Curriculum Vitae

Personal Information

Name: **Maurizia Palummo**
ORCID: https://orcid.org/0000-0002-3097-8523
Researcher ID: AAC-1949-2021
Website: https://www.fisica.uniroma2.it/elenco-telefonico/palummo/
Scholar : https://scholar.google.it/citations?user=LSIkynsAAAAJ&hl=en

Work Experience

- **2024–Present**: Full Professor, Department of Physics, University of Rome 'Tor Vergata'
- **2017–2024:** Associate Professor, Department of Physics, University of Rome 'Tor Vergata'
- **2004–2017:** Researcher, Department of Physics, University of Rome 'Tor Vergata'
- **1999–2004**: INFM fixed-term Researcher, Department of Physics, University of Rome 'Tor Vergata'
- **1996–1998**: Research Fellow, Department of Physics, University of Rome 'Tor Vergata'
- **1995–1996**: Research Fellow, ENEA Casaccia Research Center
- **1994–1995**: INFM Research Fellow, Department of Physics, University of Rome 'Tor Vergata'
- **1991–1994:** PhD in Physics, University of Rome 'Tor Vergata'

Education and Training

- PhD in Physics, University of Rome 'Tor Vergata', 1991–1994
- Laurea in Physics 'cum laude', University of Rome 'Tor Vergata', December 1989

Scientific Experience

Summary: Expert in first-principles simulations (DFT, GW, BSE) and electronic structure theory. Research topics include 2D materials, perovskites, nanostructures, excitonic effects and applications in energy materials. Developer and advanced user of the YAMBO code.

More Detailed description : After an initial research period in experimental condensed matter physics, focused on the optical properties of defects and color centers in insulating matrices, I have been working for many years in the field of first-principles calculations of the structural, electronic, and optical properties of materials.

During my PhD thesis, I began focusing on ab-initio calculations within density functional theory (DFT) and many-body perturbation theory (MBPT), studying the electronic properties of wide band-gap semiconductor compounds, such as GaN, including electronic self-energy corrections. Since 1996, I have worked on the electronic and linear and nonlinear optical properties of various semiconductor and metallic surfaces, both bare and covered by atomic or molecular adsorbates. In particular, I became an expert in calculating reflectance anisotropy spectra (RAS) and surface differential reflectivity (SDR) spectra.

After 2005, my research focused on first-principles studies of many-body effects in the surfaces of semiconductor materials with both wide and narrow band gaps, as well as on the dielectric response and electronic excitations of low-dimensional systems such as Ge and Si nanowires. In recent years, my main research interests have shifted to two-dimensional materials, organic compounds, and materials for energy applications such as perovskites.

Through my work, I have gained expertise in computational physics and familiarity with the most modern theories and computational tools for first-principles electronic structure calculations (Car-Parrinello, GW method, BSE exciton calculations, parallel computing). I am a member of the developer/superuser team of the many-body code **Yambo** (www.yambo-code.org).

Main research topics of the last 15 years :

2024–2021
i) Theoretical characterization of out-of-plane excitons in lead-free layered perovskites; calculation of the fine structure of excitons in two-dimensional layered tin- and lead-based perovskites (invited talks n. 45, 44, 43, 40; publications n. 152, 149, 146, 138)
ii) Extension and application of the spinorial BSE formulation to monolayers of transition metal dichalcogenides (TMDs) (invited talk n. 42, publication n. 131)
iii) Study of electronic and optical properties using DFT and, in some cases, post-DFT methods, of new two-dimensional materials and van der Waals homo- and hetero-bilayers of 2D materials for optoelectronic applications (invited talks n. 41, 39, 38, 37; publications n. 153, 150, 148, 145, 143, 142, 140, 137, 135, 134)
iv) Theoretical–experimental study of excitonic instability and exciton condensation in T' phase TMDs (invited talk n. 40, publication n. 139)

2020–2018
i) Study of many-body effects in double perovskites and two-dimensional layered hybrid perovskites (invited talks n. 38, 36; talks n. 18, 19; publications n. 124, 122, 112, 110)
ii) Development of an ab-initio approach to calculate radiative lifetimes of materials from 0D to 3D (invited talk n. 37; publications n. 117, 115, 111)
iii) Study of the electronic and optical properties and excitonic instability of T' phase TMDs in distorted tetragonal form (invited talk n. 35; publication n. 128, 116)
iv) Characterization of excitonic properties of 2D interfaces based on phosphorene for photocatalysis applications (invited talks n. 37, 32; publications n. 130, 114)
v) Study using DFT and post-DFT methods of linear and nonlinear electronic and optical properties of two-dimensional and layered materials (invited talks n. 32, 31, 30, 29; publications n. 123, 119, 118)

2017–2014
i) Study of many-body effects in layered hybrid perovskites (invited talk n. 29; talks n. 18, 19; publication n. 112)
ii) Development of an ab-initio approach to calculate radiative lifetimes in 2D materials, with special attention to 2D-TMDs (invited talks n. 30, 26, 19, 18; publication n. 102)
iii) Ab-initio nonradiative electron–phonon lifetimes in oxide and 2D-TMD materials (invited talks n. 26, 24, 17, 15; publication n. 103)
iv) Ab-initio study of the electronic properties of group IV nanowires and their polytypism and its influence on electronic and optical properties (invited talks n. 30, 14; publications n. 107, 104, 99, 95); excitons and their optical signatures in bulk and anatase-form TiO_2 nanosheets (invited talks n. 30; publications n. 108, 105, 91)

2013–2011
i) Ab-initio simulation of ground and excited states of porphyrin crystals and oligomers (publications n. 97, 96, 89)
ii) Spin-resolved GW calculations on doping levels in silicon nanowires
iii) Self-energy and excitonic effects in two-dimensional materials (TMDs, hybridized boron nitride and carbon, 2D TiO_2-based materials) (invited talks n. 13, 12, 11, 10, 9; talks n. 17, 16; publications n. 87, 88)
iv) Photovoltaic conversion efficiency of 2D-TMD heterobilayers and graphene/TMD bilayers for ultrathin excitonic solar cells using DFT and MBPT ab-initio simulations (invited talks n. 13, 12, 11, 10; publications n. 92)
v) Theoretical study of the electronic properties of porphyrin oligomers and tautomerization of free-base porphyrins deposited on substrates (publications n. 89, 96)

2010–2009
i) Theoretical study of the electronic and optical properties of free-base porphyrins based on density functional theory and many-body perturbation theory (invited talks n. 8, 16; publication n. 70)
ii) Study of the electronic and optical properties of Si, Ge, and SiGe nanowires (invited talks n. 6, 7, 8, 9; talk n. 9; publications n. 79, 78, 77, 76, 75, 74, 71, 68, 66)

Major External (to UniToV) Collaborations

- G. Giorgi (Univ. Perugia), K. Yamashita (Tokyo Univ.), D. Varsano (S3-CNR Modena)
- G. Cicero and M. Re Fiorentin (Politecnico di Torino), M. Amato and A. Zobelli (Paris Sud)
- E. Cannuccia and C. Attaccalite (CNRS, Marseille), J.C. Grossman (MIT), M. Bernardi (Caltech)
- D. Sangalli and A. Marini (CNR-ISM), L. Chiodo (Campus Biomedico), R. Rurali (ICMAB)
- S. Ossicini (Univ. Modena), A. Rubio (San Sebastian), J. Even (Rennes)

Scientific Impact

Author of over 150 scientific articles (147 indexed on ISI Web of Science), most of which published in international peer-reviewed journals

