

## CV of Maurizia Palummo

### Education/Professional Experience:

**Present position:** associate professor at the Physics Department of University of Rome "Tor Vergata" (UTOV)

**2017-2004** Researcher at Physics Dept of UTOV

**2004-1999:** INFN Researcher at Physics Dept of UTOV

**1998-1996:** Post-doc at Physics Dept of UTOV

**1996-1995:** Post-doc at the ENEA Casaccia research center

**1995-1994:** INFN Post-doc at Physics Dept of UTOV

**1994-1991:** PhD fellow in Physics at UTOV

**December 1989:** "Laurea cum laude" in Physics at UTOV

### Scientific expertise:

After a stage in experimental Condensed Matter Physics on the optical properties of defects and color centers in insulator matrices, I am working for many years, in the field of first-principles calculations of the structural and electronic properties of materials. During the PhD thesis, I started to focus on ab-initio calculations, within the density functional theory and many-body perturbation theory, studying the electronic properties of bulk wide band-gap semiconducting compounds, including self-energy corrections. After 1996 I worked on the electronic, linear and nonlinear optical properties of several semiconducting and metal surfaces, clean or covered with atomic and molecular adsorbates. In particular I became expert of reflectance anisotropy and surface differential reflectivity spectra calculations. After 2005, my research activity focused on the first-principle study of the many-body effects of wide-gap and low-gap semiconductor surfaces and also on the dielectric response and electronic excitations of low dimensional systems like Ge and Si nanowires. In the last years two dimensional materials, organic compounds and materials for energy applications like perovskites, is the main of my research activity. Through my work, I earned expertise in computational physics and became familiar with the most modern theories and computational tools of first-principles electronic structure calculations (Car Parrinello, GW method, BSE exciton calculation, parallelization). I am member of the developers/superusers team of the many-body code yambo ([www.yambo-code.org](http://www.yambo-code.org)). A more detailed description of the main research topics of the last 10 years is given in the following:

**2020-2018** i) study of many-body effects of double perovskites and 2D layered hybrid perovskites ii) Development of an ab-initio approach to compute radiative lifetimes of 0D-to 3D materials iii) study of the excitonic instability of distorted tetragonal Transition Metal Dichalcogenides iv) characterization of the excitonic properties of 2D interfaces based on phosphorene

**2017-2014** i) study of many-body effects in layered hybrid halide-perovskites perovskites ii) Development of an ab-initio approach to compute radiative lifetimes of two-dimensional materials with a main focus on transition metal dichalcogenides 2D-TMD

iii) ab-initio electron-phonon non radiative lifetimes in oxide materials and 2D-TMD, iv) ab-initio study of polypitysm in group IV and III-V nanowires and its influence on the electronic and optical properties v) Excitons and their optical peaks in anatase bulk and nanosheets

**2013-2011** i) ground-state and excited state first-principles simulation of crystals and oligomers of porphyrines ii) spin-resolved GW calculations on dopant levels in Si-nanowires

iii) self-energy and excitonic effects in two-dimensional materials (TMD, Hybridized Carbon Boron Nitride, tio2-sheets) iv) photoconversion efficiency of 2D-TMD hetero-bilayers and TMD/graphene bilayers for ultra-thin excitonic solar cells by ab-initio DFT and MBPT simulations

### Main collaborations external to UTOV:

G. Giorgi (Univ. Perugia), K. Yamashita (Tokyo Univ.), D. Varsano (S3-CNR Modena), G. Cicero (PoliTO), M. Amato (Paris Sud), A. Zibelli (Paris Sud), J.C. Grossman (MIT), M. Bernardi (Caltech), D. Sangalli (CNR-ISM), A. Marini (ISM-CNR Rome), L. Chiodo (Campus Biomedico Roma), R. Rurali (ICMAB, Barcelona), S. Ossicini (Modena Univ.), A. Rubio (San Sebastian, Spain)

### Scientific Keywords:

ab-initio, DFT, GW, BSE, excitons, surfaces, interfaces, organic compounds, nanomaterials, photovoltaics

Investigation tools: ground and excited state ab-initio simulations: Plane-wave codes:

Quantum-espresso, ABINIT, VASP; Many-body codes: YAMBO, EXC, DP etc

Programming Languages: f90, script shell languages, python

**Scientific Impact** (Orcid <https://orcid.org/0000-0002-3097-8523>):

Author of more than 130 articles, most of them in international peer-reviewed journals, several book chapters and 3 review articles (see the full list at the end of this CV). 120 on scopus among them 1 Nat nanotechnology, 1 Nat Comm, 1 Chem Rev, 2 Advanced Functional Materials, 2 ACS nano, 1 ACS energy letter, 5 Nano Letters, 2 JPCL, 2 JPCC, 5 PRL, 2 JCP, 27 PRB; **Indices:** Total number of citations (scopus/ISI/scholar) : 3913/3.815/4829 (3606 without self-citations on ISI); h-index: 31 (scopus/ISI Web); 33 (Google Scholar)

### List of the 10 most relevant publications of the last 10 years:

*10 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)

*9 Optical Properties of Lead-Free Double Perovskites by Ab Initio Excited-State Methods* **M. Palummo**, Eduardo Berrios, Daniele Varsano, Giacomo Giorgi ACS Energy Letters 5,457 (2020)

*8 Nature of the Electronic and Optical Excitations of Ruddlesden-Popper Hybrid Organic-Inorganic Perovskites: The Role of the Many-Body Interactions* G Giorgi, K Yamashita, **M Palummo** The journal of physical chemistry letters 9 (19), 5891-5896 (2018)

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- 7 *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)
- 6 *Strongly bound excitons in anatase TiO<sub>2</sub> single crystals and nanoparticles* E. Baldini; L. Chiodo; A. Dominguez, **M. Palummo** et al. Nature Communications 8, 13 (2017)
- 5 *Optical emission in hexagonal SiGe nanowires* X Cartoixa, **M Palummo**, HIT Hauge, EPAM 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 materials* M Bernardi, **M Palummo**, JC Grossman Nano letters 13 (8), 3664-3670 (2013)

**International conferences/workshops/schools** : 7 posters, **19 orals** and **24 Invited talks** (of these two keynote talks, one talk at MRS-Fall and two talks at EMRS-Fall meetings), **12 invited seminars/lectures** at national and foreign institutions, **9 outreach seminars** for High School and Bachelor Degree students)

