

Olivia Pulci Curriculum Vitae

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Languages: Italian (mother tongue), English (fluent), German (basic)
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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:

30/12/2021–today	Full Professor in Solid State Physics
2017-2023	National qualification for Full Professor 02/B2 (call 1532/2016)
23/12/2010-29/12/2021	Associate Professor at the University of Rome Tor Vergata
01/09/2005-22/12/2010	Researcher at the University of Rome Tor Vergata
05/2003-08/2005	INFM Researcher, Univ. of Modena and Reggio Emilia and Univ. of Rome Tor Vergata
09/2001-04/2003	INFM post-doc (assegno di ricerca), University of Rome Tor Vergata
01/2001-08/2001	post-doc (assegno di ricerca), University of Rome Tor Vergata
06/2000-12/2000	post-doc Research Associate, 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)
10/1998-03/1999	Post-doc Research Associate, Ecole Polytechnique, Paris (Prof. Lucia Reining)
03/1997-09/1998	Post-doc Research Associate, IFTO, Friedrich–Schiller–Universität, Jena, Germany (Prof. F. Bechstedt)

Visiting

- Visiting Prof Friedrich Schiller Universitaet Jena (August 2010)
- Visiting scientist at the Friedrich Schiller Universitaet Jena (August 2014)
- Visiting Prof. at the Belarus State University, Minsk (17-29 June 2016)
- Visiting Prof at the Friedrich Schiller Universitaet Jena (18 August-4 September 2016)
- Visiting Prof. at the Belarus State University, Minsk (19-26 June 2017)
- Visiting scientist at the Friedrich Schiller Universitaet Jena (18 August-2 September 2017)
- Visiting Prof. at the Belarus State University, Minsk (18-22 February 2019)

- Visiting Professor at the Chemnitz Technische Universitaet, Germany (17-31 August 2019)

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** and **2-dimensional materials**. Some highlights are given by publications n.13, 39, 87, 89, 98, 105, 122, 132) and by 3 chapters in books (n.64, n.134, n. 140). A 4th chapter is under preparation. Publication n.13 is the first calculation of Reflectance Anisotropy of a surface with GW Many-Body effects. Publication n.16 is the first non-perturbative GW calculation on a surface. Publication n. 87 represents the first TDDFT calculation on the optical properties of surfaces (selected as Editor's Suggestion). Among the two-dimensional materials I am studying **Dirac systems** (*graphene* and its cousins silicene, germanene, stanene) and other 2-D new materials, in particular **group III-Nitrides** (n.123, 138, 151). This research topic is carried on in tight collaboration with Prof. Bechstedt, Friedrich Schiller Universitaet, Jena.

Since 2003, thanks to a strong collaboration with the University of Modena Reggio Emilia (Prof. Stefano Ossicini) my research interests have expanded to the study of **nanocrystals** and **nanodots** (Highlights: n.114, 61, 77, 58).

In 2005 I opened a new research line, thanks to a fruitful collaboration with the biochemists Michele Cascella (now at Oslo University) and Paolo Carloni (now Forschungszentrum Jülich, Germany), and with Leonardo Guidoni (now at the University of L'Aquila). In particular, I studied **water, ice and biological molecules** (highlights: 113, 69, 51, 68). 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, 68). *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 have touched. 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 (QM/MM plus Many-Body) (highlight: publication n. 69)

In 2010 I opened a new research line in my group, in strong collaboration with the experimental group of Dr. Mauro Missori (CNR-ISC), on the application of our theoretical methods to understand the yellowing of ancient paper. This new line is of great interest both for **cultural heritage** applications and for basic research. Our study of degradation of cellulose (highlight: 97) and application to Leonardo da Vinci self portrait (highlight: 112) has been internationally recognized with interviews, articles, invitations to TV programs and so on.

Since 2012 my research has mainly focused on 2-D systems and on the Topological aspects of Matter: **Weyl, Dirac, topological insulators**. Highlights: n.124, 128, 133, 137

More recently (2020), **1-D** systems came to my attention: carbon based nanoribbons, nanotubes, and carbon chains (Highlights: 154, 159)

I am co-author of the post-processing program **pw2gw.x** inserted in the Quantum Espresso suite, which calculates the optical properties of any material.

My expertise has been recognized at international level: among other activities and duties, I was beamline responsible scientist at the European Theoretical Spectroscopy Facility (ETSF) for the **Optical Beamline** from 2007 to 2016.

I have been involved in the education of 40 students (during their diploma Thesis, and/or PhD Thesis, or stage). At the moment, I am responsible scientist of a small group composed of 4 PhD students and 1 post-laurea fellow.

Since 2003 I teach at Laurea Magistrale in Material Science and in Physics.

Expertise and scientific interests

- **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 (Reflectance Anisotropy and Surface Differential Spectroscopy) of surfaces. Effect of steps.

- **Nanocrystals, nanodots:**

Absorption and emission spectra of 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; study of ice.

- **Graphene and other 2-D systems**

Study of graphene, silicene and germanene pristine and functionalized. Effects of the substrates. Effects of twist angles. Study of 2D-Nitrides.

- **Cultural Heritage:**

Theoretical investigations of degradation of cellulose. Study of Leonardo Da Vinci self-portrait.

- **Software development:**

co-author of the post-processing code pw2gw.x, in the Quantum Espresso suite, for the calculations of the optical properties of matter.

- **Topological aspects of Matter: Dirac, Weyl fermions, topological insulators**

Study of 3-dimensional Dirac and Weyl systems. Transitions from topological to trivial insulators, driven by an external electric field.

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, Bethe Salpeter Equation.