Contributions include: Several book chapters, 4 review articles. Publications in top journals, such as: *Nature Physics*, *Nature Nanotechnology*, *Nature Communications*, *Chemical Reviews Advanced Functional Materials* (2), *ACS Nano* (2), *ACS Energy Letters*, *Nano Letters* (5), *npj 2D Materials and Applications* (2), *Advanced Optical Materials* (2), *Journal of Physical Chemistry Letters* (5), *Physical Review Letters* (5), *Journal of Physical Chemistry C* (2), *Journal of Chemical Physics* (2), *Physical Review B* (29)

Citation Metrics:
Total citations (ISI / Google Scholar): 6,702 / 8,090
Citations excluding self-citations (ISI): 6,414
Average citations per article (ISI): 45.59
h-index (ISI / Google Scholar): 38 / 42

Main Publications (last 15 years):

10. *Excitons and light emission in semiconducting $MoSi_2X_4$ two-dimensional materials*
M. Sun, M. Re Fiorentin, U. Schwingenschlögl, M. Palummo
npj 2D Materials and Applications, 6, Article number: 81 (2022)

9. *A monolayer transition metal dichalcogenide as a topological excitonic insulator*
D. Varsano, M. Palummo, E. Molinari, M. Rontani
Nature Nanotechnology, 15(5), 367–372 (2020)

8. *Optical properties of lead-free double perovskites by ab initio excited-state methods*
M. Palummo, E. Berrios, D. Varsano, G. Giorgi
ACS Energy Letters, 5, 457 (2020)

7. *Nature of the electronic and optical excitations of Ruddlesden–Popper hybrid organic–inorganic perovskites: The role of many-body interactions*
G. Giorgi, K. Yamashita, M. Palummo
The Journal of Physical Chemistry Letters, 9(19), 5891–5896 (2018)

6. *Theory and ab initio computation of the anisotropic light emission in monolayer transition metal dichalcogenides* H.Y. Chen, M. Palummo, D. Sangalli, M. Bernardi
Nano Letters, 18(6), 3839–3843 (2018)

5. *Optical emission in hexagonal SiGe nanowires*
X. Cartoixà, M. Palummo, H.I.T. Hauge, E.P.A.M. Bakkers, R. Rurali
Nano Letters, 17(8), 4753–4758

4. *Crystal phase effects in Si nanowire polytypes and their homojunctions*
M. Amato, T. Kaewmaraya, A. Zobelli, M. Palummo, R. Rurali
Nano Letters, 16(9), 5694–5700 (2016)

3. *Exciton radiative lifetimes in two-dimensional transition metal dichalcogenides*
M. Palummo, M. Bernardi, J.C. Grossman Nano Letters, 15(5), 2794 (2015)

2. *Silicon–germanium nanowires: chemistry and physics in play, from basic principles to advanced applications* M. Amato, M. Palummo, R. Rurali, S. Ossicini
Chemical Reviews, 114(2), 1371–1412 (2014)

1. *Extraordinary sunlight absorption and one-nanometer-thick photovoltaics using two-dimensional monolayer materiali* M. Bernardi, M. Palummo, J.C. Grossman
Nano Letters, 13(8), 3664–3670 (2013)

Editorial and Reviewing Activities

- Guest Editor of the Focus Collection *"Focus on Photocatalytic Water Splitting"*, Nanotechnology, IOP Science.
  https://iopscience.iop.org/collections/nano-231020-395
- Guest Editor of the Special Issue *"Focus on Excitonic Properties of Two-Dimensional Materials"*, Journal of Physics: Condensed Matter, 2023.
  https://iopscience.iop.org/collections/jpcm-230901-338
- Guest Editor of the Special Issue *"Theoretical Study of Two-Dimensional Materials for Photocatalysis and Photovoltaics"*, Frontiers in Chemistry, 2022.
  https://www.frontiersin.org/research-topics/32734/theoretical-study-of-two-dimensional-materials-for-photocatalysis-and-photovoltaics/magazine#articles
- Guest Editor of the Special Issue *"Optoelectronic Properties and Applications of Nanomaterials"*, Nanomaterials (MDPI), 2021.
  https://www.mdpi.com/journal/nanomaterials/special_issues/Nano_Optoe_App
- Guest Editor of the volume *Current Opinion in Green and Sustainable Chemistry*, Elsevier, 2019.
- Member of the Editorial Board of *Scientific Reports* (Nature Publishing Group).
- Reviewer for journals of APS, ACS, RSC, IOP, and Elsevier.
- Reviewer of competitive research proposals including: Several ISCRA-B (CINECA) projects, 2 NSF (USA) project, 1 Estonian national project, 2 Austrian Science Fund projects, 1 ANR (French National Research Agency) project, 2 DFG (German Research Foundation) projects, 1 PRACE project, 1 ERC Consolidator Grant proposal

Conferences/Schools/Workshops/seminars:

36 Invited talks (2 keynote talks,1 talk Psik-2022, 2 talks a IEE-NANO2023 and IEE-NANO2021, 1 MRS-Fall-meeting, 4 talks al EMRS-Fall meetings,1 talk al 242nd ECS meeting), **17 invited seminars/lectures** at national and foreign institutions, **20 orals,** 7 posters, **13 outreach seminars**

Invited Talks:

- **53 Invited Seminar** *Ab-initio Insights into the Opto-Electronic Properties of Emerging 2D and Layered Materials* CNR-ISM Area Tor Vergata 5-5-2025
- **52 Invited Talk** *Quasi-Particles and Excitons in 2D/Layered Materials—Insight by Ground and*

Excited State Simulations MRS Spring Meeting 1-7 April 2025 Seattle https://www.mrs.org/meetings-events/annual-meetings/2025-mrs-spring-meeting

- **51 Invited Talk** *Excitonic properties of 2D-layered materials by DT+GW+BSE simulations* Toulouse 2-4 October 2024 Cecam Flagship Workshop Green's function methods: the next generation **(**https://www.cecam.org/workshop-details/greens-function-methods-the-next-generation-6-1286**)**
- **50 Invited Keynote Talk** *Excited state properties of novel 2D/layered materials by ab-initio DFT + MBPT methods* The meeting of the condensed matter theory Italian community Bressanone 28-30 August 2024 https://cmtconference.it/
- **49 Invited Seminar** *Quasi-particles and excitons in 3D and 2D halide perovskites by ab-initio ground and excited state methods* YCU Minatomirai Campus Yohokama 4 July 2024
- **48 Invited Seminar** *Ab-initio DFT+GW+BSE methods: excited state properties of 2D/layered materials for opto-electronic applications* Japan Women's University Tokyo 1 July 2024
- **47 Invited Talk** *Electronic and optical properties of novel 2D/layered materials by ab-initio DFT and post-DFT methods* Nanoscience & Nanotechnology conference 3-6 June 2024 National Laboratories of Frascati (Rome), Italy https://agenda.infn.it/event/38963/
- **45 Invited talk** *"Opto-electronic properties of solar-harvesting 2D/layered materials by ab-initio methods: from TMDs to halide perovskites"* NMDC 2023 22-25 Ottobre 2023 Paestum Italy https://ieeenmdc.org/nmdc-2023/
- **44 Invited talk** *"Opto-electronic properties of 2D/layered materials by DFT and post-DFT methods: from TMDs to halide perovskites"* al simposio J **"**Exploring the potential of bidimensional materials for energy and optoelectronics" del EMRS Fall Meeting Warsaw 18-21 Settembre 2023 https://www.european-mrs.com/meetings/2023-fall-meeting
- **43 Invited talk** *"Novel materials for energy applications: insight by ab-initio ground and excited state simulations*" Nanoscience & Nanotechnology conference Maggio 29, 2023 al 1 Giugno, 2023 LNF (Frascati), Italia https://agenda.infn.it/event/34629/
- **42 Invited lecture** *"The Bethe-Salpeter equation: derivations and main physical concepts"* at the international YAMBO school "Ab initio many-body perturbation theory: from equilibrium to time-resolved spectroscopies and nonlinear optics" Roma Maggio 22-26 2023 https://www.yambo-code.eu/2023/02/18/yambo-school-2023/
- **41 Invited talk** "*Excited State Properties of Low-Dimensional Materials: Insight By Ab-Initio DFT + Mbpt Simulations*" al Simposio D06" Quantum Dot Science and Technology" del 242nd ECS Meeting 9-13 october 2022 https://www.electrochem.org/242
- **40 Invited talk** "*Novel materials for energy applications: insight by ab-initio ground and excited state simulations***"** del Simposio "Materials for Energy" Psi-k 2022 Conference in Lausanne (Switzerland) https://www.psik2022.net/, Agosto 21-25 2022
- **39 Invited talk** "*Excitons in 2D/Layered Materials by DFT plus MBPT Methods*" al Simposio "The Rise of Low Dimensionality Materials: Opportunities and Challenges from Cutting-Edge Computational Investigations" of the PACS22 conference 27-29 Giugno 2022 https://pasc22.pasc-conference.org/program/minisymposia/