#### **Invited talks/seminars/lectures at National and International conferences/institutions/schools:**

- Invited talk Symposium "Materials for Energy" Psi-k Conference to be held in Lausanne (Switzerland) 14-17 September 2020 <https://www.psi2020.net/>, postponed to August 2022 for Covid
- Invited talk IEEE Nano 2020 sulla nanotecnologia a Montreal, 29-31 July 2020 (<https://2020.ieeenano.org/>) postponed to July 2021 for Covid
- Invited talk 8th edition of the International Meeting 'Nanostructures Self-Assembly, NanoSeA 2020, Rome, University La Sapienza, 8-12 June, 2020 <https://nanosea2020.it/> postponed for Covid to June 2021
- **Invited talk** *Novel Materials for energy applications: insight by ab-initio ground and excited state methods* Sezione 2 - Congresso SIF 14-18 September 2020 <https://www.sif.it/attivita/congresso/106>
- **Invited talk** "Role of Quasi-particle and excitons in 3D and 2D halide perovskites" at the Symposium "Theory and Computation of Halide Perovskites" (ComPer) of NanoGe online conference 8-9 September 2020 (<https://www.nanoge.org/ComPer/home>)
- **Invited talk** *Quasi-particle and excitons with Yambo* Max Webinar 16-June 2020 <http://www.max-centre.eu/events/max-webinar-yambo-code>
- Invited talk Symposium "2D-materials for energy applications" EMRS Spring Conference to be held in Strasbourg (France) 25-28 May 2020 Prof. Rajeev Ahuja (renounced for personal reasons)
- **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/>
- **Invited seminar** "Opto-electronic properties of novel 2D materials from DFT + post-DFT methods", ICQMS Shanghai University 5 June 2019
- **Invited seminar** "Novel 2D materials for opto-electronic applications: insight from refined ab-initio simulations" University of Paris-Sud Orsay 4 March 2019 <https://www.lps.u-psud.fr/spip.php?article3257&lang=fr>
- **Keynote Invited talk** "Fundamental properties of materials from ab-initio methods" Nanoscience and Nanodevices Frascati 18-20 December 2018 <https://agenda.infn.it/event/17167/timetable/?print=1&view=nicecompact>
- **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/>
- **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](https://www.nanoinnovation.eu/2018/pdf/Programme_NanoInnovation_2018.pdf)
- **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>
- **Invited seminar** '2D Transition Metal Dichalcogenides: fundamental properties and applications' 23/2/18 Department of Chemistry University of Perugia <https://www.clhyo.org/scientific-events/seminars.html>
- **Invited talk** 'MoS<sub>2</sub> and its family : fundamental properties and applications' Osi12 26-29 June 2017 Dublin <http://osi12conference.com/>
- **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/>
- **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>
- **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>
- **Invited lecture** on *how to use the code YAMBO for GW and BSE calculations* Dept of Applied Physics Caltech Univ. Pasadena USA , 1 August 2016 from 01-08-2016 till 01-08-2016
- **Invited Lecture** "*Theoretical lesson on the GW approach*" Dept of Applied Physics Caltech Pasadena USA, 4 August 2016
- **Invited seminar** "*Transition Metal Dichalcogenides: a novel class of 2D materials*" Dipartimento di Fisica Università di Cagliari 21/06/2016
- **Invited seminar** "*Two-dimensional Transition Metal Dichalcogenides for opto-electronics*" Dept of Chemistry, Univ. Tokyo 8 Marzo 2016
- **Invited seminar** "*Transition metal dichalcogenides: a novel class of two-dimensional materials for opto-electronics*" ICN2, Institut Catala' de Nanociencia i Nanotecnologia, Barcelona 21/1/2016
- **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 April 2015 Cecam Lausanne <https://psi-k.net/psi-k-workshops-2015/>
- **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/>
- **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
- **Invited talk** '*Novel layered Materials for solar harvesting applications*', EMRS-2014 Fall Meeting Warsaw 15-19 September 2014 <https://www.european-mrs.com/2014-fall-symposium-european-materials-research-society>
- **Invited talk** '*Two-Dimensional Materials for ultrathin optoelectronic devices*', ETSF Meeting Luxemburg 1-4 October 2013 [www.etsf.eu](http://www.etsf.eu)
- **Invited talk** "*Novel nanoscale materials for optoelectronic and Solar Energy Harvesting applications*" NanoCenter Annual Conference 2013, Royal Rimonim Dead Sea Hotel April 3-4 2013
- **Invited talk** "*Monolayer materials for tunable polymer-free excitonic solar cells*", Crystal & Graphene Science Symposium-2012 Waltham, 5-6 September 2012 <http://www.expressgenes.com/crystalss2012/main.html>
- **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 November-3 December 2010 <https://www.mrs.org/fall2010>
- **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/>
- **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/>
- **Invited talk** "*Quasi-particles and excitons in Silicon Nanowires: effect of Doping and Surface Termination*" Cecam Workshop 6-8 July 2009 Lausanne [www.cecama.org](http://www.cecama.org)
- **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>
- **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/>
- **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/>
- **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>
- **Invited talk** "*First-principles optical spectra of semiconductor surfaces: from one-particle to many-body approach*", Epioptics-7 20-26 July 2002 <http://www.csem.infn.it/csem2002/Cricenti2002.html>

## Orals

- **Talk** "*Strongly-bound excitons in Organic-inorganic 2D Perovskites: a DFT + post-DFT study*" Materials.it 2018 Bologna, 22-28 October 2018
- **Talk** "*Strongly bound excitons in organic-inorganic 2d perovskites : a dft+ mbpt study*" Symposium A3 IMRC 2018 Cancun Mexico August 2018
- **Talk** "*Excitons at the (001) surface and nanosheets of anatase TiO<sub>2</sub> : optical signatures and spatial behavior*" OSI-IX "Akumal, Mexico 19-23 September 2011
- **Talk** "*Excitonic Behavior in 2-D TiO<sub>2</sub> Anatase Systems: A First-principles Investigation*", "MRS Fall Meeting" Boston, 29 November-3 December 2010
- **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
- **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
- **Talk** "*Energy Loss Spectra of nanowires, nanotubes and nanolayers of Silicon:an ab-initio study*", "Nanosea 2006" Aix-en-Provence, 2-7 July 2006
- **Talk** "*Dielectric Response of clean and covered surfaces from first-principles approaches*", Congresso INFM Genova 8-10 June 2004