Personal Skills

- Ability to coordinate large research consortia
- Ability to attract students
- Ability to collaborate with experimentalists
- Problem Solving
- Relational skills
- Adaptability
- Critical thinking

Teaching experience:

Supervision/training of students/early stage researchers:

1. 1999: Supervisor of the theoretical part of the Diploma Thesis of Kathy Lüdge, TU Berlin, Germany, during her stay at the IFTO, Jena

2. June -December 2000 Supervisor diploma thesis of Philip Eggert FHI Berlin
3. July-October 2002: Supervisor of the student Patrick Hahn (Marie Curie Training site Fellow from Germany) during his stay in Rome Tor Vergata
4. 2004–2005: Training: Dr. Paola Gori (CNR-ISM)
5. January 2003-February 2005: co-supervisor of the PhD Thesis of Margherita Marsili, Universita' di Roma Tor Vergata, Italy
6. September 2003-March 2004: Supervisor of the student Andreas Hoglund (Marie Curie Fellow) during his stage in Rome Tor Vergata
7. January 2004-February 2007: Supervisor for the theoretical part of the PhD thesis of Viviana Garbuio
8. 2004 Supervisor of the PhD student Eleonora Luppi (University of Modena and Reggio Emilia) during her stage at Roma Tor Vergata
9. 2005 Supervisor of the student Ariadna Sanchez (from UNAM, Mexico DF) during her stage in Roma Tor Vergata
10. September 2006- December 2006: Supervisor of the student Tonatiuh Rangel (from Mexico) during his stage at Roma Tor Vergata
11. March 2007-September 2007: tutor of Diploma Thesis of Elena Cannuccia
12. Nov 2009-Feb 2010: Training of Markus Roepischer, ISAS, Berlin, Title: Optical properties of III-nitride superlattices
13. March 2010-Feb2011: training of the early stage researcher Dr. Mariella Ippolito (Caspur, Rome) Title: Optical properties of silicon nanocrystals
14. October 2010-May 2011: Supervisor of the Diploma Thesis of Alessia De Vito
15. October 2010-July 2011: External Supervisor of the Diploma Thesis in Chemistry (from Roma 1 La Sapienza) of Daniele Meggiolaro
16. February 2011-September 2011: Supervisor of the Diploma Thesis of Claudia Violante
17. November 2011-October 2014: Supervisor of the PhD thesis of Claudia Violante (Physics)
18. January 2011-December 2011: Tutor of the Marie Curie Fellow Lars Matthes (from Germany) (supervisor for part of his PhD Thesis)
19. 2012-2015: supervisor of the theoretical part of the PhD thesis of Lorenzo Teodonio
20. 2014-2015: tutor of the Diploma Thesis of Luca Retattino (Physics)
21. 2014-2015: Supervisor of the Diploma Thesis of Stella Prete (Physics)

22. 2015-January 2016: tutor of the Diploma Thesis of Marco Polimeni (Physics)
23. November 2014-April 2015: Supervisor of the fellow Claudia Violante (Physics)
24. November 2015-April 2019 Supervisor of the PhD thesis of Stella Prete
25. March 2016–September 2016: Supervisor of the Diploma Thesis (Master Thesis) of Davide Grassano (Material Science)
26. March 2016–Supervisor of the Diploma Thesis (Master Thesis) of Gianluca Tirimbo' (Physics)
27. March 2016–December 2016: Supervisor of the Diploma Thesis (Master Thesis) of Valerio Armuzza (Physics)
28. November 2016–October 2019: Supervisor of the PhD thesis of Davide Grassano (Material Science)
29. June 2016–September 2017 : External Supervisor of the PhD Thesis of Mousa Bejanii (University of Tabriz, Iran)
30. March 2018–October 2018: Supervisor of the Diploma Thesis of Simone Grillo (Laurea Triennale in Physics)
31. 25 February 2018-24 May 2018 : training of the Early Stage researcher Vasil Saroka (INP-BSU, Minsk, Belarus State University, MSCA action)
32. November 2018-February 2019: training of the student Matteo Elviretti (stage, Material Science)
33. October 2017-March 2018: Supervisor of the training of the student Andrea Pianetti (stage, Material Science)
34. October 2018 – May 2019: Supervisor of the Diploma thesis (Master thesis) of Alessandro Giuliani (Physics)
35. April 2019–July 2019: training of the Early Stage researcher Sonya Voronovich-Solonevich (INP-Belarus State University) (MSCA action)
36. 1 September 2019–30 September 2019: training of the early stage researcher Aleksandr Melnikau (INP-BSU, Minsk, Belarus State University)
37. November 2019–January 2020: supervisor of the post-graduate fellowship Davide Grassano
38. 1st October 2019–11th June 2020: Supervisor of the Master thesis of Simone Brozzesi (Material Science)
39. Since November 2020– Supervisor of the PhD thesis of Simone Brozzesi
40. December 2020–June 2021: Supervisor of the Master thesis of Simone Grillo (Physics)

41. May 2021–November 2021 Supervisor of the post-laurea fellowship Roberto Cardia
42. Since November 2021– Supervisor of the PhD thesis of Simone Grillo
43. 1 March 2022–30 May 2022 Supervisor of the post-laurea fellowship Roberto Cardia
44. March 2022–July 2022: Supervisor of the Master Thesis of Domenico Corona
45. April 2022–October 2022: Supervisor Master thesis Alessia Muroi
46. June 2022–May 2023: Supervisor of the post-laurea fellowship of Ihor Kupchak
47. Since November 2022: supervisor PhD Thesis Domenico Corona
48. since November 2022: supervisor PhD Thesis Alessia Muroi
49. May 2023–May2025 Responsible of the postdoc contract Ihor Kupchak
50. since February 2023: supervisor of the Marie Curie Fellow Vasil Saroka
51. 1 November 2024–31 January 2025: supervisor of the fellowship of Simone Grillo

Lectures in Foreign Institutions:

-Belarus State University: "Ab-initio methods in Solid State Physics": lectures to PhD students of the Graduate School and scientists of the "Institute for Nuclear Problems of Belarussian State University", Minsk, Belarus (17-29 June 2016, 19-26 June 2017, 18-22 February 2019).

