Margherita Marsili

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EDUCATION

2006 **University of Rome 'Tor Vergata',** Rome (Italy)
PhD in Physics (Ottimo)
Thesis: "*Electronic and optical properties of the (111)2x1 diamond surface: an ab-initio study.*"
Supervisor: Prof. R. Del Sole

2002 **University of Rome 'La Sapienza'**
Master's Degree in Physics (110/110)
Thesis: "*Study of the two bands Hubbard model with the use of the slave-bosons technique*"
Supervisor: Prof. M. Grilli

ACADEMIC POSITIONS

July 2022- **Assistant Professor**,
Physics Department, Alma Mater Studiorum University of Bologna

Development of methodologies for the automatic and high-throughput study of mechanical and tribological properties of solid-solid interfaces.
Computational material design for surface and interface optimization.
High-entropy alloy surface and interface properties.
Fundamental studies on the relation between electronic and mechanical properties of material subject to uniaxial load.

Nov 2018-July 2022 **Postdoctoral Research Associate,**
Chemistry Department, University of Padova, Padova (Italy)
Contracts: Borsa di ricerca 03/10/2021- ; Assegno di ricerca (L. 240/2010) 31/10/2018-02/10/2021 including 5 months of maternity leave.

Interface of GW-BSE, Stochastic Schrodinger Equation and PCM methods for the description of plasmon driven hot electron dynamics. Study of plasmon enhanced photocatalysis of CO_2 methanation on Rh nanocubes. Supervisor: Prof. Stefano Corni

Nov 2017-Oct 2018 **Ecole Polytechnique,** Palaiseau (France)
Contract: Chercheur en physique 01/11/2017-31/10/2018

I/O optimization and parallelization of the dp-code. This code is devoted to the calculation of optical properties of materials at the RPA, TDDFT and BSE level. Supervisor: Dr. Francesco Sottile

April 2014-August 2015 **CNR-NANO S3,** Modena (Italy)
Contract: Assegno di ricerca (L. 240/2010) 01/04/2014-31/08/2015

First-principle simulations of ultra-fast transient absorption spectra in single layers of transition-metal dichalcogenides. Study of the electronic and optical properties of lead halide perovskites, of organic dyes on TiO2 clusters, porphyrins, and 2D crystals. Supervisor: Dr. Deborah Prezzi

April 2012-March 2014 **Astronomy and Physics Department, University of Padova,** Padova (Italy)
Contract: Assegno di ricerca (L. 240/2010) 01/04/2012-31/03/2014

Development and implementation of a first-principle code for the calculation of optical properties of materials through the solution of the Bethe-Salpeter equation within the

Quantum-Espresso Suite. The implemented approach is particularly suited for treating large systems. Study of the electronic structure of porphyrin thin films in collaboration with the experimentalists of ELETTRA synchrotron, and study of efficient formulation for the calculation of the Fock term in extended systems. Supervisor: Prof. Paolo Umari

Dec 2006-June 2011 **University of Rome 'Tor Vergata',** Rome (Italy)
Contracts: Assegno di ricerca universita' (L 449/97) 01/10/2010-30/06/2011; Assegno di ricerca universita' (L. 449/97) 15/09/2009-14/09/2010; Assegno di ricerca universita' (L. 449/97) 15/09/2008-14/09/2009; Assegno di ricerca CNR (L. 449/97) 17/09/2007-16/09/2008; Borsa di studio CNISM 01/07/2006-30/06/2007

Determination of the electronic and optical properties within many-body perturbation theory of 2D systems such as hydrogenated silicene, germanene, and graphane; study of the effect of steps on the optical properties of diamond surfaces; study of the electronic and optical properties of free-standing and embedded Si and Ge nanocrystals; determination of the adsorption geometry of ethylene on Si(100) surface by optical properties calculations. Supervisor: Prof. Del Sole

May-November 2006 **Ecole Polytechnique,** Palaiseau (France)
Contracts: Borsa di studio CNISM 01/07/2006-30/06/2007, Borsa di studio Egide 11/05/2006-10/11/2006, Borsa di studio Angelo della Riccia

Efficient formulation for the exchange and correlation kernel of time-dependent density-functional theory for extended systems. Supervisor: Dr. Francesco Sottile