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- **Talk** "*Many-body effects on the optical properties of the (100) Diamond and Silicon surface*", Nanophase workshop, Lyon (France), October 12-13 2001
- **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.
- **Talk** "*Calculations of the spectroscopic properties of real materials*", Workshop "Modelling through Numerical Simulations" Roma, 'Tor Vergata' 17 - 18 January 2000
- **Talk** "*Optical properties of Germanium nanocrystals*", SIO'99 St. Maxime, France, May 4-8 1999
- **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
- **Talk** "*Calculation of the dielectric function of Si beyond the Local Density Approximation*", II congresso Nazionale dell'INFM, Rimini 25-30 June 1998
- **Talk** "*Electronic properties of semiconductors and insulators: computing the behaviour of complex systems*", Lione Francia, September 1994
- **Talk** "*First-principles calculation of the self-energy corrections to the bandstructure of cubic GaN*", XVII Annual Meeting Advances in Surface and Interface
- **Talk** "*Self energy corrections for excited states and localized states*", European Community Workshop, Parigi, Francia, Settembre 1992
- **Talk** "*Calcolo ab-initio con pseudopotenziali a norma conservata delle proprietà di stato fondamentale e di stato eccitato del GaN*", Wide-Band-Gap Semiconductors" Trieste, June 1992
- **Talk** "*Studio dei livelli VUV di eccitazione del Cr<sup>3+</sup> in un cristallo di Na<sub>3</sub>In<sub>2</sub>Li<sub>3</sub>F<sub>12</sub>*", Congresso SIFTrento 8-13 October 1990

#### Outreach Seminars

- "La scienza dei Materiali" Liceo Scientifico Touschek 15/12/2020 Grottaferrata (zoom platform)
- "Fisica della materia: dal macro al nanomondo" 9/4/19 Pizza Seminars Univ. Tor Vergata
- "Alla scoperta del nanomondo" 27/02/2019 Scienza Orienta Univ. Tor Vergata
- "La scienza dei materiali" Liceo Classico-Linguistico Cicerone 31/1/2019 Frascati
- "La scienza dei materiali" Liceo Scientifico Cartesio 10/3/2017 Olevano Romano
- "La scienza dei materiali" Liceo Classico Seneca 9/2/2016 Roma
- "La scienza dei materiali" Liceo Scientifico Touschek 27/10/2015 Grottaferrata
- "La scienza dei materiali" Liceo Scientifico Pietro Bono 10/12/2015 Alatri
- "La scienza dei materiali" Liceo Classico Plauto 7/5/2015 Roma

#### Editorial/Referee activities:

- Guest Editor of a volume of Current opinion in Green and Sustainable Chemistry Elsevier (2019)
- Editorial Board member of Scientific Reports (Nature publishing group)
- Referee for APS, ACS, RCS and IOP and Elsevier journals;
- Project reviewer for 2 American NSF projects, 1 Estonian and 2 Austrian Science foundation projects, 1 French National Agency project, 1 DFG German project, 2 IS CRA-B Cineca projects and 1 PRACE project.

#### Professional recognitions:

- National Scientific Qualification as Full Professor, application n.62439, (2018, up to 2024) - Bando D.D. 1532/2016, 02/B2 Theoretical condensed Matter Physics
- Winner of the MIUR "Finanziamento delle attività base di ricerca" as Associate Professor (2017)
- Winner as PI of a PRACE-H2020 European project (XVI call) and co-PI of other PRACE-H2020 projects (XIX call)
- Winner of an Endeavour fellowship from Australian Government (<https://endeavour.education.gov.au>), to carry out research on 2D materials in Australia (4 months, 2017). Declined for personal reasons
- Winner of a CNRS visit grant for a research period at Orsay-Paris Sud 15 June-3 July 2020 (not used yet for covid)
- Winner of ESF Short Visit Grant award to collaborate with Dr. E. Cannuccia in Grenoble, 1 week July 2013
- Visiting scientist at ICQMS Group Prof. W. Ren Shanghai University, 2-8 June 2019 (funded by the hosting group)
- Visiting scientist at CNRS-Orsay Group Dr. A. Zobelli Paris Sud 4-8 March 2019 (funded by the hosting group)
- Visiting scientist at the Dept of Applied Physics Caltech Univ. Group Prof. M. Bernardi (9/7/2017-5/8/2017) (funded by the hosting group)
- Visiting scientist at the Dept of Applied Physics Caltech Institute of Technology Group. Prof. M. Bernardi (13/7/2016-13/8/2016) (funded by the hosting group)
- Visiting scientist at the Dept. of Chemistry Univ. of Tokyo Group Prof. K. Yamashita (1-11 March 2016, funded by the hosting group)
- Visiting scientist at MIT Department of Materials Science Group Prof. J.C. Grossman: Summer 2012 (3 months MIT official contract), January 2013 (funded by the hosting group), July 2014 (funded by the hosting group), March 2015 (funded by the hosting group), July 2018 (funded by the hosting group)
- Jury member for the doctoral thesis defense of Dr. A.R. Kshirsagar Univ. Grenoble-Alps France, 24 March 2021
- International Referee of the PhD thesis and Jury member the thesis defence of Dr. Arnaud Lorin, Ecole Polytechnique Palaiseau France, 17 December 2020
- External referee of the PhD thesis of Dr. Paola Mocci, University of Cagliari 2019
- External Referee of the PhD thesis of Dr. M. Atambo University of Modena and Reggio 2018

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- External PhD examination committee member at the Faculty of Science of Lund University, Sweden Candidate E. Bostrom 4-6 June 2017
- External referee of the PhD thesis of Dr. Roberto Cardia, University of Cagliari 2016
- External PhD examination committee member of the final PhD exam of Dr. Leonardo Espinosa, San Sebastian Spain 22/10/2013
- International Referee of the PhD thesis of Dr. Matteo Govoni 2013 Ecole Polytechnique, Paliseau France (2012)
- External Referee PhD Thesis Dr. F. Iori, Univ. Modena and Reggio (2008)
- Member of "Collegio dei docenti del Dottorato di Ricerca in Fisica" at UTOV 30 Sept 2011- 31 December 2013
- Member of "Collegio dei docenti del Dottorato di Ricerca in Fisica" at UTOV from 01-03-2017 up today
- Member of the committee for the final PhD exam Dottorato di Ricerca in "Physics and Nanosciences" Modena Year 2021 (dates to be established)
- Member of the committee for the final PhD exam Dottorato di Ricerca in "Physics and Nanosciences" Modena Year 2020 (dates of exams 13/01/2020 and 4/9/2020)
- Member of the committee for the final PhD exam Dottorato di Ricerca in "Physics and Nanosciences" Modena, Year 2019 (dates of exams 18/2/19 and 29/8/19)
- Member of the committee of the final exam for the PhD course "in Physics and Nanoscience" Univ. Modena and Reggio Emilia, 18/2/2018
- Member of the committee of the final exams for the PhD course "in Physics and Nanoscience" Univ. Modena and Reggio Emilia, 3/2/2015
- Member of the committee for the admission exam to the PhD course "Modelli matematici per ingegneria, elettromagnetismo e nanoscienze" Univ. Roma La Sapienza 6/10/2014
- Member of a national commission to select one RTDA at the Physics Dept of the Università di Milano (02/B2 n 4042 G.U. n. 51 del 28/06/2019)
- Member of a national commission to select two RTDB at Politecnico di Milano (02/B1 n. 2018/RTDB\_PS\_FIS14) (2019)
- Member of a national commission to select one RTDB at Università di Milano (02/B2 D.R. 1875/2018 n. 3761 (2018)
- Research related to excitons in anatase bulk and nanocrystals (Nat Comm 2017) featured on <https://phys.org/news/2017-04-absorption-titanium-dioxide.html>, <http://www.azonano.com/article.aspx?ArticleID=4471>, <https://idw-online.de/en/news672925>
- Research related to Ultra-thin Photo-Voltaics based on monolayer materials, published on Nano Letters 2013, featured on MIT homepage (<http://web.mit.edu/newsoc/2013/thinner-solar-pan-0626.html>) materials online (<http://www.materials360online.com/newsDetails/40780>), optics news (<http://optics.org/news/4/7/10>), and other web sites like photonics news; climate change website; breaking energy An interview appeared on Hungton Post of 28 June 2013 (<http://www.hungtonpost.it>)
- Research on Si/Ge Nanowires for PV applications featured on (<http://www.lobbyinnovazione.it>)
- Several publications selected for the Virtual Journal of Nanoscale Science & Technology