-Friedrich Schiller Universität: lectures to the PhD students of the Graduate school and scientists of the Friedrich Schiller Universität, Jena, Germany (15/10/2010-15/11/2010, 24/08/2014-14/09/2014)

Teaching in Tor Vergata University:

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 nanostruttura'

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 nanostruttura' (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)

Academic year 2013-2014:

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 nanostruttura' (20 lessons)

Module at University course in Material Science (Laurea Specialistica) 'Theory of Solids and Molecular Models' held by Dr.ssa Palummo: DFT and TDDFT (20 lessons)

Academic year 2014-2015:

Module at University course in Material Science (Laurea Magistrale) 'Theory of Solids and Molecular Models' held by Dr.ssa Palummo: 22 hours

Module at University course in Physics (Laurea Magistrale) 'Struttura 2' held by Dr.ssa Palummo: 6 hours

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

Academic year 2015-2016:

-Classes for the PhD School in Physics: 2CFU

"Teoria dei Solidi e Modelli Molecolari" (Material Science) 4CFU

"Teoria quantistica dei solidi" (Physics) 4CFU

"Struttura2" (Physics) 6 lessons

Academic year 2016-2017:

-Classes for the PhD School in Physics: 2CFU

"Teoria dei Solidi e Modelli Molecolari" (Material Science Master Course) 26 lessons

"Teoria quantistica dei solidi" (Physics) 24 lessons

”Struttura2” (Physics) 6 lessons

Academic year 2017-2018 ”Teoria dei Solidi e Modelli Molecolari” (Material Science Master Course) 26 lessons

”Teoria quantistica dei solidi” (Master students, Physics) 14 lessons (co-chair with Prof. Feodor Kusmartsev, Visiting prof at the University of Rome Tor Vergata)

”Struttura2” (Physics) 6 lessons

Academic Year 2018-2019 24 hours in ”Teoria dei Solidi e Modelli Molecolari” (co-chair with Prof. Palumbo), 6 hours Struttura2, 24 hours Teoria Quantistica della Materia

Academic Year 2019-2020 4 hours Struttura della Materia 2 26 hours Teoria dei Solidi e Modelli Molecolari (co-chair with Prof. Palumbo) 42 hours Teoria QUantistica della Materia

Academic Year 2020-2021 ”Teoria dei Solidi e Modelli Molecolari” (Material Science Master Course) 6 hours Struttura della Materia 2, 28 hours Teoria dei Solidi e Modelli Molecolari (co-chair with Prof. M. Palumbo) -in the 2nd semester I will give classes in Teoria QUantistica della Materia (6CFU), chair

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. Invited talk at the international conference NANO 2010 (Rome La Sapienza 13-17 September 2010)
22. Invited talk at the 2nd International School on Nanophotonics and Photovoltaic, Tsakhadzor, Armenia (16-22 September 2010) (best talk award female prof.)
23. Invited talk at ICSFS15 (Beijing, China 5-10 October 2010)
24. Invited talk at the first meeting of the Mediterranean Institute of Fundamental Physics (MIFP) Marino, ROME 16-19 March 2011
25. Invited talk at the School of Nanophotonics Maratea (September 2011)
26. Invited talk at the workshop CMCSN on water, Seattle 10-12 February 2012

27. Invited talk at the ESF Polaronic workshop, Marino March 20-23, 2012
28. Invited talk at OSI10 (9-13 September 2013 Chemnitz)
29. Invited talk at the International Workshop on Surface Sensitive Optical Spectroscopy Tianjin University (China) November 3-5, 2013 "Excitonic effects in 2D systems"
30. Invited talk at the MIFP meeting (Marino, Rome, April 2014)
31. Invited talk at METANANO conference (Varadero, Cuba, 24 April - 1 May 2014)
32. Invited talk at EPIOPTICS ERICE school July 2014 (two invited classes)
33. Invited talk at METANANO conference (Varadero, Cuba, 5-12 April 2015)
34. Invited talk at SPP2015: Surface Plasmonics and Plasmonic Workshop (S. Margherita Ligure, 7-10 June 2015)
35. Invited talk at 5th International School on Nanophotonics and Photovoltaics (Cefalu' September 2015)
36. Invited talk at FisMat2015 conference (Palermo, September 2015)
37. Invited to IW2DC international workshop (Campofelice di Roccella, 29 May-4 June 2016)
38. Invited talks (2 classes) at the EPIOPTICS 2016 school (Erice, 24-30 July 2016)
39. Invitation to "Functional and Nanostructured Materials" Workshop (Tbilisi, Georgia, 6-10 September 2016) (could not participate)
40. Invited talk at the annual March meeting of MIFP 8-10 March 2017: "Electronic and optical properties of topological semimetals"
41. Invited talk (Plenary) at the Conference "Optical NanoSpectroscopy IV", Lisboa 28-31st March 2017.
42. Invited talk at the conference "Terametananano" (May 2017, Venice)
43. Invited talk at the mini-workshop "From experiments to Theory and models. A computational challenge for Biophysics", University of Tor Vergata, Rome, 5 December 2017
44. Invited talk at the Psi-k workshop *2D layered materials for opto-electronics: a theoretical/computational perspective* (Rome 18-19 December 2017)
45. Invited talk at the 2D-BN workshop, Malta, 30 May 2018
46. Invited talk at the NATO conference FANEM2018, MINSK, Belarus (4-8 June 2018)

47. Invited talk at the NPO2018 conference, Savonlinna, Finland (6-11 August 2018)
48. Invited talk at the EPIOPTICS school, Ettore Majorana Center, ERICE, Italy (15-20 July 2018)
49. Invited talk at the "Nanoinnovation" conference (Rome, September 11th-14th)
50. Invited talk at "ACSIN-14" conference, Japan, Sendai, 21-25 October 2018
51. Invited talk at the MIFP March meeting, Marino, Italy, March 2019
52. Invited talk at the MIFP March meeting, Castel Gandolfo, March 2022
53. Invited talk at EPIOPTICS school, ERICE 3-9 July 2022
54. Keynote invited speaker at the International Conference on Physics of Two-Dimensional Crystals (ICP2DC) Tirana 18-22 September 2023
55. Invited talk La Sapienza TOPOLOGY 29-31 January, 2024
56. Invited talk at ERICE 2024 July 2024
57. Invited talk at NPO24 Finland August 2024
58. Invited talk at CMD31 (Braga, Portugal) September 2024

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. Seminar at the University of Rome Tor Vergata, Italy (May 20, 1997) Title 'Optical properties of Surfaces with the Tetrahedron Method'
4. Invited seminar at the Laboratoire CEA, Saclay, France (16 December 1998)
5. Invited seminar at the Laboratoire de Physique des Solides Université Paris-Sud, Orsay, France (18 March 1999)
6. Invited seminar at the Fritz-Haber Institut, Berlin (Germany), (24 June 1999)
7. Invited seminar at the University of Modena (20 February 2002)
8. Invited seminar at ENEA (Casaccia, Rome) (27 February 2002)
9. Invited seminar at SISSA, Trieste (12/12/2002)