- **38 Invited talk** IEEE Nano 2021 online conference 28 Luglio 2021 "*Novel 2D/layered materials for energy applications: insight by ab-initio ground and excited-state methods"* https://2021.ieeenano.org/speakers/
- **37 Invited talk** *Novel Materials for energy applications: insight by ab-initio ground and excited state methods* Sezione 2 - Congresso SIF 14-18 Settembre 2020 https://www.sif.it/attivita/congresso/106
- **36 Invited talk** *"Role of Quasi-particle and excitons in 3D and 2D halide perovskites"* al Simposio "Theory and Computation of Halide Perovskites" (ComPer) of NanoGe online conference 8-9 Settembre 2020 (https://www.nanoge.org/ComPer/home)
- **35 Invited talk** *Quasi-particle and excitons with Yambo* Max Webinar 16-Giugno 2020 http://www.max-centre.eu/events/max-webinar-yambo-code

- 34 Invited talk Symposium “2D-materials for energy applications” EMRS Spring Conference, Strasbourg (France) 25-28 May 2020 Prof. Rajeev Ahuja (rinunciato per motivi personali)
- **33 Invited Lecture** “The Bethe-Salpeter Equation for optical properties of materials: common approximation and practical implementations” & “Hands-on Tutorial on BSE and the yambo code”, ICTP Yambo-School 2020 27-31 January 2020 http://indico.ictp.it/event/9018/
- **32 Invited seminar** “*Opto-electronic properties of novel 2D materials from DFT + post-DFT methods*”, ICQMS Università di Shanghai 5 Giugno 2019
- **31 Invited seminar** “*Novel 2D materials for opto-electronic applications: insight from refined ab-initio simulations*” Università di Paris-Sud Orsay 4 Marzo 2019 https://www.lps.u-psud.fr/spip.php?article3257&lang=fr
- **30 Keynote Invited talk** “*Fundamental properties of materials from ab-initio methods*" Nanoscience and Nanodevices Frascati 18-20 Dicembre 2018 https://agenda.infn.it/event/17167/timetable/?print=1&view=nicecompact
- **29 Invited talk** '*Novel 2D materials for opto-electronic applications: insight from parameter-free quantum mechanical methods*' 10-12/9/18, NanoMaterials for Devices Montreal, Canada http://nanomaterialsfordevices.ism.cnr.it/
- **28 Invited talk** '*Novel 2D materials for opto-electronic applications: insight from parameter-free quantum mechanical methods*' 11-14/9/18 NanoInnovation2018, Rome Italy 2019 https://www.nanoinnovation.eu/2018/pdf/Programme_NanoInnovation_2018.pdf
- **27 Invited talk** '*Transition Metal Dichalcogenides: a new class of 2D materials for opto-electronics*' 2/3/18 MIFP march meeting Marino Italy https://www.mifp.eu/images/stories/events/meetings/mifp2018/mifp-mm-2018.pdf
- **26 Invited seminar** '*2D Transition Metal Dichalcogenides: fundamental properties and applications*' 23/2/18 Dipartimento di Chimica Università di Perugia https://www.clhyo.org/scientific-events/seminars.html
- **25 Invited talk** '*MoS2 and its family: fundamental properties and applications*' Osi12 26-29 Giugno2017 Dublino http://osi12conference.com/
- **24 Invited lecture** '*Ab-initio optical properties of materials: BSE usual approximations and practical implementation*' Cecam school Lausanne 24-28 Aprile 2017 https://psi-k.net/advanced-computing-excited-state-properties-solids-nanostructures-yambo-cecam-hq-24-28-april-2017/
- **23 Invited talk** "*Fundamental properties of Transition Metal Dichalcogenides:a novel class of 2D materials for opto-electronic applications*" Nanoscience and Nanotechnology meeting 2016 26-29 Settembre 2016 https://agenda.infn.it/event/11337/sessions/1330/#20160926
- **22 Invited talk** "*Transition Metal Dichalcogenides: 2D materials for next generation opto-electronic devices*" Fall Meeting EMRS 2016 Settembre 18-22 2016 http://www.european-mrs.com/carbon-and-materials-energy-applications-emrs
- **21 Invited lecture** on *how to use the code YAMBO for GW and BSE calculations* Dept of Applied Physics Caltech Univ. Pasadena USA , 1 Agosto 2016 dal 01-08-2016 al 01-08-2016
- **20 Invited Lecture** *"Theoretical lesson on the GW approach"* Dept of Applied Physics Caltech Pasadena USA, 4 Agosto 2016
- **19 Invited seminar** *"Transition Metal Dichalcogenides: a novel class of 2D materials"* Dipartimento di Fisica Università di Cagliari 21/06/2016
- **18 Invited seminar** *"Two-dimensional Transition Metal Dichalcogenides for opto-electronics"* Dept of Chemistry, Univ. Tokyo 8 Marzo 2016
- **17 Invited seminar** "*Transition metal dichalcogenides: a novel class of two-dimensional materials for opto-electronics"* ICN2, Istitut Catala' de Nanocienca i Nanotecnlogia, Barcelona 21/1/2016
- **16 Invited Lecture** "'*Ab-initio optical properties of materials: BSE usual approximations and practical implementation*'" & “Hands-on Tutorial on BSE calculations with the YAMBO code” 13-17 Aprile 2015 Cecam Lausanne https://psi-k.net/psi-k-workshops-2015/
- **15 Invited talk** '*Light absorption and exciton radiative lifetimes in two-dimensional transition metal dichalcogenides*' Nanoscience and Nanotechnology 2015 INFN Frascati 28 Sept-2 Oct 2015 http://www.lnf.infn.it/conference/nn2015/
- **14 Invited Lecture** *"Optical absorption and the Bethe-Salpeter Approach"* & “Hands-on Tutorial on Excited State Spectroscopy: GW and BSE using the Yambo code" Roma 7-9 May 2014