#### Organization and Managements:

- Co-chair of two scientific sessions at the conference "Nanoscience & Nanotechnology" at INFN-LFN Frascati 15-19 October 2019 <https://agenda.infn.it/event/19925/timetable/#20191015>
- Co-chair of a scientific Symposium at IMRC2018 conference (Cancun 2018) (<http://www.mrs-mexico.org.mx/imrc2018/symposium-A4>)
- Local organizer of a Psik-funded workshop OPTEL2D on 2D materials (Rome 18-19 Dec 2017) <https://psi-k.net/scientific-report-psi-k-workshop-2d-layered-materials-opto-electronics-theoretical-computational-perspective/>
- Local co-organizer of the "ETSF Collaboration Team on Electron-Vibrational Coupling" Roma 15-16 January 2015, ([www.yambo-code.org](http://www.yambo-code.org))
- Co-organizer "40 Years of the GW Approximation for the Electronic Self Energy: Achievements and Challenges" (GW2005), Bad Honnef, Germany, 2005.
- Local co-organizer "Theory and Modeling of Electronic Excitations in Nanoscience", Acquafredda di Maratea, Italy, (2004, [www.etsf.eu](http://www.etsf.eu))
- Co-organizer "Ab initio Electron-Excitations Theory: Towards systems of Biological Interest" BIOEXC, San Sebastian, Spain, (2003, [www.etsf.eu](http://www.etsf.eu))
- Co-organizer of "Ab initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials" Lyon, France, CECAM (2002, [www.etsf.eu](http://www.etsf.eu))
- Co-organizer 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.cecama.org/workshop-details/598>)
- Co-organizer of several schools (Yambo school 2020 ICTP/Psi-k Max, Yambo School Psik/Cecam 2017, Yambo School Psik/Cecam 2015, Yambo school Psi-k/Cast Cineca 2014, see [www.yambo-code.org](http://www.yambo-code.org)).
- Co-organizer of a symposium on Optical Properties of materials ICSFS16 conference 1-6 July 2012 Genoa, Italy <http://www.icsfs16.eu/>

Since 2001, I participated in drafting several scientific national and European and bilateral projects, as member of the Rome node or as PI, in particular, during the last 10 years:

- A PRIN2020 n. deadline of submission 26/1/2021 (PI of the local node)
- A Nato multi-years project *Ultralight, wearable solar cells as portable electricity source* deadline 15/1/2021 (member)

RP

- A Regione Lazio Research project n. A0375-2020-36676 submitted 28/10/2020 (member, under evaluation)
- An INFN research project "TIME2QUEST" iniziativa specifica gruppo 4 (member, accepted)
- An INFN research project "NOWID" section 5 (as node leader, not funded)
- an ANR-France Project "Bonaspes" 2019-2022 (as Partner's scientific leader) (ongoing started 1/2020 funded for 480 keuro)
- a "beyond-borders" Project of the university of Rome Tor Vergata (co-PI, partially funded)
- a "Mission sustainability" Project of the university of Rome Tor Vergata (3/2018-8/2019-- PI, funded for 21 keuro)
- an "Uncovering excellence" project of the university of Tor Vergata (member, not funded)
- an INFN research project NEMESYS of "Iniziativa Specifica-group VI" (member, funded from 2017-2020)
- two MISTI-bilateral projects <https://misti.mit.edu/> 2016 and 2017 (PI, not funded)
- PRIN2017 (PI of a local node, not funded)
- PRIN2015 (national PI, not funded)
- an Italy/USA bilateral project n. PGR01381 (co-PI with G. Cicero, PI: J.Grossman, not funded)
- two Italy/France bilateral Galileo projects 2013 and 2015 (co-PI, not funded)
- a Samsung GRO 2015 with M.Bernardi (CIT,USA) project (co-PI, not funded)
- 1 Psi-k grant for funding the organization of the international workshop 2dopt Rome 2017 (PI, funded 3k€)
- 1 Psi-k/Max-Center & ICTP grants for funding the organization of Yambo school 2020 (co-PI, 9.2k€ funded)
- 1 Psi-k grant for the organization of Hands-on Tutorial on Excited State Spectroscopy: GW and BSE using the Yambo code, Rome, Italy, 7-9 May 2014 (co-PI, funded 6k€)
- 1 CECAM & ESF/Psik grant for the organization of the workshop "Theory, simulation and modeling of SiGe nanostructures: from nanoelectronics to renewable energy", 3-6 June 2013, Cecam Lausanne (co PI, funded 18 k€)
- an European H2020-MSCA-RISE-2018 DiSeTCom n. 823728 (member, funded 690k€)
- an European H2020-MSCA-RISE-2017 OPTMAT (member, not funded)
- an European H2020-MSCA-RISE-2014 COEXAN (member funded 1ML€)
- an European H2020-FETPROACT-2016-20 n. 73204 (member, not funded)
- an European FP7-NMP-2011 n. 280723 project "White Light Emitting hybrid ZnO Nanostructures" (2011) (PI of a local node, not funded, first excluded)
- an European FP-NMP.2001.4.05 "Nanoscale simulations for Photovoltaics" project (2011) (member, not funded)
- a FIRB n. RBFR129YPH004 project (2010) (member, not funded but first excluded)