10. 'Ab-initio calculations of electronic and optical properties of surfaces', invited seminar at CNR ISM (Rome), 18 November 2004
11. Invited seminar at the Universidad Nacional Autonoma del Mexico (UNAM) 26 January 2005
12. 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
13. Invited seminar at CNR Montelibretti 7 May 2012 'Strong excitonic effects in graphene-like 2D honeycomb systems"
14. Invited lectures (2) at the annual group meeting of the Semiconductor research Group of Prof. D. R. T. Zahn, TU-Chemnitz, held in Karlovy Vary 28 September-1 October 2014
15. Invited lectures (2) at the Belarus State University, Minsk (June 2016)
16. Invited lecture at IFTO, Friedrich Schiller Universitaet, Jena, 31st August 2016
17. Invited seminar at the Universidad Nacional Autonoma del Mexico (UNAM) 26th May 2017
18. Invited Lecture at the Belarus State University, Minsk (June 2017)
19. Invited seminar at the Chemnitz University, Germany (August 2019)
20. Invited talk at the University of Rome Tor Vergata for the day of light, 16 May 2022 Leonardo Da Vinci Self-portrait

Presentations at Conferences (oral contribution, posters)

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. *Surface and Interface Optics 1997* (SIO97), Aalesund, Norway (June 1997) (oral)
6. EXCAM workshop 1997: Electronic Exchange and Correlation in Advanced Materials; CECAM, Lyon, France (September 1997) (oral)
7. Seminar at the University of Rome Tor Vergata, Italy (5 June 1998)
8. *EPIOPTICS 5 (international school of Solid state physics, 14th Workshop*, Erice, Italy (June 1998) (poster)
9. *INFMeeting* (Italian Institute Material Science workshop) Rimini, Italy (June 1998) (poster)
10. IX Workshop on Computational Material Science, Cagliari (Italy), (10-13 September 1999) (poster)
11. SEMAT 99 (Structure Electronique et Materiaux) Strasbourg 12-13 october 1999 (oral)
12. X Workshop on Computational Material Science, Cagliari (Italy), (7-12 September 2000) (poster)
13. Optical Spectroscopy at Interfaces (OSI2001), Bad Honnef, Germany (21-23 May 2001) (poster)
14. INFMeeting 2001 (Annual workshop of the Italian Material Science Society), Rome, Italy (18-22 June 2001) (poster)
15. CMS2001 (XI Computational Material Science Workshop), Villasimius, Cagliari (Italy) (17-23 September 2001) (poster)
16. XXI Workshop of Theoretical Physics and Solid State Matter, Fai della Paganella, (21-24 March 2002) (poster)
17. INFMeeting 2002 (Annual workshop of the Italian Material Science Society), Bari, Italy (24-28 June 2002) (poster)
18. Ab initio Theoretical approaches to the electronic and optical spectra of materials (CECAM/Psi-k workshop), Lyon, France (23-25 September 2002) (poster)
19. CMS2002 (XII Computational Material Science Workshop), Villasimius, Cagliari (Italy) (23-29 September 2002) (oral)
20. XI International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, ICTP, Trieste (16-18/1/2003) (poster)
21. OSI5: Optics of Surfaces and Interfaces, 26-30 May 2003 Leon, Mexico (oral presentation + poster presentation)

22. INFMeeting 23-25 June 2003, Genova, Italy (poster)
23. *CMS2003* 13-18 September 2003, Cagliari, Italy (poster)
24. *BIOEX: Ab initio Electron-Excitations Theory: Towards systems of Biological Interest*, DIPC, S. Sebastian, Spain, 21-24 September 2003 (poster)
25. PSIK meeting 2004 "Ab Initio Modeling in Biological Sciences" hold in Trieste, Italy May 15th-16th, 2004 (oral)
26. Oral presentation at ICFSI-10 (Aix en Provence, France, 3-8 July 2005) 'Ab initio study of the Ge(111):Sn surface'
27. Oral presentation at Nanocose3, Villa Mondragone (Frascati) 3-5 October 2005: 'from Silicon Nanocrystals to liquid water'
28. Seminar at the University of Rome Tor Vergata (15 February 2006) 'First principles characterization of complex systems'
29. Poster at ABR2006 (Acta Biophysica Romana) *Ab-initio study of the excited state properties of liquid water*, Rome Tor Vergata 22-24 February 2006
30. 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".
31. Talk at the CSFI2008 workshop (Rimini 27-31 May 2008) 'Ab initio calculation of the optical properties of liquids: the case of water'
32. Talk at the PLMCN9 conference (Lecce, Italy, 16-20 April 2009) 'Electronic and optical properties of Silicon and Germanium nanocrystals: an ab-initio study'
33. 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*
34. Talk at the CNR workshop 'NANOFASICI', CNR, Rome, 26-28 October 2015
35. Talk at the CNISM-CNR workshop 'MATERIALS.IT', Catania, 11-16 December 2016. Title of the talk: "Topological semimetals: the case of Cd_3As_2 "
36. Talk at the CNISM-CNR workshop 'MATERIALS.IT', Catania, 11-16 December 2016. Title of the talk: "Ab-initio study of 2D Nitrides"
37. Talk at the Nanoscience & Nanotechnology Conference, 13-14 December 2022, INFN National Laboratories of Frascati. "Transitions in Xenon between excitonic, topological and trivial insulator phases: influence of screening, band dispersion and external electric field"

38. Talk at the ETSF meeting, Amsterdam, May 2023
39. Talk at the E-MRS spring meeting (Strasbourg 2023) "Transitions in Xenon between excitonic, topological and trivial insulator phases"

Referee activities:

- Evaluator for the Centre Europeen de Calcul Atomique et Moleculaire CECAM (www.cecam.org) of proposals for CECAM financed Scientific Schools/workshops
- 2014-2017: Associate Editor of the journal "Frontiers in Materials", belonging to the Nature publishing group
- since 2014: I belong to the Referees Panel for the European projects PRACE
- 2014: referee for the Austrian Science Fund (FWF) START projects
- 2013: Referee for the German Research Foundation (DFG)
- Referee of international journals (Phys. Rev. Lett., Appl. Phys. Lett., Surf. Science, Physical Review B, Thin Solid Films, Physica Status Solidi, Superlattices and Microstructures, The Journal of Physical Chemistry).
- 2007-2009: Member of the national evaluation panel for CINECA-INFN super-computer projects
- 2010: evaluator of proposals to the CEA-Eurotalents projects
- since 2011: Reviewer for CINECA ISCRA projects

Organization of conferences:

1. 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, 23-25 September 2002.
2. Organizer and Member of the Scientific and Advisory Board of the conference "Ab initio Electron-Excitations Theory: Towards systems of Biological Interest", DIPC, S. Sebastian, Spain, 21-24 September 2003.