- **13 Invited talk** '*Novel layered Materials for solar harvesting applications'*, EMRS-2014 Fall Meeting Warsaw 15-19 Settembre 2014 https://www.european-mrs.com/2014-fall-symposium-european-materials-research-society
- **12 Invited talk** '*Two-Dimensional Materials for ultrathin optoelectronic devices*', ETSF Meeting Luxemburg 1-4 Ottobre 2013 www.etsf.eu
- **11 Invited talk** "*Novel nanoscale materials for optoelectronic and Solar Energy Harvesting applications*" NanoCenter Annual Conference 2013, Royal Rimonim Dead Sea Hotel Aprile 3-4 2013
- **10 Invited talk** "*Monolayer materials for tunable polymer-free excitonic solar cells*", Crystal & Graphene Science Symposium-2012 Waltham, 5-6 Settembre 2012 http://www.expressgenes.com/crystalss2012/main.html
- **9 Invited talk** "*Silicon and Germanium nanostructures for opto-electronic and photo-voltaic applications: ab-initio results*", Symposium Group IV Semiconductor Nanostructures and Applications "MRS Fall Meeting" Boston, 29 Novembre-3 Dicembre 2010 https://www.mrs.org/fall2010
- **8 Invited talk** "*Materials for opto-electronic applications: ab-initio calculations and modelling*", "Nanoscience and Nanotechnology workshop N&N2010" INFN, Frascati 20-23 September 2010 http://www.lnf.infn.it/conference/nn2010/
- **7 Invited talk** "*Quasi-particles and excitons in Silicon Nanowires: effect of Doping and Surface Termination and mixing*" OSI-VIII 7-11 September 2009 Ischia http://osi8.roma2.infn.it/
- **6 Invited talk** "*Quasi-particles and excitons in Silicon Nanowires: effect of Doping and Surface Termination*" Cecam Workshop 6-8 July 2009 Lausanne www.cecam.org
- **5 Keynote Invited talk** "*Electronic properties and dielectric response of semiconducting surfaces and nanostructures from ab-initio approaches*" Nanosea2008 7-10 July 2008 Monte Porzio Catone, Rome Italy http://nanosea.roma2.infn.it/2008/programme/programme-full.pdf
- **4 Invited talk** "*Semiconducting nanowires: from one-particle to many-body approaches*" Cecam-Psi-K Workshop 9-12 June 2008 Lyon France https://psi-k.net/psi-k-workshops-2008/
- **3 Invited talk** "*First-principles optical spectra of semiconducting surfaces and nanowires: the role of the excitonic effects*", 12th Nanoquanta Workshop 18-22 September (2007), Aussois France http://etsf.grenoble.cnrs.fr/events/nanoquanta-workshop07/
- **2 Invited talk** "*Semiconductor nanowires: ab-initio electronic and optical properties beyond the one-particle approach*", OSI 2005, Aalborg, Denmark 6-10 June, (2005) https://vbn.aau.dk/en/activities/conference-on-optics-of-surfaces-and-interfaces-osi-vi-2
- **1 Invited talk** "*First--principles optical spectra of semiconductor surfaces: from one-particle to many-body approach*", Epioptics-7 20-26 July 2002 http://www.ccsem.infn.it/ccsem2002/Cricenti2002.html

Orals (20):

- **20 Talk** *Electronic and Optical Properties of Novel 2D/Layered Materials by Parameter Quantum-Mechanical Ground and Excited State Methods* MRS Fall Meeting 1-6 December 2024 Boston https://www.mrs.org/meetings-events/annual-meetings/2024-mrs-fall-meeting
- **19 Talk** *"Strongly-bound excitons in Organic-inorganic 2D Perovskites: a DFT + post-DFT study"* Materials.it 2018 Bologna, 22-28 October 208
- **18 Talk "**Strongly bound excitons in organic-inorganic 2d perovskites : a dft+ mbpt study" Symposium A3 IMRC 2018 Cancun Mexico August 2018
- **17 Talk** *"Excitons at the (001) surface and nanosheets of anatase TiO2 : optical signatures and spatial behavior" OSI-IX* "Akumal, Mexico 19-23 September 2011
- **16 Talk** *"Excitonic Behavior in 2-D TiO2 Anatase Systems: A First-principles Investigation",* "MRS Fall Meeting" Boston, 29 November-3 December 2010
- **15 Talk** *"Excitons in pure and doped Silicon Nanowires: a first principle study"*, E-MRS Symposium K of the E-MRS Spring Meeting, 12-06-2009 Strasbourg 8-12 June 2009 , France

- **14 Talk** *"Doping and Codoping in Silicon Nanowires"*, CMD-22 The 22nd General Conference of the Condensed Matter Division of the European Physical Society, 25-29 August 2008 , Rome Italy
- **13 Talk** *"Energy Loss Spectra of nanowires, nanotubes and nanolayers of Silicon:an ab-initio study",* "Nanosea 2006" Aix-en-Provence, 2-7 July 2006
- **12. Talk** "*Dielectric Response of clean and covered surfaces from first-principles approaches"*, Congresso INFM Genova 8-10 June 2004
- **11 Talk** *"Many-body effects on the optical properties of the (100) Diamond and Silicon surface",* Nanophase workshop, Lyon (France) , October 12-13 2001
- **10 Talk** *"Ab-initio calculation of SHG at Si(100) surface",* 25th ANNUAL MEETING: ADVANCES IN SURFACE AND INTERFACE PHYSICS" MODENA (ITALY), December 18-19, 2000.
- **9 Talk** *"Calculations of the spectroscopic properties of real materials"*, Workshop "Modelling through Numerical Simulations" Roma, `Tor Vergata' 17 - 18 January 2000
- **8 Talk** *"Optical properties of Germanium nanocrystals"*, SIO'99 St. Maxime , France, May 4-8 1999
- **7 Talk** *"Ab-initio calculation of the linear and non linear optical properties of the Si(100) surface",* XXIII Annual meeting Advances in Surfaces and Interfaces Physics, Modena, December 21-22 1998
- **6 Talk** *"Calculation of the dielectric function of Si beyond the Local Density Approximation",* II congresso Nazionale dell'INFM , Rimini 25-30 June 1998
- **5 Talk** *"Electronic properties of semiconductors and insulators: computing the behaviour of complex systems",* Lione Francia, September 1994
- **4 Talk** *"First-principles calculation of the self-energy corrections to the bandstructure of cubic GaN"*, XVII Annual Meeting, Advances in Surface and Interface Trieste
- **3 Talk** *"Self energy corrections for excited states and localized states"*, European Community Workshop, Parigi, Francia, Settembre 1992
- **2 Talk** *"Calcolo ab-initio con pseudopotenziali a norma consrvata delle proprietà di stato fondamentale e di stato eccitato del GaN"*, Wide-Band-Gap Semiconductors" Trieste, June 1992
- **1 Talk** *"Studio dei livelli VUV di eccitazione del Cr3+ in un cristallo di Na3In2Li3F12"*, Congresso SIF Trento 8-13 October 1990

Outreach seminars/articles/interviews (19):