QUALIFICATION

27/01/2022 National scientific qualification as associate professor in the Italian higher education system for the disciplinary field of 02/B2 - FISICA TEORICA DELLA MATERIA

NON-ACADEMIC WORK (1 year R&D in a private company, 3 years as a maths teacher)

2021-2022 **Scuola Media Ruzante,** Padova (Italy)
2015-2017 Middle school maths and science teacher

2011-2012 **Xgroup SPA,** San Pietro in Viminario (Italy)

Position: full-time R&D employee (impiegata addetta al Settore Ricerca e Sviluppo, rapporto di lavoro a tempo pieno e indeterminato, inquadramento: VII Livello del C.C.N.L. Industria Metalmeccanica Confindustria)

Duties: responsible for the solar cell manufacturing company's research projects aiming at the technology transfer from research institutions and universities.

MATERNITY LEAVES (4 leaves, 20 months in total)

2019 July - December

2017 August - January (2018)

2009 March - August

2007 January - June

COORDINATION OF RESEARCH PROJECTS AND CPU-TIME GRANTS

2010-12 Local responsible, within XGROUP Spa, for the national project PED4PV (Pulsed Electron Deposition for Photovoltaics), funded by Ministero delle Sviluppo Economico within the "Industria 2015" framework (contract number EE01_00062, 01/03/2009). Total budget €13M

CPU-TIME GRANTS

2023 PI of the Iscra B project (HP10B0EDQ9) "Tuning the adhesion of diamond coatings through adatom adsorption" Assigned budget: 1.358.400 CPU/GPU h on LEONARDO_B

2022 PI of the Iscra C project (HP10CXFHSB) "Many-body calculations for excited state energy barriers" Assigned budget: 33.000 CPU h @g100.cineca.it

2019 PI of the Iscra C project (HP10CY9E6M) "Study of the plasmonic character of the optical excitations of metallic clusters through many-body perturbation theory"
Assigned budget: 70.000 CPU h @marconi.cineca.it

2017 PI of the Iscra C project (HP10C0956U) "Excitonic effects in the optical absorption spectra of supercooled water"
Assigned budget: 35.000 CPU h @marconi.cineca.it

2016 PI of the Iscra C project (HP10CAQLHH) "Silicongraphene heterostructures"
Assigned budget: 34.000 CPU h @marconi.cineca.it, 1.000.000 CPU h @fermi.cineca.it

2013 PI of the Iscra B project (HP10BUL24D) "Effects of Hydrogen on the electronic and optical properties of the (111) surface of diamond"
Assigned budget: 4.750.000 CPU h @fermi.cineca.it, 50.000 CPU h @eurora.cineca.it

2012 PI of the Iscra C project (HP10CDC0J2) "Study of stacking effects on the electronic properties of porphyrins films."
Assigned budget: 2.500.000 CPU h @fermi.cineca.it

PARTICIPATION TO RESEARCH PROJECTS

July 2022 - Team member of the international project H2020 ERC "Slide - Advancing solid interfaces and lubricants by first principles material design"

Oct 2021 - July 2022 Team member of the international project H2020 ProID

Nov 2018 - Sept 2021 Team member of the international project H2020 ERC "TAME Plasmons - A Theoretical chemistry approach to time-resolved molecular plasmonics"

April 2014- August 2015 Team member of the national project FIRB "Flashit - Analisi dei fenomeni ultraveloci fotoindotti alla scala nanometrica: una approccio teorico sperimentale"

Sept 2010- June 2011 European Theoretical Spectroscopy Facility (ETSF) - funded under FP7-INFRASTRUCTURES) - scientist in charge of the collaborative project "Optical properties of graphene-like silicon sheets on silver (110) and (111)" (ETSF user projects submitted to the ETSF, evaluated by external panel, and accepted for financial support by the ETSF)

CPU-TIME GRANTS

2019 Team member of the PRACE project "NANOMOLEL -Antenna-reactor nanostructures for electron injection in molecules" application proposal 2018194568

AWARDS

2005 Fondazione Angelo Della Riccia fellowship travel grant that partially funded my first post-doc appointment at Ecole Polytechnique (France)