3. 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
4. Organizer and Coordinator of the section 'Ab-initio approaches to excited states and transport' of the MMD (Matter, Materials and Devices) workshop (INFM-meeting 2005, Genova, June 22-25 2005)
5. 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
6. Member of the International Advisory and Programme Committee of ICFSI-12 (Weimer 5-10 July 2009)
7. Member of the Program Committee of PLMCN10, Cuernavaca, Mexico, 11-16 of April, 2010.
8. 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
9. Member of the Organizer Committee for NANOSEA2012 S. Margherita di Pula June 2012
10. organizer of the special session 'Optical properties' (memorial for Prof. Rodolfo Del Sole) at ICSFS16 (Genoa 1-6 July 2012)
11. Member of the International Programme Committee of the International Conference on Optics of Excitons in Confined Systems - OECS 13 (Rome 9-12 September 2013)
12. Member of the Scientific Committee of OSI 10 (Chemnitz 9-13 September 2013)
13. Member of the Organizing Committee of the CECAM/ETSF Young Research Meeting (12-14 May 2014 Rome)
14. Member of the Scientific Committee of EPIOPTICS school (26 July- 1 August 2014 Erice)
15. Member of the Scientific Committee of OSI 11 (Austin, Texas, 28 June- 3 July 2015)
16. Organizer of the miniworkshop "Collective Excitations in Advanced Nanostructures (CoExAN)" (26 July 2016 Erice) within EPIOPTICS-14 school
17. Member of the Scientific Committee of OSI 12 (Dublin, June 2017)

18. Member of the International Advisory and Program Committee of ICFSI-16
16th International Conference on the Formation of Semiconductor Interfaces
July 02–07, 2017 Hannover
19. Co-organizer of the annual ETSF workshop (Frascati 4-7 September 2017)
20. Member of the Scientific Committee of EPIOPTICS school (July 2018 Erice,
Ettore Majorana center)
21. Member of the Scientific Committee of OSI 13 (Leon, Mexico, June 2019)
22. Member of the International Advisory and Program Committee of ICFSI-17
17th International Conference on the Formation of Semiconductor Interfaces
(June 2019 Shanghai)
23. Member of the Organizing Committee of the YAMBO School May 22-26 2023,
Argiletum, Rome

Scientific coordination:

1. 2004–2005 Member of the Scientific Panel of the section 'Surfaces and Interfaces'
(IT7, WP7) for the Network of Excellence European Project 'NANOQUANTA:
Nanoscale Quantum Simulations' (FP6). (Primary coordinator of IT7: Prof.
Giovanni Onida)
2. 2005-2007: Member of the 'NANOQUANTA: Nanoscale Quantum Simulations'
(FP6) scientific committee for the organization of the European Theoretical
Spectroscopy Facility (ETSF): Integration Team Member IT1, WP1. Primary
coordinator of IT1: Dr. Lucia Reining.
3. 2007: Member of the scientific committee of NaST (Laboratorio d'Ateneo)
Rome Tor Vergata
4. Since 2007: Research Team Leader in the European Theoretical Spectroscopy
Facility (ETSF: <http://www.etsf.eu>) core node of Rome Tor Vergata
5. 2007–2016: Optical Beamline reference scientist for the European Theoretical
Spectroscopy Facility
6. 2008-2010: participant in PRIN 2007: "Many-Body and TDDFT approaches
for first-principles calculations of excited states" (coordinator: Prof. Stefano
Ossicini)
7. 2011-2012: **Principal Investigator** for the node of Rome Tor Vergata of the
EU project "ROBOCON" (Routes to Bose-Einstein Condensation at Room
Temperature) (IRSES project within FP7, Grant Agreement 230832) Budget:
271 kEuro

8. 2011-2013: **Principal Investigator** for the Rome node of the ITN (MSC actions) "CLERMONT4" (FP7, GA235114), Tor Vergata budget: 243 kEuro
9. February 2010-October 2014: **Scientific Coordinator** of the IRSES European Project "New Century of Superconductivity: Ideas, Materials, Technologies" (SIMTECH), FP7, project n. 246937. Beneficiaries: University of Rome Tor Vergata (Coordinator), and Bordeaux University, France. Partner Organizations: Bogolyubov Institute, Kiev, Ukraine; Institute for Physics of Microstructures, and Landau Institute, Russia. Amount of financing: 712.800 Euro
10. 1st October 2015–30 September 2019: **Scientific Coordinator** of the RISE "Collective Excitations in Advanced Nanostructure", CoExAN (MSC actions in HORIZON2020, GA644076). Beneficiaries: University of Rome Tor Vergata (Italy) (coordinator); University of Exeter (UK); University of Eastern Finland (Finland); University of Iceland (Iceland); CNR-SPIN (Italy). Partner Organizations: Yerevan State University (Armenia), De La Salle University (Philippines), ISP-NAS-Kiev (Ukraine), Belarusian State University (Belarus). Within such project, the innovation initiative "Carbon-based materials for microwave -THz radiation absorbers" has been selected by EU (see <https://www.innoradar.eu/>). Moreover, in 2018 the project entered the Graphene Flagship as partnering project. Amount of financing: 1.003.500 Euro
11. 2017-2020 INFN project NEMESYS (participant)
12. October 2018-January 2020: Task leader in the project ADAMO of the DCT Lazio (Distretto Tecnologico dei Beni Culturali) n. B86C18001220002
13. 1st March 2019-31 December 2023: **Principal Investigator** for the Rome node of the EU project DiSetCOm (MSCA RISE HORIZON2020 GA823728), duration: 48 months. Tor Vergata budget: 101 kEuro
14. November 2018-October 2020: Task leader for the Physics node of the project GRAFION (financed by Regione Lazio) (project number 85-2017-15125)
15. since 2019: ENEA Project on Sodium Batteries "1.2 Sistemi di accumulo, compresi elettrochimico e power to gas, e relative interfacce con le reti", financed by MiSE PTR 2019-2021, **PI** for the task *Calcoli teorici su materiali elettrodici e loro interfaccia con l'elettrolita* (Tor Vergata budget: 75 kEuro).
16. 2020: winner of the HPC EUROPA3 Transnational Access with the project: *Novel materials for energy storage: sodium-based batteries, ref.HPC17JFXQS*. Role: **Principal Investigator** (I could not travel because of COVID-19 lockdown)
17. 2020: INFN project TIME2QUEST (participant)