- **19. Article** "Le infinite possibilità della scienza dei Materiali" articolo divulgativo apparso sul numero "Infinito" della collana Uninews dell' Università di Roma Tor Vergata 2024 https://online.flippingbook.com/view/282293380/15/
- **18.** Seminar "Dal liceo classico alla carriera accademica in Fisica della Materia" STEM al femminile ispirazione e percorsi di donne nella scienza 4 Febbraio 2025 Macroarea Scienze Univ. di Roma Tor Vergata
- **17.** Seminar "La scienza dei materiali all' università di Roma Tor Vergata" Giornata Orientamento Liceo F. D'Assisi Roma 11-12-2024
- **16** Seminar "L' invisibile bellezza della materia alla scala atomica: dal sogno di Feynman ai nuovi materiali del futuro, Dipartimento di Fisica Roma Tor Vergata 17-5-2024
- **15.** Seminar "From physics to materials science: The extraordinary world of materials" Euromath & Eurosciences Università di Roma Tor Vergata 14/3/2024
- **14.** Seminar "La scienza dei materiali all' università di Roma Tor Vergata" Evento organizzato dal Liceo M.T. Cicerone Frascati 24/2/2024
- **13.** Seminar "La scienza dei materiali all' università di Roma Tor Vergata" Evento iniziale Lab2go 2023-2024 18/12/2023
- **12.** Seminar " Lo straordinario mondo dei materiali", 24 Settembre 2021 durante l'evento "Notte Europea dei Ricercatori" (zoom platform)
- **11.** Seminar " La scienza dei Materiali" Liceo Scientifico Touschek 15/12/2020 Grottaferrata (zoom platform)

- **10.** Seminar “Fisica della materia: dal macro al nanomondo” 9/4/19 Pizza Seminars Univ. Tor Vergata
- **8.** “Alla scoperta del nanomondo” 27/02/2019 Scienza Orienta Univ. Tor Vergata
- **7.** Seminar “La scienza dei materiali” Liceo Classico-Linguistico Cicerone 31/1/2019 Frascati
- **6.** Interview on research activities appeared on the annual report of European PRACE-HPC Initiative 2018 https://prace-ri.eu/wp-content/uploads/2019/08/PraceAnnualReport2018.pdf
- **5.** Seminar “La scienza dei materiali” Liceo Scientifico Cartesio 10/3/2017 Olevano Romano
- **4.** Seminar “La scienza dei materiali” Liceo Classico Seneca 9/2/2016 Roma
- **3.** Seminar “La scienza dei materiali” Liceo Scientifico Touschek 27/10/2015 Grottaferrata
- **2.** Seminar “La scienza dei materiali” Liceo Scientifico Pietro Bono 10/12/2015 Alatri
- **1.** Seminar “La scienza dei materiali” Liceo Classico Plauto 7/5/2015 Roma

Awards, Fellowships, Visiting Positions, and Committee Memberships

Professional Recognitions:

- Member of the Psi-k Working Group C6 (Nanoscale Structures) since June 2024
- Selected in the list of the World’s Top 2% Scientists by Stanford University 2023 https://ecebm.com/2023/10/04/stanford-university-names-worlds-top-2-scientists-2023
- National Scientific Qualification as Full Professor (first level), application no. 62439 (2018, valid until 2028) – Call D.D. 1532/2016, sector 02/B2 Theoretical Physics of Matter
- Winner of the MIUR Prize "Funding for basic research activities" as Associate Professor (2017)
- Principal Investigator and winner of a European PRACE-H2020 project (Call XVI)
- Awarded an Endeavour Research Fellowship from the Australian Government (2017, 4 months) for research on 2D materials in Australia (declined for personal reasons)
- Visiting scientist at Laboratoire Physique des Interactions Ioniques et Moléculaires (PIIM), Aix-Marseille University, group of Dr. Elena Cannuccia, 2–16 September 2023 (funded by the host institution)
- Visiting scientist at CNRS-Orsay, group of Dr. A. Zobelli, Paris Sud University, 11–23 March 2023 (funded by the host group)
- Awarded a CNRS grant for research at Orsay-Paris Sud, 15 June–3 July 2020 (not used due to COVID)
- Visiting scientist at ICQMS Group, Prof. W. Ren, Shanghai University, 2–8 June 2019 (funded by the host group)
- Visiting scientist at CNRS-Orsay, group of Dr. A. Zobelli, Paris Sud University, 4–8 March 2019 (funded by the host group)
- Visiting scientist at the Department of Applied Physics, Caltech, group of Prof. M. Bernardi, 9 July – 5 August 2017 (funded by the host group)
- Visiting scientist at the Department of Applied Physics, Caltech, group of Prof. M. Bernardi, 13 July – 13 August 2016 (funded by the host group)
- Visiting scientist at the Department of Chemistry, University of Tokyo, group of Prof. K. Yamashita, 1–11 March 2016 (funded by the host group)
- Visiting scientist at the Department of Materials Science, MIT, group of Prof. J.C. Grossman: Summer 2012 (official 3-month MIT contract), January 2013, July 2014, March 2015, July 2018 (all funded by the host group)

Doctoral Jury and Evaluation Activities:

- International referee and jury member for the PhD thesis of Dr. Elisa Serrano, Université Paris Saclay, France, 19 November 2024
- International opponent and jury member for the PhD defence of Dr. Mikkel Sauer, Department of Materials and Production, Aalborg University, 9 October 2023
- Member of the HDR (Habilitation à Diriger des Recherches) committee for Dr. George (Yorgos) Volonakis, Rennes, 22 May 2023

- Jury member for the PhD defence of Dr. A.R. Kshirsagar, Université Grenoble-Alpes, France, 24 March 2021
- International opponent and jury member for the PhD thesis of Dr. Arnaud Lorin, École Polytechnique, Palaiseau, France, 17 December 2020
- External referee for the PhD thesis of Dr. Felice Conte, University of Naples Federico II, October 2021
- External referee for the PhD thesis of Dr. Paola Mocci, University of Cagliari, 2019
- External referee for the PhD thesis of Dr. M. Atambo, University of Modena and Reggio Emilia, 2018
- International opponent and jury member for the PhD defence of candidate E. Bostrom, Faculty of Science, Lund University, Sweden, 4–6 June 2017
- External referee for the PhD thesis of Dr. Roberto Cardia, University of Cagliari, 2016
- International opponent and external jury member for the PhD defence of Dr. Leonardo Espinosa, San Sebastián, Spain, 22 October 2013
- International referee for the PhD thesis of Dr. Matteo Govoni, École Polytechnique, Palaiseau, France (2012)
- External advisor for the PhD thesis of Dr. F. Iori, University of Modena and Reggio Emilia (2008)

Academic Committees and Selection Panels:

- Member of the Doctoral Board in Physics at UTOV, 30 September 2011 – 31 December 2013
- Member of the Doctoral Board in Physics at UTOV since 2017
- Member of the Excellence Pathway Selection Committee for the Bachelor's and Master's Degrees in Physics at UTOV, 2020 – present
- Member of the final examination committee for the PhD in "Physics and Nanoscience" at the University of Modena: 2021 (28 October), 2020 (13 January and 4 September), 2019 (18 February and 29 August), 2018 (18 February), 2015 (3 February)
- Member of the admission exam committee for the PhD in "Mathematical Models for Engineering, Electromagnetism and Nanoscience", University of Rome La Sapienza, 6 October 2014

National Academic Recruitment Committees:

- Member of the national selection committee for a Researcher (RTT) at the Department of Physical and Chemical Sciences, University of L'Aquila (PHYS-04, Rectoral Decree 40/2025)
- Member of the national selection committee for a Researcher (RTT) at the Department of Engineering, University of Modena and Reggio Emilia (02/B2, Rectoral Decree 378/2024, 29 April 2024)
- Member of the national selection committee for a Researcher (RTDA) at the Department of Physics, University of Padua (02/B2, Rectoral Decree 4530, 28 October 2022)
- Member of the national selection committee for a Researcher (RTDB), University of Milan (02/B2, Official Gazette No. 17, 1 March 2022, no. 4956/2022)
- Member of the national selection committee for a Researcher (RTDA), Department of Physics, University of Milan (02/B2, no. 4042, Official Gazette No. 51, 28 June 2019)
- Member of the national selection committee for two RTDB positions, Politecnico di Milano (02/B1, no. 2018/RTDB_PS_FIS14)
- Member of the national selection committee for an RTDB position, University of Milan (02/B2, Rectoral Decree 1875/2018, no. 3761/2018)