WORKSHOPS AND CONFERENCES ORGANISATION

2015 Member of the organising committee of the international workshop "Excitations in Realistic Materials using Yambo on Massively Parallel Architectures", CECAM-HQ-EPFL, Lausanne, Switzerland 13-17 April

2011 Member of the organising committee of the international workshop "16th ETSF workshop on Electronic Excitations - Bridging theory and experiment", Turin, Italy, September 27-30

2010 Member of the organising committee of the international workshop "15th ETSF Workshop on Electronic Excitations - New Frontiers in Theoretical Spectroscopy and Quantum Transport", Berlin, Germany, October 12-15 (http://etsf.polytechnique.fr/etsfconference2010/Organisers)

2006 Member of the organising committee of the international workshop "3rd Nanoquanta Young Researchers Meeting" Rome, Italy, May 3-5

METHODOLOGICAL DEVELOPMENTS, CODE IMPLEMENTATION AND OPTIMIZATION

Part of my research work has been devoted to methodological developments and implementations in open-source publicly distributed codes (under GPL licence) such as Quantum Espresso, and WaveT-TDPLAS. This work is documented in publications n. 41, 38, 32, and 31 (see the publication list below). Since 2014 I have been a member of the Yambo-project team (open-source, GPL licence) as an expert user applying and supporting the debugging activity of novel implementations (see publications n. 37, 33, and 30).

2022- Developer of Tribchem (https://gitlab.com/triboteam/tribchem) a software specifically designed to perform the high-throughput study of solid-solid interfaces.

2019- Developer of the interface between MOLGW (http://www.molgw.org/) and the WaveT-TDPLAS (http://www.tame-plasmons.eu/, https://github.com/stefano-corni/WaveT_TDPlas).

2018- Optimization of the dp code (http://dp-code.org/)

2014- Member of the Yambo-project team (http://www.yambo-code.org)

2012-14 Developer of the GWW-BSE code within the Quantum Espresso suite (https://www.quantum-espresso.org/)

2006-07 Contributor of the *exc* scientific code (http://theory.polytechnique.fr/codes/exc/)

PUBLICATIONS

(To date bibliometric indices from SCOPUS: total 39 regular articles, 2 review and 6 conference papers on international peer reviewed journals, h-index 19; total citations 6661)

46. G Dall'Osto, M Marsili, M Vanzan, D Toffoli, M Stener, S Corni, E Coccia *"Peeking into the Femtosecond Hot-Carrier Dynamics Reveals Unexpected Mechanisms in Plasmonic Photocatalysis"* J. Am. Chem. Soc, 146, 3, 2208 (2024)

45. N. Domenica, P. Grobas Illobre, M. Marsili, M. Stener, D. Toffoli, E. Coccia *"Time evolution of plasmonic features of pentagonal Ag clusters"* Molecules 28, 5671 (2023)

44. A. N. Koya, M. Romanelli, J. Kuttruff, N. Henriksson, A. Stefancu, G. Grinblat, A. De Andres, F. Schnur, M. Vanzan, M. Marsili, M. Rahaman, A. V. Rodríguez, T. Tapani, H. Lin, B. D. Dana, J. Lin, G. Barbillon, R. Proietti Zaccaria, D. Brida, D. Jariwala, L. Veisz, E. Cortes, S. Corni, D. Garoli, N. Maccaferri "*Advances in ultrafast plasmonics"* Applied Physics Reviews 10, 021318 (2023)

43. A. Ciniero, G. Fatti, M. Marsili, D. Dini, M.C. Righi, "*Defects drive the tribocharging strength of PTFE: An ab-initio study*", Nano Energy 112, 108502 (2023)

42. P. Restuccia, G. Losi, O. Chehaimi, M. Marsili, M.C. Righi, "*High-Throughput First-Principles Prediction of Interfacial Adhesion Energies in Metal-on-Metal Contacts*", ACS Applied Materials & Interfaces 15, 19624 (2023)

41. M. Marsili and S. Corni *"Electronic Dynamics of a Molecular System Coupled to a Plasmonic Nanoparticle Combining the Polarizable Continuum Model and Many-Body Perturbation Theory"* J. Phys. Chem. C , 126, 8768 (2022)