18. 2020: Participant in "progetti Fondo Integrativo Speciale per la Ricerca", FIRS-I fase: FIRS_2020IP_02585: SFIDE, a Smart Framework for vIrus Detection; durata: 6mesi (P.I.prof Giovanni Betta, Universit degli Studi di cassino e del lazio Meridionale; PI Unit dellUniversit degli Studi di Roma Tor Vergata: prof.ssa Laura Micheli).
 19. 2022-2025: PRIN 2020 PHOTO (PI for the ToV node; coordinator: Prof. Stefano Lupi, La Sapienza)
 20. 2023-2025: PI of the MSCA -Individual Fellowships within HORIZON EUROPE: "TERAEXC" 188.590 Euro
 21. 2023-2025: PRIN 2022 IRIDE (PI for the ToV node)
 22. 2022-2024: ENEA project on batteries (Coordinator: Dr. Margherita Moreno) PTR22-24 MASE (Ministry of Ambient and Energetic Security). O.P. responsible for the Task: WP1.20 "Calcoli teorici da principi primi su materiali elettroici innovativi."
- I have been coordinator or participant in more than 30 projects for CPUtime requests at CINECA HPC center

Institutional Activities

- Since November 2019 Coordinator of the CAST (Centro di Ateneo per il Calcolo nella Scienza e nella Tecnica) <https://www.fisica.uniroma2.it/sezioni/ricerca/centri-di-ricerca/centro-di-ateneo-per-il-calcolo-nella-scienza-e-nella-tecnica/>
- Since March 2010: Member of 'Collegio dei Docenti di Dottorato' (PhD school) in Physics of Tor Vergata University for the PhD in Physics
- 2011-2012: Adjoint Member of the PhD School 'Material for Health, Environment and Energy'
- Since December 2014: Reference Scientist for the ERASMUS programme at Tor Vergata, for the students of 'Material Science and Technology' Laurea course.
- 2014-2015: member of the Council of the CECAM-La Sapienza node
- Since 2017-: member of the Council of the CECAM-IT-SIMUL node of the Centre Europeen de Calcul Atomique et Moleculaire (CECAM, www.cecama.org) CECAM-IT-SIMUL at present comprises six members: Polytechnic University of Milan, Polytechnic University of Turin, University of Rome Tor Vergata, University of L'Aquila, University of Rome 'La Sapienza and the Istituto Italiano di Tecnologia. O.P. is the reference scientist for Tor Vergata (<https://cecamsimul.eu/>)

- 2018-2022: Member of the "Giunta del Dipartimento"
- Since November 2020: Member of the "Commissione Didattica Ristretta" for the Physics course
- Since May 2023: Vice-coordinator of the PhD School in Physics, University of Rome Tor Vergata

Commissions of Trust

- 2016 Member of the Committee for a researcher (RTDb) position, Politecnico di Milano
- 2018 Member of the Committee for a researcher (RTDa) position, Padova
- 2019 Member of the Committee for a researcher (RTDb) position, Biocampus, Rome
- 2019 Member of the Committee for a postdoc position, CNR, Adamo project
- 2019 Member of the Committee for a postdoc position, Engineer, Tor Vergata, Grafion project
- 2019 Member of the Committee for a researcher (RTDa) position, Milano Bicocca
- 2020 Member of the Committee for the final PhD examination, Milano Bicocca
- 2020 Member of the Committee for a researcher position (RTDb) Milano Bicocca
- 2021 Member of the Committee for a researcher (RTDa) position, Biocampus, Rome
- 2021 Member of the Committee for a researcher (RTDa) position, University of Naples, Italy
- 2022 Member of the Committee for a full professor, Politecnico di Torino
- Since 2010: Member of the Committee for PhDs positions in Physics, Tor Vergata
- Head or Member of the Committee for several post-docs and post-laurea fellowships, Tor Vergata
- AA 2021/22-and 2022/23: Member of the Committee for the final PhD examination, University of Modena and Reggio Emilia
- 27 October 2023: Member of the Committee for the final PhD examination of Pierre Lechiffart, University of Marseille, France
- 2023 Member of the Committee for a researcher (RTDB) university of Rome Tor Vergata
- 11 October 2024: Member of the Committee for the final PhD examination of Iskander Mukatayev, University of Grenoble, France

Member of the committee for numerous fellowships, post-doc positions, research and professorship

Memberships

- Member of the European Theoretical Spectroscopy Facility (ETSF, www.etsf.eu)
- Member of the Mediterranean Institute for Fundamental Physics (MIFP, www.mifp.eu)
- Member of the American Chemical Society (ACS, Membership number 30604339) (2014-2019)

Scientific Associations

- Associated to INFN (National Institute Nuclear Physics)

Scientific Responsibility of Research Projects:

ETSF Users projects and ETSF Training Projects: O.P. has been given the responsibility by the European Theoretical Spectroscopy Facility (ETSF) to carry on the research collaborative study of the following users projects, approved by the experts reviewers of the external evaluation panel, and financed by the ETSF:

- Scientific Responsible for the ETSF user Project n.71. Proponent: Dr. Leonardo Guidoni (Roma, La Sapienza) 1.11.2009–31.10.2010 Title: The optical spectra of rhodopsin by many body theory
- Scientific Responsible for the ETSF user project n.113. Proponent: Prof. Yves Borenztein (Jussieu, Paris) 4.june.2009-1 April 2010 Title: "The puzzle of the SiC(001): optical properties versus reconstructions understanding"
- Scientific Responsible for the ETSF user project n.173. Proponent: Dr. Maria Antonietta Loi (Groningen, The Netherlands) Feb.2010—2011 " Title "Electronic properties of PbS nanocrystals"
- Scientific Responsible for the ETSF user project n.211. Proponent: Dr. Mauro Missori (ISC, CNR, Rome) 1.4.2010-31.12.2010. Title: Understanding the ancient paper yellowing and degradation.
- Scientific Responsible for the ESTF user project n.232. Proponent: Dr. Leonardo Guidoni (Roma, La Sapienza) May 2010-June 2011. Title: The optical spectra of rhodopsin by many body theory. (follow up of project n.71)

- Scientific Responsible for the ETSF user project n.373. Proponent: Dr. Michele Cascella, Departement für Chemie und Biochemie Universität Bern 2/2011–June 2011. Title: Solvent effects on the optical properties of acetone and formamide.
- Scientific Responsible for the ETSF user project n. 306. Proponent: Prof. Peter Weightman University of Liverpool 9/6/2010-12/2010. Title: "Tackling real surfaces:the effect of steps on the optical properties of C(001):H"

Other scientific responsibilities:

- 2011: Scientific Responsible for the post-doc fellowship of Adriano Mosca Conte on "Ab-initio study of optical properties for organic photovoltaic" (D.R.2239 23/08/2011)
- 2014: Scientific Responsible for the post-laurea fellowship of Cluadia Violante on "Ab-initio calculations of properties and infrared spectra in cellulose" (D.R. 1608 17/07/2014)
- 2015: Scientific Responsible for the post-laurea fellowship of Ihor Kupchak on "Ab-initio study of excitons in 2D systems" (D.R. 1375 06/05/2015)
- 2016: Scientific Responsible of the post-laurea fellowships of Marco Polimeni on "Ab-initio study of relativistic electrons in Cd3As2" (D.R.584 03/03/2016)
- 2017: Scientific Responsible for the post-laurea fellowship of Ihor Kupchak "Ab-initio computational study of new 2D materials" (D.R. 2584 24/11/2016)
- 2018: Scientific Responsible for the post-doc fellowship of Stella Prete on "Ab-initio simulations on optical properties of cellulose" (GELARTE project by CNR-ISC, n. ADR ISC RMSAP 07 2018)
- 2018, 2019: Scientific Responsible for the post-laurea fellowship of Ihor Kupchak on "Theoretical studies on the TDDFT Kernel" (D.R. 174 29/01/2018, renewed with D.D. n.199 05/03/19)
- 2019: Scientific Responsible for the post-laurea fellowship of Sergey Sharapov "Effect of strain on the impurity levels of graphane" (D.R. 187 28.01.2019)
- 2019: Scientific Responsible for the post-laurea fellowship of Valery Gusynin on "Landau levels in 3D Dirac materials" (D.R. 185 28/01/2019)
- 2020 Scientific Responsible for the post-laurea fellowship of Davide Grassano on "Topological transitions in 2D Materials" (D.R. 2129 06/09/2019)
- 2015-2019: Responsible scientist for WP1 of the EU RISE project CoExAN (MSC actions in HORIZON2020, GA644076)
- 2018-2020: Task leader in the project ADAMO of the DCT Lazio (Distretto Tecnologico dei Beni Culturali) project of Regione Lazio n. B86C18001220002

- 2018-2020: Task responsible for the ab-initio calculations in GRAFION (financed by Regione Lazio, n.85-2017-15125)
- since 2019: ENEA Project on Sodium Batteries "1.2 Sistemi di accumulo, compresi elettrochimico e power to gas, e relative interfacce con le reti", financed by MiSE PTR 2019-2021, task responsible for the workpackage *Calcoli teorici su materiali elettrodici e loro interfaccia con l'elettrolita*
- since 2019: responsible of the ab-initio calculations part in the EU project DiSET-CoM (MSCA RISE HORIZON2020 GA823728)
- Responsible of the Theory part in PRIN 2022 IRIDE

Outreach and Third mission

- ESTF training project n.175. Proponent: Dr. Christoph Cobet (ISAS, Berlin, Germany) Nov 2009-Feb 2010 Training project for the student Markus Roeppischer, Title: Optical properties of III-Nitrides superlattices
- ETSF training project n.302. Proponent: Mariella Ippolito (Caspur, Rome) 29/3/2010-Feb2011. Training project for the early stage researcher Mariella Ippolito. Title: "Optical properties of silicon nanocrystals"
- Publication about "Carbon nanocircuits" on the broad audience journal *Platinum* (28 November 2016, page 86)
- Press release on the national newspaper La Repubblica about the Leonardo Da Vinci self-portrait:
http://www.repubblica.it/scienze/2014/06/16/news/lautoritratto_di_leonardo_sta_svanendo_cos_possiamo_salvarlo_dal_tempo-88650028/ (16 June 2014)
- 11th April 2019 seminar for the "Percorso di Eccellenza Laurea Magistrale in Fisica": "The Marie-Sklodowska-Curie projects in HORIZON2020", University of Tor Vergata
- "Costruirsi la carriera attraverso la mobilita': dall'ERASMUS ai progetti RISE" Tor Vergata, 22 Ottobre 2020 (Seminario divulgativo per i Percorsi d'eccellenza)
- 3rd February 2021 Solid State physics seminars for bachelor students Tor Vergata
- "Costruirsi la carriera attraverso la mobilita': dall'ERASMUS ai progetti RISE" Tor Vergata, 24 March 2022
- 13 December 2023 La fisica incontra la citta', University of Roma 3, invited seminar "Flatland, the wonderful 2dimensional world"

Prizes/Honoris/Awards:

- Prize: "Best talk female professor Award" for her Invited talk at the 2nd International School on Nanophotonics and Photovoltaic, Tsakhadzor, Armenia (16-22 September 2010)
- Prize "Honoris Causa" at MIFP, 2018 2nd of March