The list of other older financed projects are: PRIN2002 (member), PRIN2005028257\_004 (member), PRIN20079XA4HW\_004 (member), INNESCO 2003-2005 (member), Eu-Nanophase HPRN-CT-2000-00167 (member), Eu-Nanoquanta NMP4-CT-2004-500198 (member), Eu-I3-ETSFn. RI-211956 (member); 4 ESF/Psi-k grants to organize the ETSF conferences (co-PI)

In the last ten years I was PI (5) or co-PI/staff member (8) of several national and European HPC-supercomputing projects on the basis of competitive and peer reviewed selection (*for PRACE (Iskra-B) :1ML core-hours are equivalent to about 5.5keuro (6keuro) as indicated by Cineca*)

- PI of a PRACE-H2020project optel2d *Opto-electronic properties of 2D Transition Metal Dichalcogenides with DFT and post-DFT simulations* 2018 (49ML core-hours on Marconi).
- PI of a IS CRA-B project EXSEM2D *Excitons in 2D semiconducting materials by refined ab-initio methods* (10ML core-hours on Marconi, 2019)
- PI of a IS CRA-B project NWPOLY *Polytypism in Group III-V and IV nanowires : an ab-initio perspective* 2015 (650k core-hours on Fermi)
- PI of a IS CRA-B project Ex-natio n. HP10BUJ6VJ *Ab-initio investigation of EXcited-state properties of NAnostructured TIO2-based materials* (2011) (650k core-hours on fermi)
- PI of a IS CRA-B project OPSANN n. HP10B2DDQJ *A New Perspective in Semiconductor Nanoscience: Optoelectronic Properties of SiGe Alloyed Nanocrystals and Nanowires* (136k core-hours on SP62010)
- Co-PI of a PRACE-H2020 Project *Extend" EXcitonic instability in two dimensional tungsten Ditelluride"* 2019 (45ML core-hours on Marconi2)
- Member of a PRACE Project *Ancient\_Rome -Study of mANy body exCitations in dEfective titaNium dioxide maTeRials by ab-initio Methods* 2019 (30 ML core-hours on Marconi2)
- Member of a PRACE-DECI-7-FP7 project 7 2011 "DIAVIB: Effect of electron-phonon coupling on the electronic structure of small diamond cages"
- Member of a PRACE-DECI-6- FP7 project 2010 "The optical properties of group IV semiconductor nanocrystals an ab initio many body perturbation approach"
- Member of Iskra-B project n. hp10bbznp SPERE *Single Photon emission from point defects in 2D materials* 1.5 ML cpu-hours on Marconi2 (2020)
- Member of Iskra-B project n. HP10BEBZU4 *PiBifree* (1.5ML cpu-hours on marconi2) (2019)
- Member of Iskra-B project 2D-OIHPs n. HP10BGUJ6X *Insights in the 2D Organic-Inorganic Hybrid Perovskites (OIHPs) and their heterocomposites. A first principle analysis* (4ML core-hours on Marconi, 2018)
- Member of a IS CRA-B Project n. HP10B4SQA4 "Atomistic simulations of nanostructured silicon interfaces" 2013

Other projects awarded:

- PI of a Iscra-C project GeSOPT n. HP10C8NU7N “Germanium Disulphide: an ab-initio study of the electronic and optical properties by DFT+MBPT methods” (2020)
- PI of ISCRA-C project n. HP10COI5O6 2DASP “*Optoelectronic features of 2D AsP layered structures up to the inclusion of many-body effects*” 2019
- PI of ISCRA-C project n. HP10CLLJPF EXCMOIRE *Exciton modulation by Moire' patterning in bilayer boron nitride* (2018)
- PI of ISCRA-C project n. HP10CP60YK LESiNW *Light-emission in Silicon Nanowires* (2017)
- PI of ISCRA-C project n. HP10C7TJJP OPFLOW *Optical properties of porphyrin thin films and low dimensional structures* (2015)
- PI of ISCRA-C project n. HP10CXGIQB T2DTMD “*Radiative lifetimes of two-dimensional Transition Metal Dichalcogenides*” (2014)
- PI of ISCRA-C project n. HP10C80NSA TAPOG “*Tautomeric forms of Porphyrines on Graphite: energetics, electronic and optical properties*” (2013)
- PI of ISCRA-C project n. HP10CMAA6K TEXCAB “*Tunable Polymer-Free Excitonic Solar Cells from Ab-Initio Calculations*” (2012)
- Staff Member of other 19 ISCRA-C projects
- PI/member of the scientific teams of 10 ETSF collaborative and/or training proposals [www.etsf.eu](http://www.etsf.eu)
- Host of two European researchers (M. Voros 2011 and F. Iori 2010) within the HPC-Europa2 Transnational Access Programme

#### Department organization Duties

- I am responsible for Materials Science and Technology of the new web page of degree course and social channels (facebook, Instagram)
- I am responsible for organizing the Materials Science seminars
- I have been a member until 2019 of the restricted teaching commission of the degree course in Physics
- I am member of the restricted teaching commission of the degree course in Materials science

#### Teaching experience:

Bachelor, Master and PhD Thesis:

- Alessandro Moreci Bachelor Thesis in Physics ongoing, Univ. Tor Vergata 26 February 2021, supervisor)
- Sara Postorino (PhD ongoing since 2018 Univ. Tor Vergata, supervisor)
- Simone Brozzesi Master Thesis in Materials Science (Univ. Tor Vergata) A.A. 2019-2020 (co-supervisor)
- Alessandro Graziani Master Thesis in Physics (Univ. Tor Vergata) A.A. 2018-2019 (co-supervisor)
- Simone Grillo Bachelor Degree in Physics Thesis (Univ. Tor Vergata) A.A. 2017-2018 (co-supervisor)
- Sara Postorino Master Thesis in Physics (Univ. Tor Vergata) A.A. 2017-2018 (co-supervisor)
- Riccardo De Gennaro Master Thesis in Physics (Univ. Tor Vergata) A.A. 2016-2017 (co-supervisor)
- Antonio D'Auria Bachelor Degree Thesis Univ. Tor Vergata A.A. 2015-2016 (supervisor)
- Giovanni Bellucci Master Degree in Materials Science Univ. Tor Vergata A.A. 2015-2016 (supervisor)
- Emanuele Tomo Bachelor Degree in Physics A.A. 2011-2012 (supervisor)
- Paolo Bagala Master Thesis in Physics (Univ. Tor Vergata) A.A. 2008-2009 (co-supervisor)
- Michele Amato PhD Thesis in Nanoscience Univ. di Modena e Reggio A.A. 2009-2010 (co-supervisor)
- Mauro Bruno PhD Thesis in Physics Univ. di Tor Vergata A.A. 2007-2008 (co-supervisor)

Since 2010 Professor of Solid State Physics (6 cfu Master Degree in Physics, UTOV)