40. Z. Xu, D. Ferraro, A. Zaltron, N. Galvanetto, A. Martucci, L. Sun, P. Yang, Y. Zhang, Y. Wang, Z. Liu, J. D. Elliott, M Marsili, Luca Dell'Anna, P. Umari, and Michele Merano *"Optical detection of the susceptibility tensor in two-dimensional 2 crystals"* Communication Physics 4, 215 (2021)

39. M. Vanzan, M. Marsili[+], and S. Corni "*Study of the rate determining step of Rh catalyzed CO_2 reduction: insight on the hydrogen assisted molecular dissociation"* Catalysts 11, 538 (2021) [+] corresponding author

38. P. Grobas Illobre, M. Marsili[+], S. Corni, M. Stener, D. Toffoli, and E. Coccia, *"Time-resolved excited-state analysis of molecular electron dynamics by TDDFT and Bethe-Salpeter formalisms"* Journal of Chemical Theory and Computation*, 17, 6314 (2021)* [+] corresponding author

37. M. Marsili, A. Molina Sanchez, M. Palummo, D. Sangalli, and A. Marini *"Many-Body perturbation theory in a non-collinear spinorial basis: spin properties of the excitonic states in paradigmatic Transition Metal Dichalcogenides"* Phys. Rev. B 103 (15), 155152 (2021)

36. E. Coccia, J. Fregoni, C. A. Guido, M. Marsili, S. Pipolo, and S. Corni *"Theoretical models for nanophotonics"* Journal of Chemical Physics 153, 200901 (2020)

35. J. D. Elliott, Z. Xu, P. Umari, G. Jayaswal, M. Chen, X. Zhang, A. Martucci, M. Marsili, and M. Merano, *"Surface susceptibility and conductivity of MoS2 and WSe2 monolayers: A first-principles and ellipsometry characterization"* Phys. Rev. B 101, 045414 (2020)

34. J. D. Elliott, N. Colonna, M. Marsili, N. Marzari, P. Umari, *"Koopmans meets Bethe-Salpeter: Excitonic optical spectra from GW-free simulations"* Journal of Chemical Theory and Computation 15, 3710 (2019)

33. D Sangalli, A Ferretti, H Miranda, Claudio Attaccalite, I Marri, E Cannuccia, P Melo, M Marsili, F Paleari, A Marrazzo, G Prandini, P Bonfa, MO Atambo, F Affinito, M Palummo, A Molina-Sánchez, C Hogan, M Grüning, D Varsano, A Marini *"Many-body perturbation theory calculations using the yambo code"* Journal of Physics Condensed Matter 31, 325902 (2019)

32. P. Giannozzi et al. *"Advanced capabilities for materials modelling with Quantum ESPRESSO"* , Journal of Physics: Condensed Matter 29 (46), 465901 (2017)

31. M. Marsili, E. Mosconi, F. De Angelis, P, Umari "*Large scale GW-BSE calculations with N3 scaling: excitonic effects in dye sensitised solar cells"*, Phys. Rev. B 95, 075415 (2017)

30. E. A. A. Pogna*, M. Marsili*, D. De Fazio, S. Dal Conte, C. Manzoni, D. Sangalli, D. Yoon, A. Lombardo, A. C. Ferrari, A. Marini, G. Cerullo, and D. Prezzi *"Photo-Induced Bandgap Renormalization Governs the Ultrafast Response of Single-Layer MoS2"*, ACS nano 10 (1), 1182-1188 (2016)
* the two authors contributed equally to the work

29. O. Pulci, M. Marsili, V. Garbuio, P. Gori, I. Kupchak, and F. Bechstedt, *"Excitons in two-dimensional sheets with honeycomb symmetry",* Physica Status Solidi 252, 72 (2015)

28. M. Marsili, P.Umari, G. Di Santo, M. Caputo, M. Panighel, A. Goldoni, M. Kumar, and M. Pedio *"Solid state effects on the electronic structure of H2OEP",* Phys. Chem. Chem. Phys. 48, 27104 (2014)

27. C. Verdi, E. Mosconi, F. De Angelis, M. Marsili, and P. Umari, "*Alignment of energy levels in dye/semiconductor interfaces by GW calculations: effects due to co-adsorption of solvent molecules",* Physical Review B 90, 155410 (2014)