Highlighted Research Featured Online:

- Research on the excitonic insulator WTe_2 featured on CNR NANO website
- Research on MoS_2-T' excitonic and topological order featured on CNR NANO website
- Research on excitons in anatase bulk and nanocrystals (Nat. Commun. 2017) featured in:
  - Phys.org, AzoNano, IDW Online
- Research on ultrathin photovoltaics based on monolayer materials (Nano Letters 2013), featured in:
  - MIT homepage, Materials360Online, Optics.org
  - Various websites on photonics, climate change, Breaking Energy
  - Interview featured on the Huffington Post (28 June 2013)
- Research on Si/Ge nanowires for photovoltaic applications featured on Lobby Innovazione

- Various publications selected for the Virtual Journal of Nanoscale Science & Technology

Organization and Scientific Management

International Conferences, Workshops, and School Organization

- **Co-organizer** of the symposium *"2D Heterostructures: electronic structure and spectroscopic response, from theory to experiment"* at FISMAT2025, Venice, 7–11 July 2025. https://eventi.cnism.it/fismat2025/thematic-workshop
- **Co-chair** of two scientific sessions at the conference *"Nanoscience & Nanotechnology"*, INFN-LNF Frascati, 15–19 October 2019. https://agenda.infn.it/event/19925/timetable/#20191015
- **Co-chair** of the scientific symposium A4 at the international conference *IMRC2018*, Cancún, Mexico. http://www.mrs-mexico.org.mx/imrc2018/symposium-A4
- **Local organizer** of the international Psi-k workshop *"OPTEL2D: 2D materials from a theoretical and computational perspective"*, Rome, 18–19 December 2017. https://psi-k.net/scientific-report-psi-k-workshop-2d-layered-materials-opto-electronics-theoretical-computational-perspective
- **Co-local organizer** of the ETSF workshop *"Electron-Vibrational Coupling"*, Rome, 15–16 January 2015. http://www.yambo-code.org
- **Co-organizer** of the international workshop *"40 Years of the GW Approximation for the Electronic Self Energy: Achievements and Challenges"*, Bad Honnef, Germany, 2005. http://www.etsf.eu
- **Organizing committee member and local organizer** of the international conference *"Theory and Modeling of Electronic Excitations in Nanoscience"*, Acquafredda di Maratea, Italy, 2004. http://www.etsf.eu
- **Organizing committee member** of the international conference *"Ab initio Electron-Excitations Theory: Towards Systems of Biological Interest (BIOEXC)"*, San Sebastián, Spain, 2003. http://www.etsf.eu
- **Organizing committee member** of the international conference *"Ab initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials"*, Lyon, France, CECAM, 2002. http://www.etsf.eu
- **Organizer/committee member** of four international workshops on nanowires:
  - NW2010: http://www.iesl.forth.gr/conferences/nw2010/default.html
  - NW2011: http://www.iesl.forth.gr/conferences/nw2011/default.html
  - NW2012: http://www.pdi-berlin.de/nanowires-2012
  - CECAM 2013: https://www.cecam.eu/workshop-details/598
- **Co-organizer** of several international Yambo schools (2014–2025) on many-body perturbation theory and the use of the Yambo code:
  - Yambo School 2025 (Modena)
  - Yambo School 2023 (lRome, local organizer)
  - Yambo Schools 2022 (ICTP/Max), 2021 (CECAM/Max, online), 2020 (ICTP/Psi-k/Max)
  - Yambo Schools 2017, 2015 (Psi-k/CECAM), 2014 (Psi-k/Cast Cineca) http://www.yambo-code.eu
- **Co-organizer** of the symposium *"Optical Properties of Materials"* at the international conference ICSFS16, Genoa, 1–6 July 2012.

Research Project Coordination and Participation

Since 2001, I have participated in the drafting of numerous national, European, and bilateral scientific projects (and carried out/coordinated research activities in the funded ones), both as a member of the Rome node and as Principal Investigator (PI).
In particular, in the last 15 years:

- **Japan–Italy HANAMI** Project (participant, HORIZON-EUROHPC-JU-2022-INCO-04)
- PLUTO Italy–Turkey High Relevance Project (PI of Italian node, submitted Nov 2024)
- **PRIN2022 IRIDE** (scientific collaborator, funded)
- **EcoE-III HORIZON-EUROHPC-JU-2023-COE-01** (WP leader funded, WP2 Materials, €5.998.787)
- **Spoke 6 – Multiscale Modelling** (WP leader, funded with a 2-year post-doc)
- **TIMES** Doctoral Network (WP leader, funded, starting 03/2024)
- PRIN-PNRR LEGOS (local PI, evaluated 94/100, not funded, first excluded)
- Bilateral project Italy–USA PGR11276 (member, PI D. Sangalli, not funded)
- PRIN2022 HEROES (local PI, evaluated 93/100, funded after re-evaluation in 2024)
- **Japan–Italy NEDO project** (PI of Italian node, funded, 2021–2024)
- PRIN2020 ARCHITECTURING (local PI, evaluated 90.3/100, not funded)
- **NATO** project on wearable solar cells (member, funded €273K)
- **Lazio Region project "High mobility 2D polymers"** (local PI, funded €150K, 2021–2023)
- **INFN TIME2QUEST** (member, funded)
- **ANR France BONASPES** (Partner scientific leader, funded €480K, 2020–2024)
- **Beyond Borders project,** Univ. Roma Tor Vergata (co-PI, funded €5K)
- **Mission Sustainability project**, Univ. Roma Tor Vergata (PI, funded €21K, 2018–2019)
- Uncovering Excellence project, Univ. Roma Tor Vergata (member, not funded)
- **INFN NEMESYS** project (member, funded, 2017–2020)
- Two bilateral MIT–MISTI projects 2016–2017 (PI of one node, not funded)
- PRIN2017 (local PI, well evaluated, not funded)
- PRIN2015 (national PI, well evaluated 12/15, not funded)
- PRIN2012 (local PI, well evaluated, not funded)
- Bilateral project PGR01381 Italy–USA (co-PI with G. Cicero, not funded)
- Galileo bilateral projects 2013/2015 (co-PI, not funded)
- Samsung GRO 2015 (PI of one node, not funded)
- **Psi-k grant 2DOPT** workshop Rome 2017 (PI, funded €3K)
- **Psi-k/Max & ICTP grant** Yambo School 2020 (co-PI, funded €9.2K)
- **Psi-k grant GW/BSE** tutorial 2014 (co-PI, funded €6K)
- **CECAM/ESF grant** SiGe workshop 2013 (co-PI, funded €18K)
- **H2020-MSCA-RISE DiSeTCom** (member, funded, €690K)
- H2020-MSCA-RISE OPTMAT (member, not funded)
- **H2020-MSCA-RISE COEXAN** (member, funded, €1M)
- **H2020-FETPROACT-2016-20** (member, funded)
- FP7-NMP-2011 ZnO nanostructures (local PI, not funded, well evaluated, first among excluded)
- FP-NMP.2001 Photovoltaics project (member, not funded)
- FIRB RBFR129YPH004 (member, not funded, well evaluated, first among excluded) (member, not funded, well evaluated, first among excluded)

Earlier funded contributions (pre-2010): PRIN2002, PRIN2005, PRIN2007, INNESCO (2003–2005), EU projects Nanophase, Nanoquanta, I3-ETSF; 4 FSE/Psi-k grants (co-organizer of ETSF conferences).