Since 2012 Professor of Solid State Theory and molecular models, (4 cfu Master Degree in Material Science, UTOV)

Since 2012 Series of Lectures in “Quantum Theory of Solids” course- Prof. O. Pulci, (for a total of about 14 frontal hours Master Degree in Physics, UTOV)

A.A. 2011-2013, Series of Lectures "Introduction to Many-Body Perturbation Theory", PhD in Physics courses, UTOV

A.A. 2004-2005, Professor of Mathematical Methods for Material Science, (6 cfu Bachelor Degree in Material Science, UTOV)

A.A. 2005-2006, Professor of Mathematical Methods for Material Science, (6 cfu Bachelor Degree in Material Science, UTOV)

A.A. 2002-2011 Assistant Professor of Atomic and Molecular Physics (Prof. Fanfoni, Bachelor Degree in Material Science, UTOV) and Structure of Matter (Bachelor Physics Degree UTOV) for a total of about 20 frontal hours

A.A. 2000-2001 and 2001-2002, Assistant Professor of Classical Physics for Biologists (Bachelor Degree UTOV) for a total of about 16 frontal hours

For more info see the personal web page [www.fisica.uniroma2.it/~palummo](http://www.fisica.uniroma2.it/~palummo), for the full list of publications see also google-scholar or ISI-WEB

#### Full list of Scientific Publications

**137)** *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 under review on Physical Review B (2021)

**136)** *First-principle exciton radiative lifetimes in monolayer graphitic carbon nitride* Michele Re Fiorentin, Francesca Risplendi, **Maurizia Palummo**, Giancarlo Cicero

under review on ACS Applied Nano Materials 2021

**135) On the Nature of Optical Excitations in Porphyrin Crystals: a Joint Experimental and Theoretical Study**

**Maurizia Palummo**, Luisa Raimondo, Conor Hogan, Silvia Trabattoni, Claudio Goletti, Adele Sassella  
Accepted on the Journal of Phys. Chem. Letters (2021)

**134) Ab Initio Theory of Interband Transitions**

Conor Hogan, **Maurizia Palummo**, Olivia Pulci, Carlo Maria Bertoni (2020) in Springer Handbook of Surface Science, 2020

**133) Theoretical Aspects of Point Defects in Semiconductor Nanowires**

R Rurali, **M Palummo**, X Cartoixà Fundamental Properties of Semiconductor Nanowires, 349-367 (2020) Springer

**132) Close-Packed Arrangements of Flat-On Free-Base Porphyrins Driven by van der Waals Epitaxy**

M Campione, C Hogan, **M Palummo**, A Bossi, R Yivlialin, G Bussetti Crystal Growth & Design 20 (11), 7450-7459 2020

**131) Spatially indirect excitons in black and blue phosphorene double layers**

MR Fiorentin, G Cicero, **M Palummo** Physical Review Materials 4 (7), 074009 2020

**130) Ab initio studies of the optoelectronic structure of undoped and doped silicon nanocrystals and nanowires: the role of size, passivation, symmetry and phase** S Ossicini, I Marri, M Amato, **M Palummo**, E Canadell, R Rurali

Faraday discussions 222, 217-239 2020

**129) A monolayer transition-metal dichalcogenide as a topological excitonic insulator**

D Varsano, **M Palummo**, E Molinari, M Rontani Nature Nanotechnology 15 (5), 367-372 10 2020

**128) Impact of Impurities on the Electrical Conduction of Anisotropic Two-Dimensional Materials**

J Sun, M Passacantando, **M Palummo**, M Nardone, K Kaasbjerg, A Grillo, ..L.Camilli Physical Review Applied 13 (4), 044063 5 2020

**127) A Scalable Method for Thickness and Lateral Engineering of 2D Materials**

J Sun, G Giorgi, **M Palummo**, P Sutter, M Passacantando, L Camilli Acs Nano 14 (4), 4861-48704 2020

**126) Strain-induced effects on the electronic properties of 2D materials**

S Postorino, D Grassano, M D'Alessandro, A Pianetti, O Pulci, **M.Palummo**  
Nanomaterials and Nanotechnology 10, 1847980420902569 5 2020

**125) Optical Properties of Lead-Free Double Perovskites by Ab Initio Excited-State Methods**

**Maurizia Palummo**, Eduardo Berrios, Daniele Varsano, Giacomo Giorgi ACS Energy Letters 5 (5), 457 7 2020

**124) Interlayer bound wannier excitons in germanium sulfide**

S Postorino, J Sun, S Fiedler, LO Lee Cheong Lem, **M Palummo**, L Camilli Materials 13 (16), 3568 2020

**123) Halide Pb-Free Double-Perovskites: Ternary vs. Quaternary Stoichiometry**

**M Palummo**, D Varsano, E Berrios, K Yamashita, G Giorgi Energies 13 (14), 3516 2020

**122) Precise radiative lifetimes in bulk crystals from first principles: the case of wurtzite gallium nitride**

VA Jhalani, HY Chen, **M Palummo**, M Bernardi Journal of Physics: Condensed Matter 32 (8), 084001 5 2019

**121) First-Principles Nonequilibrium Green's Function Approach to Ultrafast Charge Migration in Glycine**

E Peretto, D Sangalli, **M Palummo**, A Marini, G Stefanucci Journal of chemical theory and computation 15 (8), 4526-4534 5 2019

**120) Second-harmonic generation in single-layer monochalcogenides: A response from first-principles real-time simulations**

C Attaccalite, **M Palummo**, E Cannuccia, M Grüning Physical Review Materials 3 (7), 074003 6 2019

**119) Out-of-plane excitons in two-dimensional crystals**

I Guilhon, M Marques, LK Teles, **M Palummo**, O Pulci, S Botti, F Bechstedt Physical Review B 99 (16), 161201 11 2019

**118) Ab initio calculations of exciton radiative lifetimes in bulk crystals, nanostructures, and molecules**

Hsiao-Yi Chen, Vatsal A. Jhalani, **Maurizia Palummo**, Marco Bernardi Phys. Rev. B 100, 075135 7 2019

**117) Tailoring the optical properties of MoS2 and WS2 single layers via organic functionalization**

**M Palummo**, N A D'Auria, J C Grossman, Giancarlo Cicero J. Phys.: Condens. Matter 31, 235701 5 (2019)

**116) Many-body perturbation theory calculations using the yambo code**

D Sangalli, A Ferretti, H Miranda, C Attaccalite, I Marri, E Cannuccia, P Melo, M Marsili, F Paleari, A Marrazzo, G Prandini, P Bonfà, M O Atambo, F Affinito, **M Palummo**, A Molina-Sánchez, C Hogan, M Grüning, D Varsano and A Marini