26. A. Compagnin, M. Meneghini, V. Giliberto, M. Barbato, M. Marsili, A. Cester, E. Zanoni, G. Meneghesso *"Thermal and electrical characterization of catastrophic degradation of silicon solar cells submitted to reverse current stress"*, Photovoltaic Specialists Conference (PVSC), 2013 IEEE 39th , 1826 (2013)

25. M. Marsili, S. Botti, M. Palummo, E. Degoli, O. Pulci,H-C Weissker, M.A.L. Marques, S. Ossicini, R. Del Sole, *"Ab-Initio Electronic Gaps of Ge Nanodots: The Role of Self-Energy Effects",* Journal of Physical Chemistry C 117 14229 (2013)

24. M. Marsili and P. Umari, "*Method for the fast evaluation of Fock exchange for non-localized wave functions"* Phys. Rev. B 87, 205110 (2013)

23. V. Garbuio, M. Cascella, R. Del Sole, M. Marsili, and O. Pulci *"Excited state properties of formamide in water solution: an ab-initio study"* J. Chem. Phys. 137, 164317 (2012)

22. P. Gori, O. Pulci, M. Marsili, and F. Bechstedt, *"Side-dependent electron escape from graphene- and graphane-like SiC layers"* Appl. Phys. Lett. 100, 043110 (2012)

21. O. Pulci, P. Gori, M. Marsili, V. Garbuio, R. Del Sole, F. Bechstedt, *"Strong excitons in hydrogenated two-dimensional group-IV crystals"* Europhysics Letters 98, 37004 (2012)

20. M. Pesce, M. Maugeri, M. Marsili, M. Zarcone, D. Tonini, C. Bottosso , M. Galiazzo, and A. Tomasi, *"Technological and economic assessment of two-steps printing processes in a mc-Si solar cells production environment"* Energy Procedia 21, 24 (2012)

19. A.I. Shkrebtii, M. Marsili, E. Heritage, O. Pulci, R. Del Sole and F. Bechstedt *"Defect induced modification of the surface gap and optical properties of C(111)2×1 surface"* Physica Status Solidi A, 209 669 (2012)

18. R. Guerra, M. Marsili,O. Pulci, and S. Ossicini "*Local-Field Effects in Silicon Nanoclusters"* Phys. Rev. B 84, 075342 (2011)

17. M. Schwitters, D. S. Martin, P. Unsworth, T. Farrell, J. E. Butler, M. Marsili, O. Pulci, and P. Weightman *"The contribution of steps to the optical properties of vicinal Diamond (100):H surfaces ".* Phys. Rev. B 83, 085402 (2011)

16. M. Marsili and O. Pulci *"The fascinating physics of carbon surfaces: first-principles study of hydrogen on C(001), C(111), and graphene."* J. Phys. D: Appl. Phys. 43 374016 (2010)

15. O. Pulci, P. Gori, M. Marsili, V. Garbuio, A. P. Seitsonen, F. Bechstedt , A. Cricenti, R. Del Sole *"Ab initio calculations of electronic and optical properties of group IV 2-dimensional materials".* Phys. Stat. Solidi (a). 207, 291 (2010)

14. R. Guerra, E. Degoli, M. Marsili, O. Pulci and S. Ossicini *"Local-fields and disorder effects in free-standing and embedded Si nanocrystallites".* Phys. Stat. Solidi (b) 247, 2113 (2010)

13. O. Pulci, E. Degoli, F. Iori, M. Marsili, M. Palummo, R. Del Sole, and S. Ossicini "*Electronic and optical properties of Si and Ge nanocrystals: an ab-initio study***"** Superlattices and Microstructures 47, 178 (2010)

12. A. Mosca Conte, V. Garbuio, M. Marsili, E. Ippoliti, R. Del Sole, P. Carloni, and O. Pulci *"Excited state properties calculations: applications to biological systems"* Nuovo Cimento C, 32, 73 (2009)

11. M. Marsili, O. Pulci, M. Palummo, P. L. Silvestrelli, R. Del Sole "*Electronic and optical properties of acetylene and ethylene on Si(001)"* Superlattices and Microstructures 46, 240 (2009)

10. M. Marsili, O. Pulci, F. Bechstedt, and R. Del Sole *"Tight-binding calculations of quasiparticle wave functions for C(111)2x1"* Phys. Rev. B 78, 205414 (2008)