HPC Projects (PI, Co-PI, and Staff Roles)

Over the last 15 years, I have served as PI (7 projects) or Co-PI/staff member (8 projects) in various national and European HPC projects, including several PRACE allocations, selected through competitive, peer-reviewed processes. (1 million core-hours is equivalent to approx. €6.25k, according to Cineca).

As Principal Investigator (PI):

- **ISCRA-B "Strano"** – Strain modulation of the electronic and optical properties of vdW hetero-structures (200k core-hours on M100, 2022)
- **ISCRA-B "Dieci2D"** – Direct and indirect excitons in chalcogen-based 2D materials: a DFT+MBPT study (HP10BKKCCV, 720k core-hours on M100, 2020)
- **PRACE-H2020 "optel2d"** – Optoelectronic properties of 2D TMDCs using DFT and post-DFT (49 million core-hours on Marconi-KNL, equivalent to €306k, 2018)
- **ISCRA-B "EXSEM2D"** – Excitons in 2D semiconductors via advanced ab-initio methods (10 million core-hours on Marconi, 2019, equivalent to €62.5k)
- **ISCRA-B "NWPOLY"** – Polytypism in III-V and IV nanowires (650k core-hours on Fermi, 2015)
- **ISCRA-B "Ex-natio"** – Excited-state properties of TiO_2 nanostructures (HP10BUJ6VJ, 650k core-hours on Fermi, 2011)
- **ISCRA-B "OPSANN"** – Optoelectronic properties of SiGe nanocrystals and nanowires (HP10B2DDQJ, 136k core-hours on SP6, 2010)

As Co-PI or staff member:

- ISCRA-B "P2DFET" (HP10BAE9TU, 444.8k standard core-hours on Leonardo)
- ISCRA-B "Symmetry and Optoelectronics in 2D Hybrid Organic-Inorganic Halide Perovskites" (50k node-hours on M100)
- PRACE-H2020 "Extend" – Excitonic instability in 2D WTe_2 (45 million core-hours on Marconi2, 2019)
- ISCRA-B "PiBifree" (HP10BEBZU4, 1.5 million CPU-hours on Marconi2, 2019)
- ISCRA-B "2D-OIHPs" – Analysis of hybrid 2D perovskites and composites (HP10BGUJ6X, 4 million core-hours on Marconi, 2018)
- ISCRA-B "SPERE" – Single-photon emission from defects in 2D materials (HP10BBZNPY, 1.5 million CPU-hours on Marconi2, 2020)
- PRACE "Ancient_Rome" – Many-body excitations in defective TiO_2 materials (30 million core-hours on Marconi2, 2019)
- PRACE-DECI-7-FP7 "DIAVIB" – Electron-phonon coupling in diamond nanocages (2011)
- PRACE-DECI-6-FP7 – Optical properties of group IV nanocrystals via MBPT (2010)
- ISCRA-B "Silicon Interfaces" (HP10B4SQA4, atomistic simulations of nanostructured Si interfaces, 2013)

Departmental Roles and Responsibilities

- Since 3 March 2023, elected Coordinator of the Bachelor's and Master's Degree Programs in Materials Science at the University of Rome Tor Vergata
- Member (2017–2019) of the restricted teaching committee for the Bachelor's Degree in Physics at the University of Rome Tor Vergata
- Member of the evaluation committee for students enrolled in the "Excellence Pathway" of the Bachelor's and Master's Degree Programs in Physics at the University of Rome Tor Vergata
- Member of the restricted teaching committee for the Degree Program in Materials Science at the University of Rome Tor Vergata

- Member of the PhD Board in Physics at the University of Rome Tor Vergata (2011–2013 and since 01/03/2017)
- Responsible for the Materials Science and Technology area of the degree program website and its social media channels (Facebook, Instagram, LinkedIn, TikTok)
- Responsible for organizing the Materials Science seminar series at the Department of Physics, University of Rome Tor Vergata

Teaching Experience

Theses Supervision (Bachelor's, Master's, and PhD):

- Simone Grillo – PhD in Physics, 2021–2024 (co-supervisor), *"Ground-State and Many-Body Properties of Low-Dimensional Materials"*, defense: 21 January 2025
- Andrea Sette – MSc in Materials Science, *"An ab initio study: electronic and optical properties of N-heterocyclic carbenes"*, 26 May 2022 (supervisor)
- Stefano Lista – BSc in Physics, *"Ab-initio simulations of a novel 2D polymer with Dirac cones and linear dispersion"*, 18 December 2021 (supervisor)
- Alessandro Moreci – BSc in Physics, *"First-principles simulations of pure and doped graphitic carbon nitride"*, 26 February 2021 (supervisor)
- Sara Postorino – PhD in Physics (Cycle XXXIV), *"Electronic and Excitonic Properties of Two-Dimensional Chalcogen-based Materials by Ab-initio Ground and Excited State Methods"*, 2018–2022 (supervisor)
- Simone Brozzesi – MSc in Materials Science, 2019–2020 (co-supervisor)
- Alessandro Graziani – MSc in Physics, 2018–2019 (co-supervisor)
- Simone Grillo – BSc in Physics, 2017–2018 (co-supervisor)
- Sara Postorino – MSc in Physics, 2017–2018 (supervisor)
- Riccardo De Gennaro – MSc in Physics, 2016–2017 (supervisor)
- Antonio D'Auria – MSc in Physics, 2015–2016 (supervisor)
- Giovanni Bellucci – MSc in Materials Science, 2015–2016 (supervisor)
- Emanuele Tomo – BSc in Physics, 2011–2012 (supervisor)
- Paolo Bagalà – MSc in Physics, 2008–2009 (co-supervisor)
- Michele Amato – PhD in Nanoscience, University of Modena and Reggio Emilia, 2009–2010 (co-supervisor)
- Mauro Bruno – PhD in Physics, University of Rome Tor Vergata, 2007–2008 (co-supervisor)

Teaching Activities:

- Since 2023: Lecturer of the course *2D Materials* (MSc in Materials Science, 6 ECTS, 3 co-taught)
- Since 2010: Lecturer of the course *Structure of Matter 2* (MSc in Physics, University of Rome Tor Vergata, 6 ECTS)
- 2012–2022: Lecturer of the course *Solid-State Theory and Molecular Models* (MSc in Materials Science, 4 ECTS)
- 2012–2021: Guest Lecturer, course *Quantum Theory of Solids* – Prof. O. Pulci (approx. 16 hours total, MSc in Physics)
- Academic Years 2011–2013: Lecture Series *Introduction to Many-Body Perturbation Theory*, PhD in Physics (6 hours total)
- Academic Years 2004–2006: Lecturer of *Mathematical Methods for Materials Science* (BSc in Materials Science, 6 ECTS)
- 2002–2011: Co-lecturer of *Atomic and Molecular Physics* (Prof. Fanfoni) and *Structure of Matter* (BSc in Physics and Materials Science, approx. 20 hours)
- Academic Years 2000–2002: Co-lecturer of *Classical Physics for Biology* (BSc in Biology, approx. 16 hours)

FULL LIST OF SCIENTIFIC PUBLICATIONS

162) "*Optical absorption in hexagonal-diamond Si and Ge nanowires: insights from STEM-EELS experiments and ab initio theory"* Tizei, Luiz et al. Nano Letters 2025 **(IF =10.8)**

161) Giant Light Emission Enhancement in Strain-Engineered InSe/MS_2 (M = Mo or W) van der Waals Heterostructures E Blundo at al. Nano Letters 2025 **(IF =10.8**)