Journal of Physics: Condensed Matter 76 2019

**115) Ice-Assisted Synthesis of Black Phosphorus Nanosheets as a Metal-Free Photocatalyst: 2D/2D Heterostructure for Broadband H<sub>2</sub> Evolution**

Qingzhe Zhang Shengyun Huang JiuJun Deng Deepak Thrithamarassery Gangadharan Fan Yang Zhenhe Xu Giacomo Giorgi **Maurizia Palummo** Mohamed Chaker Dongling Ma  
Advanced Functional Material 36 2019

**114) A route for minimizing emissions: sun-mediated processes and clean batteries**

G Giorgi, K Yamashita, **M Palummo**, S Fabris  
Current Opinion in Green and Sustainable Chemistry Elsevier (2019)

**113) On the Nature of the electronic and optical excitations of Ruddlesden–Popper hybrid organic–inorganic perovskites: The role of the many-body interactions** G Giorgi, K Yamashita, **M Palummo** The journal of physical chemistry letters 9 (19), 5891-5896 24 2018

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

**111) Two-dimensional optical excitations in the mixed-valence Cs<sub>2</sub>Au<sub>2</sub>I<sub>6</sub> fully inorganic double perovskite**  
G Giorgi, K Yamashita, **M Palummo** Journal of Materials Chemistry C 6 (38), 10197-10201 14 2018

**110) Optical and Electronic Properties of Two-Dimensional Layered Materials**

Marco Bernardi, Can Ataca, **Maurizia Palummo** and Jeffrey C. Grossman Nanophotonics vol.6, 2 (2017)

**109) Role of Quantum-confinement in Anatase nanosheets**

D Varsano, G Giorgi, K Yamashita, **M Palummo** The journal of physical chemistry letters 8 (16), 3867-3873 13 2017

**108) Optical emission in hexagonal SiGe nanowires**

X Cartoixà, **M Palummo**, HIT Hauge, EPAM Bakkers, R Rurali Nano letters 17 (8), 4753-4758 36 2017

**107) Le matrici tridiagonali in matematica e la loro applicazione in fisica**

M Fanfoni, S Trapani, A Sgarlata, **M Palummo**, M Tomellini IT 58 (4), 309-322 (2017)

**106) Strongly bound excitons in anatase TiO<sub>2</sub> single crystals and nanoparticles**

E. Baldini, L. Chiodo, A. Dominguez, **M. Palummo**, S. Moser, M. Yazdi-Rizi, G. Auböck, B.P.P. Mallett, H. Berger, A. Magrez, C. Bernhard, M. Grioni, A. Rubio & M. Chergui Nature Communications volume 8, Article number: 13 (2017)

**105) 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 32 2016

**104) Temperature-dependent excitonic effects in the optical properties of single-layer MoS<sub>2</sub>**

A Molina-Sánchez, **M Palummo**, A Marini, L Wirtz Physical Review B 93 (15), 155435 76 2016

**103) Exciton Radiative Lifetimes in Two-Dimensional Transition Metal Dichalcogenides**

**Maurizia Palummo**, Marco Bernardi JC Grossman Nano Letters 15 (5), 2794 403 2015

**102) Ab initio energy loss spectra of Si and Ge nanowires**

**M Palummo**, C Hogan, S Ossicini Physical Chemistry Chemical Physics 17 (43), 29085-29089 3 2015

**101) Early oxidation stages of the strained Ge/Si (105) surface: A reflectance anisotropy spectroscopy study**

C Goletti, L Fazi, C Hogan, L Persichetti, A Sgarlata, **M Palummo**, et al Physica status solidi (b) 252 (1), 87-94 2015

**100) Understanding doping at the nanoscale: the case of codoped Si and Ge nanowires**

M Amato, R Rurali, **M Palummo**, S Ossicini Journal of Physics D: Applied Physics 47 (39), 394013 7 2014

**99) Electronic and optical properties of pure and modified diamondoids studied by many-body perturbation theory and time-dependent density functional theory**

T Demján, M Vörös, **M Palummo**, A Gali The Journal of chemical physics 141 (6), 064308 23 2014

**98) Probing two-dimensional vs three-dimensional molecular aggregation in metal-free tetraphenylporphyrin thin films by optical anisotropy**

G. Bussetti, M. Campione, L. Ferraro, L. Raimondo, B. Bonanni, C. Goletti, **M. Palummo**, C. Hogan, L. Duò, M. Finazzi, and A. Sassella The Journal of Physical Chemistry C 118 (29), 15649-15655 17 2014

**97) Stable alignment of tautomers at room temperature in porphyrin 2D layers**

Gianlorenzo Bussetti Marcello Campione Michele Riva Andrea Picone Luisa Raimondo Lorenzo Ferraro Conor Hogan **Maurizia Palummo** Alberto Brambilla Marco Finazzi Lamberto Duò Adele Sassella Franco Ciccacci *Advanced Functional Materials* 24 (7), 958-963 45 2014

**96) 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 16 2014

**95) SiGe nanowires for thermoelectrics applications** M Amato, **M Palummo**, S Ossicini, R Rurali *Nanoscale Thermoelectrics*, 497-515 2 2014

**94) Intermixing and buried interfacial structure in strained Ge/Si (105) facets**  
L Fazi, C Hogan, L Persichetti, C Goletti, **M Palummo**, A Sgarlata, A. Balzarotti  
*Physical Review B* 88 (19), 195312 16 2013

**93) Extraordinary sunlight absorption and one nanometer thick photovoltaics using two-dimensional monolayer materials** M Bernardi, **M Palummo**, JC Grossman *Nano letters* 13 (8), 3664-3670 1388 2013

**92) Minority surfaces of anatase and their derived nanosheets: a combined DFT and MBPT analysis**  
G Giorgi, **M Palummo**, L Chiodo, A Rubio, J Fujisawa, H Segawa, ...  
*NANOENERGY Letters* 2013

**91) Ab Initio Electronic Gaps of Ge Nanodots: The Role of Self-Energy Effects**  
M Marsili, S Botti, **M Palummo**, E Degoli, O Pulci, HC Weissker, Miguel A. L. Marques, Stefano Ossicini and Rodolfo Del Sole  
*The Journal of Physical Chemistry C* 117 (27), 14229-14234 11 2013

**90) Correlation effects in the optical spectra of porphyrin oligomer chains: Exciton confinement and length dependence** C Hogan, **M Palummo**, J Gierschner, A Rubio  
*The Journal of chemical physics* 138 (2), 01B607 30 2013

**89) Optical absorption modulation by selective codoping of SiGe core-shell nanowires**  
M Amato, **M Palummo**, R Rurali, S Ossicini  
*Journal of Applied Physics* 112 (11), 114323 9 2012