9. M. Marsili, N. Witkowski, O. Pulci, O. Pluchery, P. L. Silvestrelli, R. Del Sole, Y. Borensztein, *"Adsorption of small hydrocarbon molecules on Silicon surfaces: ethylene on Si(001)"* , Phys. Rev. B 77, 125337 (2008)

8. S. Ossicini et al., "*First Principle Study of Silicon Nanocrystals: Structural and Electronic Properties, Absorption, Emission and Doping*" Journal of Nanoscience and Nanotechnology 8, 479 (2008)

7. F. Sottile, M. Marsili, V. Olevano, L. Reining, "*Efficient ab initio calculations of bound and continuum excitons in the absorption spectra of semiconductors and insulators*", Phys. Rev. B 76, 161103(R) (2007)

6. M. Marsili, V. Garbuio, M. Bruno, O. Pulci, M. Palummo, E. Degoli, E. Luppi, R. Del Sole "*Excited state properties calculations from 0 to 3 dimensional systems*", EPIOPTICS-9, Proceedings of the 34th Course of the International School of Solid State Physics, Erice (Italy) (2007)

5. M. Marsili, O. Pulci, F. Fuchs, F. Bechstedt, R. Del Sole, "*Many body effects in the electronic and optical properties of the (111) surface of diamond*" , Surf. Sci. 601, 4097 (2007)

4. O. Pulci, M. Marsili, P. Gori, M. Palummo, A. Cricenti, F. Bechstedt, and R. Del Sole, "*Geometry and electronic band structure of surfaces: the case of Ge(111):Sn and C(111)*", Appl. Phys. A 85, 361 (2006)

3. M. Marsili, O. Pulci, F. Bechstedt, and R. Del Sole, "*Electronic structure of the (111) surface of diamond: Solution by self-consistent many body calculation*", Phys. Rev. B 72, 115415 (2005)

2. O. Pulci, M. Palummo, M. Marsili, and R. Del Sole ,"*Theory of Surface Optical Properties*" , Adv. in Solid State Phys. Vol. 45, 161-172 (2005)

1. O. Pulci, M. Marsili, E. Luppi, C. Hogan, F. Sottile, R. Magri, and R. Del Sole, "*Electronic excitations in solids: Density Functional and Green's function Theory*", Phys. Stat. Solidi (b) 242, 2737 (2005)

INVITED TALKS AT INTERNATIONAL CONFERENCES AND WORKSHOPS

"Theoretical description of photoinduced phenomena: from the basic theory to real-time electronic dynamics in complex systems" keynote lecture to the "Ladies' Day" of the DFG research unit FOR 2824 "Amorphous Molecular Materials with Extreme Non-Linear Optical Properties" INT Karlsruhe, Germany May 24th, 2024

"Plasmon enhanced photocatalysis of CO2 methanation within a GW-BSE active space". CECAM workshop "Green's function methods: the next generation 5" Tolosa, France 15-18 Nov. 2022

"Multiscale modeling of nanoparticle-molecule charge injection"
ERC TAME Plasmons Closing Workshop Virtual meeting – 22-24 Sept. 2021

"First principle insights on MoS2 ultrafast response: the role of photo-induced band gap renormalization"
at the international conference "Ultra-fast phenomena in quantum physics: a challenge for theory & experiment", April 11-16 2016 CECAM-HQ-EPFL, Lausanne (Switzerland)

"Method for an accurate determination of electronic and optical properties of large systems within GW-BSE"
at the international conference "Trends in GW-approaches for Nano-Sciences in Europe", July 25-26, 2013 Karlsruhe (Germany)

"The contribution of steps on the optical properties of C(100):H"
at the international conference "Nanoscience and Nanotechnology", Sept 20-23, 2010 Frascati (Italy)

"Electronic and optical properties of graphane and related 2-D systems"
at the European Conference on Surface Science (ECOSS 27) Aug 29-Sept 3, 2010 Groningen (Netherlands)

"Quasi-particle calculations beyond Kohn-Sham and GoWo: self-consistency and vertex corrections"
at the international conference "Epioptics-11", June 19-25, 2010 Erice (Italy)