Scientific Outcomes

178 Publications,
-1 Advanced Materials
-1 Adv. Energy Mat.
-2 Nano Letters
-5 Phy. Rev. Lett.
-1 Nature Comm.
-3 Sci. Rep.
-5 Appl. Phys. Lett.
-32 Phys. Review B
-3 Chapters in books
-1 item in Encyclopedia
-2 NPJ-2D

Full List of Publications:

- 178) L. Mosesso et al., *Evidence of high electron mobility in magnetic kagome topological metal FeSn thin films*, Nanoscale Adv. (2024), DOI: 10.1039/4D4NA00737A
- 177) I. Kupchak, F. Bechstedt, O. Pulci, and P. Gori, *Tuning the optical absorption and exciton bound states of germanene by chemical functionalization*, Sci Rep **14**, 25182 (2024)
- 176) S. Grillo, S. Postorino, M. Palummo, and O. Pulci, *Tellurene Polymorphs: A New Frontier for Solar Harvesting with Strong Exciton Anisotropy and High Optical Absorbance*, Advanced Energy Materials (2024), DOI: 10.1002/aenm.202400674
- 175) Corona, D.; Buonocore, F.; Bechstedt, F.; Celino, M.; Pulci, O. *Structural, Electronic and Vibrational Properties of B₂₄N₂₄ Nanocapsules: Novel Anodes for Magnesium Batteries*, Nanomaterials **14**, 271 (2024)

- 174) S. Brozzesi et al., *Thermodynamics and electronic structure of adsorbed and intercalated plumbene in graphene/hexagonal SiC heterostructures*, Sci. Rep. 14, 2947 (2024)
- 173) Muroi, A.; Brozzesi, S.; Bechstedt, F.; Gori, P.; Pulci, O. *Tuning Gaps and Schottky Contacts of Graphene/Phosphorene Heterostructures by Vertical Electric Field and Strain*, Nanomaterials 13, 2358 (2023)
- 172) Paraipan, A.A. et al., *Low-Frequency Vibrations of Saccharides Using Terahertz Time-Domain Spectroscopy and Ab-Initio Simulations*, Appl. Sci. 13(17), 9719 (2023)
- 171) *Transitions in Xenon between excitonic, topological and trivial insulator phases: Influence of screening, band dispersion and external electric field*, O. Pulci et al., SciPost Phys. 15, 025 (2023)
- 170) *BN endofullerenes as anode materials for Magnesium-Ion Batteries: A DFT Study*, D. Corona et al., Materials Today Chemistry (accepted)
- 169) *Two-dimensional single crystal monoclinic gallium telluride on silicon substrate via transformation of epitaxial hexagonal phase*, E. Zallo et al., npj 2D Mater Appl 7, 19 (2023)
- 168) *Covalent bonded bilayers from germanene and stanene with topological giant capacitance effects*, B. Zhang, D. Grassano, et al., npj 2D Materials and Applications 27 (2023)
- 167) *Interplay of Quantum Confinement and Strain Effects in Type I to Type II Transition in GeSi Core-Shell Nanocrystals*, I. Marri, S. Grillo, M. Amato, S. Ossicini, and O. Pulci, Journ.Phys. C 127, 1209 (2023)
- 166) C. Attacalite, M. S. Prete, M. Palummo, and O. Pulci, *Interlayer and Intralayer Excitons in AlN/WS₂ Heterostructure*, Materials 15 (2022)
- 165) Grillo, S., Pulci, O., Marri, I. *Evolution of the electronic and optical properties of meta-stable allotropic forms of 2D tellurium for increasing number of layers* Nanomaterials, 12(14) (2022)
- 164) Brozzesi, S., Attacalite, C., Buonocore, F., Giorgi, G., Palummo, M., Pulci, O. *Ab initio study of Graphene/hBN van der Waals heterostructures: Effect of electric field, twist angles and p-n doping on the electronic properties* Nanomaterials, 12(12) (2022) doi:10.3390/nano12122118
- 163) Mousa Bejani, Olivia Pulci, Naser Karimi, Elena Cannuccia, and Friedhelm Bechstedt, *Electronic structure, vibrational properties, and optical spectra of two- and three-dimensional hexagonal InSe: Layer-dependent ab initio calculations*, Phys. Rev. Materials 6, 115201 (2022)

- 162) Titubante, M., et al., *Analysis and diagnosis of the state of conservation and restoration of paper-based artifacts: A non-invasive approach*, Journal of Cultural Heritage, 55, 290-299 (2022). doi:10.1016/j.culher.2022.04.003
- 161) Gori, P., Bechstedt, F., Pulci, O. (2022). *Optical properties of xenes. Xenes: 2D synthetic materials beyond graphene* (pp. 319-352) doi:10.1016/B978-0-12-823824-0.00009-5
- 160) Bechstedt, F., Grillo, S., Pulci, O., Gori, P. (2021). *Thermal properties of dirac fermions in xenes: Model studies* Physical Review B, 104(16) (2021) doi:10.1103/PhysRevB.104.165420
- 159) L. Gontrani et al., *Detection of heavy metals in water using graphene oxide quantum dots: an experimental and theoretical study* (accepted in Molecules)
- 158) Buonocore, F., Capasso, A., Celino, M., Lisi, N., Pulci, O. *Tuning the Electronic Properties of Graphane via Hydroxylation: An Ab Initio Study*, Journal of Physical Chemistry C, 125, 16316 (2021)
- 157) F. Bechstedt, P. Gori, O. Pulci, *Beyond graphene: Clean, hydrogenated and halogenated silicene, germanene, stanene, and plumbene*, Progress in Surface Science, 2021 (in press)
- 156) A.V. Melnikov et al., *Scattering of electromagnetic waves by two crossing metallic single-walled carbon nanotubes of finite length* Physical Review B, 103, 075438 (2021)
- 155) M. Galbiati et al., *Tuning the Doping of Epitaxial Graphene on a Conventional Semiconductor via Substrate Surface Reconstruction* Journal of Physical Chemistry Letters, 12 (4), pp. 1262-1267 (2021)
- 154) S. Kutrovskaia et al., *Excitonic Fine Structure in Emission of Linear Carbon Chains*, Nano Letters 20, 6502 (2020)
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