160) *Multiple Linear Dichroism Inversions in SnO Monolayers for Polarization-Sensitive UV Photodetection* Re Fiorentin, M. Risplendi, F. Palummo, M. Cicero, G. to appear on ACS Applied Nanomaterials 2025 **(IF=5.3)**

159) *Tunable second harmonic generation in 2D materials: comparison of different strategies* S Grillo, E Cannuccia, M Palummo, O Pulci, C Attaccalite SciPost Physics Core 7 (4), 081 (2024) (**IF=5.23**)

158) *Tellurene Polymorphs: A New Frontier for Solar Harvesting with Strong Exciton Anisotropy and High Optical Absorbance.* S. Grillo, S. Postorino, M. Palummo, O. Pulci 14, Issue 44 2400674 (2024) **(IF=24)**

157) *Theoretical study of two-dimensional materials for photocatalysis and photovoltaics* K Ren, JZ Liu, M Palummo, M Sun Frontiers in Chemistry 12, 1387236 (2024) (**IF=8.5**)

156) "*Electronic Transport Modulation in Ultra-strained Silicon Nanowire Devices*" Bartmann, Maximilian; Glassner, Sebastian; Sistani, Masiar; Rurali, Riccardo; **Palummo, Maurizia**; Cartoixa, Xavier; Smoliner, Jürgen; Lugstein, Alois submitted to ACS Applied Materials & Interfaces 2024 **(IF=9.5)**

155) "*On-surface Molecular Recognition driven by Chalcogen Bonding"* L. Camilli, C.Hogan, D. Romito,L. Persichetti, A. Caporale , **M. Palummo**, M. Di Giovannantonio, D. Bonifazi JACS Au (2024) **(IF=8)**

154) *"Mechanical properties of bilayer WS_2 and Graphene-WS_2 Hybrid composites by molecular dynamics simulations"* Fan Wu, Huifeng Tan, **Maurizia Palummo** and Luca Camilli *J. Phys.: Condens. Matter* **36** 225301 (2024) **(IF=2.7)**

153) "*Strain tunable interlayer and intralayer excitons in vertically stacked MoSe2/WSe2 heterobilayers"* LL Li, R Gillen, **M. Palummo,** MV Milošević, FM Peeters Applied Physics Letters 123 (3) (2023) **(IF=3.97)**

152) *Exciton ground state fine structure and excited states landscape in layered halide perovskites from combined BSE simulations and symmetry analysis* C Quarti, G Giorgi, C Katan, J Even, **M Palummo** Advanced Optical Materials (2023) **(IF=10.05)**

151) *Exploring the range of applicability of anisotropic optical detection in axially coordinated supramolecular structures* F Goto, A Calloni, I Majumdar, R Yivlialin, C Filoni, C Hogan**, M Palummo,** et al. Inorganica Chimica Acta, 121612 (2023) **(IF=3.11)**

150) *Excitonic absorption signatures of twisted bilayer by electron energy-loss spectroscopy* Steffi Y. Woo, Alberto Zobelli, Robert Schneider, Ashish Arora, Johann A. Preuß, Benjamin J. Carey, Steffen Michaelis de Vasconcellos, **Maurizia Palummo,** Rudolf Bratschitsch, and Luiz H. G. Tizei **Physical Review B 107 (15), 155429 (2023) (IF=3.9)**

149) *Band Structure and Exciton Dynamics in Quasi-2D Dodecylammonium Halide Perovskites*
G Ammirati, F Martelli, P O'Keeffe, S Turchini, A Paladini, **M Palummo,** et al
Advanced Optical Materials, 2201874 (2023) **(IF=10.05)**

148) *Two-dimensional single crystal monoclinic gallium telluride on silicon substrate via transformation of epitaxial hexagonal phase*
E Zallo, A Pianetti, AS Prikhodko, S Cecchi, YS Zaytseva, A Giuliani, M. Kremser, N. I. Borgardt, Jonathan J. Finley, F. Arciprete, **M. Palummo,** O. Pulci, R. Calarco npj 2D Materials and Applications 7 (1), 19 (2023) **(IF=11.44)**

147) *Study of Optoelectronic Features in Polar and Nonpolar Polymorphs of the Oxynitride Tin-Based Semiconductor InSnO2N*
M Palummo, M Re Fiorentin, K Yamashita, IE Castelli, G Giorgi
The Journal of Physical Chemistry Letters 14 (6), 1548-1555 (2023) **(IF=6.88)**

146) *Plurality of excitons in Ruddlesden–Popper metal halides and the role of the B-site metal cation*
G Folpini, **M Palummo** et al Materials Advances 4 (7), 1720-1730 (2023) **(IF=5.36)**

145) *Two-dimensional borocarbonitrides for photocatalysis and photovoltaics*
W Zhang, C Chai, Q Fan, Y Yang, M Sun, **M Palummo** et al Journal of Materials Chemistry C 11 (11), 3875-3884 (2022**) (IF=6.4)**

144) *Interlayer and Intralayer Excitons in AlN/WS2 Heterostructure*
C Attaccalite, MS Prete, **M Palummo,** O Pulci Materials 15 (23), 8318 (2022) (**IF=8.06)**

143) *Excitons and light-emission in semiconducting MoSi2X4 two-dimensional materials*
M Sun, M Re Fiorentin, U Schwingenschlögl, **M Palummo** npj 2D Materials and Applications 6 (1), 1-7 (2022) (**IF = 11.44)**

142) *Ab Initio Study of Graphene/hBN Van der Waals Heterostructures: Effect of Electric Field, Twist Angles and pn Doping on the Electronic Properties* S Brozzesi, C Attaccalite, F Buonocore, G Giorgi, **M Palummo**, O Pulci Nanomaterials 12 (12), 2118 (2022) **(IF=5.44)**

141) *Advances in two-dimensional green materials for organic electronics applications*
M Palummo, K Yamashita, G Giorgi *Sustainable Strategies in Organic Electronics, 391-422 (2022)*

140) *Photo-induced lattice distortion in 2H-MoTe 2 probed by time-resolved core level photoemission*
R Costantini, F Cilento, F Salvador, A Morgante, G Giorgi, **M Palummo**, Martina Dell'Angela
Faraday Discuss., 2022,236, 429-441 (**IF=4.08)**

139) *Evidence for equilibrium exciton condensation in monolayer WTe2*
B.Sun et al Nature Physics 18 (1), 94-99 (2022) (**IF = 20.034)**

138) *Strong out-of-plane excitons in 2D hybrid halide double perovskites*
M Palummo, S Postorino, C Borghesi, G Giorgi
Applied Physics Letters 119 (5), 051103 (2021) (**IF=4)**

137) *Boosted Solar Light Absorbance in PdS2/PtS2 Vertical Heterostructures for Ultrathin Photovoltaic Devices* L Bastonero, G Cicero, **M Palummo,** M Re Fiorentin
ACS applied materials & interfaces 13 (36), 43615-43621 (2021) **(IF=10.38)**

136) *Spinorial formulation of the GW-BSE equations and spin properties of excitons in 2D Transition Metal Dichalcogenides* Margherita Marsili, Alejandro Molinas Sanchez, **Maurizia Palummo**, Davide Sangalli, Andrea Marini, Phys. Rev. B 103, 155152 2021) **(IF=3.78)**

135) *First-principles exciton radiative lifetimes in monolayer graphitic carbon nitride*
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Final Declaration

I hereby declare that all information provided in this CV is truthful and accurate, pursuant to Articles 46 and 47 of the Presidential Decree no. 445 of 2000.
Rome, 15 May 2025
Signature