"Theory of optical properties (1): single particle approach applied to ethylene on Si(100)"
at the international conference "Epioptics-10", June 20-27, 2008 Erice (Italy)

LECTURES AND TUTORING AT INTERNATIONAL SCHOOLS

"Introduction to linear response"
Ab initio many-body perturbation theory: from equilibrium to time-resolved spectroscopies and nonlinear optics, May 22-26 (2023) Rome (Italy)

Tutor for the *"Analysis of excitonic spectra, BSE solvers and convergence"* hands-on session of the "Ab-initio Many-Body Methods and Simulations with the Yambo Code" 04-08 April 2022, ICTP, Trieste Italy

"Introduction to the BSE" (lecture) *and* Co- supervisor of the hands-on session on BSE
Excitations in Realistic Materials using Yambo on Massively Parallel Architectures, April 13-17 2015 CECAM-HQ-EPFL, Lausanne, Switzerland

*"Introduction to GW in QE: the GWW code" (*lecture)
Supervisor of the hands-on session on GW.
Summer School on Atomistic Materials Modelling, Pune, India, 30 June-15 July 2014

INVITED SEMINARS

"Electronic dynamics of a molecular system coupled to a plasmonic nanoparticle combing the polarizable continuum model and many-body perturbation theory" Sept 24, 2021 ETSF online seminars

"Accurate calculations of electronic and optical properties of materials: theory, applications and perspectives."
June 23, 2017 - Dipartimento di Ingegneria civile, ambientale e meccanica - Università degli studi di Trento - Trento - Italy

"Accurate first principle calculations of electronic and optical properties of large systems"
December 17 2013, S3 CNR-INFM - Modena (Italy)

"Accurate calculations of optical spectra for large systems"
November 22 2013, INFN - Frascati (Italy)

"Accurate calculations of optical spectra for large systems"
October 16 2013, SISSA – Trieste, (Italy)

"First principle calculations of excited properties of materials: the electronic and optical properties of Si, Ge, and SiC 2dimensional crystals"
15 March 2013 IPCMS, CNRS Strasbourg (France)

"Many-body effects in Si, Ge and SiC two-dimensional crystals"
July 10 2012 University of Würzburg, Physics and Astronomy Faculty, Würzburg (Germany)

CONTRIBUTED TALKS AT INTERNATIONAL CONFERENCES AND WORKSHOPS

"High throughput first-principle prediction of tribological properties of solid-solid interfaces using VASP"
Vienna Ab-initio Simulation Package (VASP) and Applications ONLINE CONFERENCE, UNIVERSITY OF ÉVORA Feb. 14-15 2024

"High throughput first-principle prediction of interfacial adhesion energies in metal-on-metal contacts"
DPG Spring Meeting (SKM23), March 26 - 31, 2023 Dresden (Germany)

"Ultra-fast transient absorption spectra of monolayer MoS2 by first principle"
DPG Spring Meeting of the Condensed Matter Section, March 15-20 2015 Berlin (Germany)

"Effect of crystal packing on the electronic properties of free base porphyrins"
DPG Spring Meeting of the Condensed Matter Section, 30 March - 04 April 2014 Dresden (Germany)

"Many-body effects in hydrogenated Ge, Si and SiGe nanoparticles"
Theory, Simulation and Modelling of SiGe Nanostructures: from Nanoelectronics to Renewable Energy, June 3-6, 2013 CECAM-HQ-EPFL, Lausanne, Switzerland

"Accurate calculation of optical excitations for large systems"
DPG Spring Meeting of the Condensed Matter Section, March 10-15 2013 Regensburg, Germany

"The effects of steps on the optical properties of C(100):H"
European Conference on Surface Science (ECOSS 27) Aug 29-Sept 3, 2010 Groningen, Netherlands

"Quantum confinement effects on the electronic and optical properties of Ge nanocrystals"
13th Nanoquanta-ETSF Workshop on Electronic Excitations: Theoretical Spectroscopy and Quantum Transport, September 22-27, 2008 Pugnochiuso, Italy

"C(111)2×1 a tight-binding model toward quasiparticle wavefunctions"
5th Nanoquanta-ETSF Young Researchers' meeting, May 20-23, 2008 Modena, Italy

"Many body effects in the electronic and optical properties of the (111) surface of diamond"
24th European Conference on Surface Science, September 4-8, 2006 Paris, France

"Electronic band structure and optical properties of the (111) surface of diamond "
Optic of Surfaces and Interfaces (OSI-VI), June 6-10, 2005 Aalborg, Denmark

"Electronic band structure of the C(111)2X1 surface within an iterative GW scheme"
Theory and Modelling of Electronic Excitations in Nanoscience
September 19-23, 2004 Acquafredda di Maratea, Italy.