**88) Semiconducting monolayer materials as a tunable platform for excitonic solar cells**  
M Bernardi, **M Palummo**, JC Grossman *ACS nano* 6 (11), 10082-10089 89 2012

**87) The Nature of Radiative Transitions in TiO<sub>2</sub>-Based Nanosheets**  
**M Palummo**, G Giorgi, L Chiodo, A Rubio, K Yamashita  
*The Journal of Physical Chemistry C* 116 (34), 18495-18503 22 2012

**86) Band structure analysis in SiGe nanowires**  
M Amato, **M Palummo**, S Ossicini *Materials Science and Engineering: B* 177 (10), 705-711 17 2012

**85) Optoelectronic properties in monolayers of hybridized graphene and hexagonal boron nitride**  
M Bernardi, **M Palummo**, JC Grossman *Physical review letters* 108 (22), 226805 104 2012

**84) Optical properties of the long-range Si (110)-(16 × 2) reconstruction from first principles**  
E Ferraro, C Hogan, **M Palummo**, R Del Sole  
*physica status solidi (b)* 249 (6), 1148-1154 8 2012

**83) Excitons at the (001) surface of anatase: Spatial behavior and optical signatures**  
G Giorgi, **M Palummo**, L Chiodo, K Yamashita *Physical Review B* 84 (7), 073404 25 2011

**82) Coexistence of Negatively and Positively Buckled Isomers on n+-Doped Si (111)- 2 × 1**  
G Bussetti, B Bonanni, S Cirilli, A Violante, M Russo, C Goletti, ...  
*Physical review letters* 106 (6), 067601 32 2011

**81) Test of long-range exchange-correlation kernels of time-dependent density functional theory at surfaces: Application to Si (111) 2 × 1**  
O Pulci, A Marini, **M Palummo**, R Del Sole  
*Physical Review B* 82 (20), 205319 13 2010

**80) Silicon and germanium nanostructures for photovoltaic applications: ab-initio results**  
S Ossicini, M Amato, R Guerra, **M Palummo**, O Pulci  
*Nanoscale research letters* 5 (10), 1637 43 2010

MF

**79) Ab initio optoelectronic properties of SiGe nanowires: Role of many-body effects**

**M Palummo**, M Amato, S Ossicini Physical Review B 82 (7), 073305 22 2010

**78) Many-body effects on the electronic and optical properties of Si nanowires from ab initio approaches**

**M Palummo**, S Ossicini, R Del Sole  
physica status solidi (b) 247 (8), 2089-2095 7 2010

**77) Segregation, quantum confinement effect and band offset for [110] SiGe NWs**

M Amato, **M Palummo**, S Ossicini  
physica status solidi (b) 247 (8), 2096-2101 16 2010

**76) Convergence study of neutral and charged defect formation energies in Si nanowires**

R Rurali, **M Palummo**, X Cartoixa  
Physical Review B 81 (23), 235304 36 2010

**75) Giant excitonic exchange splitting in Si nanowires: first-principles calculations**

**M Palummo**, F Iori, R Del Sole, S Ossicini  
Physical Review B 81 (12), 121303 20 2010

**74) Electronic and optical properties of Si and Ge nanocrystals: An ab initio study**

O Pulci, E Degoli, F Iori, M Marsili, **M Palummo**, R Del Sole, S Ossicini  
Superlattices and Microstructures 47 (1), 178-181 3 2010

**73) Experimental and theoretical investigation of the pyrrole/Al (100) interface**

A Ruocco, L Chiodo, M Sforzini, **M Palummo**, P Monachesi, G Stefani  
The Journal of Physical Chemistry A 113 (52), 15193-15197 8 2009

**72) SiGe nanowires: Structural stability, quantum confinement, and electronic properties**

M Amato, **M Palummo**, S Ossicini  
Physical Review B 80 (23), 235333 47 2009

**71) Ab initio electronic and optical spectra of free-base porphyrins: The role of electronic correlation**

**M Palummo**, C Hogan, F Sottile, P Bagalá, A Rubio  
The Journal of chemical physics 131 (8), 08B607 144 2009

**70) Electronic and optical properties of acetylene and ethylene on Si (001)**

M Marsili, O Pulci, **M Palummo**, PL Silvestrelli, R Del Sole  
Superlattices and Microstructures 46 (1-2), 240-245 2 2009

**69) Electronic properties and dielectric response of surfaces and nanowires of silicon from ab-initio approaches**

**M Palummo**, F Iori, R Del Sole, S Ossicini  
Superlattices and Microstructures 46 (1-2), 234-239 5 2009

**68) Theory of dielectric screening and electron energy loss spectroscopy at surfaces**

C Hogan, **M Palummo**, R Del Sole  
Comptes Rendus Physique 10 (6), 560-574 7 2009

**67) Reduced quantum confinement effect and electron-hole separation in SiGe nanowires**

M Amato, **M Palummo**, S Ossicini  
Physical Review B 79 (20), 201302 48 2009

**66) Reflectance-anisotropy spectroscopy and surface differential reflectance spectra at the Si (100) surface: Combined experimental and theoretical study**

**M Palummo**, N Witkowski, O Pluchery, R Del Sole, Y Borenstein  
Physical Review B 79 (3), 035327 56 2009

**65) Novel optoelectronic properties of simultaneously n- and p-doped silicon nanostructures**

F. Iori, E Degoli, **M Palummo**, S Ossicini  
Superlattices and Microstructures 44 (4-5), 337-347 25 2008

**64) Ab-initio optical spectra of complex systems**

E Cannuccia, O Pulci, **M Palummo**, V Garbuio, RD Sole  
Physica status solidi c 5 (8), 2543-2550 2 2008

**63) EXCITED STATE PROPERTIES CALCULATIONS: FROM 0 TO 3 DIMENSIONAL SYSTEMS**



M Marsili, V Garbuio, M Bruno, O Pulci, M Palummo, E Degoli, E Luppi, ...  
EPIOPTICS-9, 41-61 2008

**62) Ab-initio electronic and optical properties of low dimensional systems: From single particle to many-body approaches**  
**M Palummo**, M Bruno, O Pulci, E Luppi, E Degoli, S Ossicini, R Del Sole  
Surface science 601 (13), 2696-2701 7 2007

**61) First-principles optical properties of silicon and germanium nanowires**  
M Bruno, **M Palummo**, S Ossicini, R Del Sole  
Surface science 601 (13), 2707-2711 58 2007

**60) From Si nanowires to porous silicon: the role of excitonic effects**  
M Bruno, **M Palummo**, A Marini, R Del Sole, S Ossicini  
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**Dichiaro che tutto quanto scritto in tale curriculum-vitae corrisponde a verità,  
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