *BIOEX: Ab initio Electron-Excitations Theory: Towards systems of Biological Interest*", DIPC, S. Sebastian, Spain, 21-24 September 2003 (poster)
26. PSIK meeting 2004 "Ab Initio Modeling in Biological Sciences" hold in Trieste, Italy May 15th-16th, 2004 (oral)
27. Oral presentation at ICFSI-10 (Aix en Provence, France, 3-8 July 2005) 'Ab initio study of the Ge(111):Sn surface'
28. Oral presentation at Nanocose3, Villa Mondragone (Frascati) 3-5 October 2005: 'from Silicon Nanocrystals to liquid water'
29. Seminar at the University of Rome Tor Vergata (15 February 2006) 'First principles characterization of complex systems'
30. Poster at ABR2006 (Acta Biophysica Romana) *Ab-initio study of the excited state properties of liquid water*, Rome Tor Vergata 22-24 February 2006
31. Poster at the "13th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods", ICTP, Trieste, Italy, 11-13 January 2007. Title of the poster: "Many-Body effects on the electronic and optical properties of liquid water".
32. Talk at the CSFI2008 workshop (Rimini 27-31 May 2008) 'Ab initio calculation of the optical properties of liquids: the case of water'
33. Talk at the PLMCN9 conference (Lecce, Italy, 16-20 April 2009) 'Electronic and optical properties of Silicon and Germanium nanocrystals: an ab-initio study'

34. Talk at the workshop 'Structure and Dynamics of Hydrogen-Bonded Systems', (ICTP Trieste, Italy, 26-27 October 2009) *Effect of proton disorder in the excited state properties of ice*

Other activities:

Referee activities:

- Referee of international journals (Phys. Rev. Lett., Appl. Phys. Lett., Physical Review B, Thin Solid Films, Physica Status Solidi, Superlattices and Microstructures, The Journal of Physical Chemistry).
- 2007-2009: Member of the evaluation panel for CINECA-INFM supercomputer projects
- 2010: evaluator of proposals to the CEA-Eurotalents projects
- since 2011: Reviewer for CINECA ISCRA projects

Organization of conferences:

- Organizer and Member of the Scientific and Advisory Board of the conference "Ab initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials", CECAM, Lyon, September 2002.
- Organizer and Member of the Scientific and Advisory Board of the conference "Ab initio Electron-Excitations Theory: Towards systems of Biological Interest", DIPIC, S. Sebastian, Spain, 21-24 September 2003.
- Organizer and Member of the Scientific and Advisory Board of the conference *Theory and Modeling of Electronic Excitations in Nanoscience*, Acquafredda di Maratea, Italy, 19-23 September 2004
- Organizer and Coordinator of the section 'Ab-initio approaches to excited states and transport' of the MMD (Matter, Materials and Devices) workshop (INFN-meeting 2005, Genova, June 22-25 2005)

- Organizer and Member of the Scientific and Advisory Board of the conference GW2005: *40 Years of the GW Approximation for the Electronic Self Energy: Achievements and Challenges* Physikszentrum Bad Honnef, Germany 12-15 September 2005
- Member of the International Advisory and Programme Committee of ICFSI-12 (Weimer 2009)
- Member of the Program Committee of PLMCN10, Cuernavaca, Mexico, 11-16 of April, 2010.
- Member of the International Advisory Board and Programme Committee for the 13th International Conference on the Formation of Semiconductor Interfaces (ICFSI-13) Prague, Czech Republic, July 3-8 2011
- Local committee member for NANOSEA2012 S. Margherita di Pula June 2012
- organizer of the special session 'Optical properties' (memorial for Prof. Rodolfo Del Sole) at ICSFS16 (Genoa July 2012)
- Member of the International Programme Committee of OECSE13 (Rome 2013)
- Member of the Scientific Committee of OSI 10 (to be held in Chemnitz in September 2013)

Scientific coordination:

- 2004-2005: Responsible scientist in interfacing the group of Prof. Del Sole with the Marie Curie Training Site Roma Tor Vergata/Milano Bicocca and in recruiting and supervising the Marie Curie PhD students.
- Since 2004 Scientific Coordinator of the section 'Surfaces and Interfaces' (IT7) for the NoE (Network of Excellence) European Project 'NANOQUANTA: Nanoscale Quantum Simulations'
- Since 2005: Member of the Nanoquanta scientific committee for the organization of the European Theoretical Spectroscopy Facility (ETSF)
- Since 2007: Member of the scientific committee of NaST (Laboratorio d'Ateneo) Rome Tor Vergata

- Since 2007: Research Team Leader in the European Theoretical Spectroscopy Facility (ETSF: <http://www.etsf.eu>) core node of Rome Tor Vergata
- Since 2008: Optical Beamline reference scientist for the European Theoretical Spectroscopy Facility
- Since February 2010: Coordinator of the IRSES European Project "New Century of Superconductivity: Ideas, Materials, Technologies" (SIMTECH), project n. 246937
- Since March 2010: Member of 'Collegio dei Docenti' (PhD school) of Tor Vergata University for the PhD in Physics
- Since February 2012: Adjoint Member of the PhD School 'Material for Health, Environment and Energy'

Rome, 10th May 2013

Olivia Pulci