"Electronic structure of the diamond (111) surface within a self-consistent GW scheme"
1st Nanophase/Nanoquanta Young Researchers' Meeting
May 6-8, 2004 Palaiseau, France

INSTITUTIONAL SERVICE ACTIVITY

2023- Member of the “Commissione per l’orientamento” del CdS di Scienza dei Materiali

2008-2011 Member of the European Theoretical Spectroscopy Facility (funded under FP7-INFRASTRUCTURES Grant agreement ID: 211956) "Improving Communication, Dissemination, and Widening Understanding" implementation team.

TEACHING (traduzione italiana)

2023-24 University of Bologna
Physics Bachelor
Class: Thermal Phenomena - 6CFU (Modulo 2, 16 h)

2023-24 University of Bologna
Materials Science Bachelor
Class: Material Science 1- 6CFU (Modulo 1, 40 h)

2022-23 University of Bologna
Physics Bachelor
Class: Thermal Phenomena - 6CFU (Modulo 2, 12 h)

2013-14 University of Padova (Italy)
Physics Lab Teaching Assistant
(Attività formative di supporto per un totale di 24h)
Class: Classical Mechanics Lab, corso di laurea di Ingegneria dell’Informazione

2013-14 University of Padova (Italy)
Physics Lab Teaching Assistant
(Attività formative di supporto per un totale di 24h)
Class: Electromagnetism Lab, corsi di laurea di Ingegneria dell’Informazione e dell’Energia

2012-13 University of Padova (Italy)
Physics Lab Teaching Assistant
(Attività formative di supporto per un totale di 24h)
Class: Classical Mechanics Lab, corsi di laurea di Ingegneria Biomedica, dell’Informazione, Elettronica e Informatica.

2012-13 University of Padova (Italy)
Physics Lab Teaching Assistant
(Attività formative di supporto per un totale di 24h)
Class: Electromagnetism Lab corsi di laurea di Ingegneria dell’Ambiente e Territorio, Civile, dell’Energia, Meccanica e Aerospaziale

2012-13 University of Rome 'Tor Vergata' (Italy)
DFT hands-on tutorial
Lessons for a total of 6 hours
Class: Solid State Physics, Corso di Laurea Magistrale di Scienze e Tecnologia dei Materiali

2007-08 University of Rome 'Tor Vergata' (Italy)
Introduction to Time Dependent Density Functional Theory
Lessons for a total of 12 hours
Class: Solid state theory, Corso di Laurea Magistrale di Scienze e Tecnologia dei Materiali

2006-07 University of Rome 'Tor Vergata' (Italy)
Atomic and structure form factor
Lessons for a total of 4 hours
Class: Solid state theory, Corso di Laurea Magistrale in Fisica

2006-07 University of Rome 'Tor Vergata' (Italy)
Introduction to Time Dependent Density Functional Theory
Lessons for a total of 12 hours
Class: Solid state theory, Corso di Laurea Magistrale di Scienze e Tecnologia dei Materiali

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SOCIAL ENGAGEMENT

2023 Organization of the event “Alla Scoperta dei Premi Nobel nella Scienza dei Materiali: i Quantum Dot” 23 Jan 2024.
The target audience of the event were high school teachers and students. Participation: more than 100 registered participants.

2021 Conceivement and development of interactive workshops for the local primary schools on internet and device safety and security.

2015 Development of small sets of laboratory classes for teaching physics and scientific reasoning in preschool and elementary school. See: https://www.pd.infn.it/main/events/cosmo_divulg_30apr.pdf

2007-09 Organization of a survey on the use of fixed-term contracts by the University of TorVergata (http://people.fisica.uniroma2.it/~pdr/index.html). The results were presented to the Physics Department Council.

Bologna 10/07/2024