Margherita Marsili

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EDUCATION

2022 **Habilitation as Italian Professor**
Associate Professor in Theoretical Condensed Matter Physics (02/B2 FIS/03)

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

2005 **Fondazione Angelo Della Riccia fellowship**

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 AND RESEARCH ACTIVITIES

July 2025- **Associate Professor**
Physics Department, Alma Mater Studiorum University of Bologna

2022-25 **Assistant Professor**,
Physics Department, Alma Mater Studiorum University of Bologna
Coordination of the development and maintenance of Tribchem, a publicly distributed software for the automatic and high-throughput study of solid-solid interfaces. Computational material design for surface and interface optimization. High-entropy alloy surface and interface properties. Electronic and mechanical properties of materials subject to uniaxial load.

2018-21 **Postdoctoral Research Associate,**
Chemistry Department, University of Padova
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

2017-18 Postdoctoral Research Associate,
Ecole Polytechnique, Palaiseau (France)
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

2014-15 Postdoctoral Research Associate,
CNR-NANO S3, Modena
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

2012-14 Postdoctoral Research Associate,
Astronomy and Physics Department, University of Padova
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

2006-11 Postdoctoral Research Associate,
University of Rome 'Tor Vergata'
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

2006 Postdoctoral Research Associate,
Ecole Polytechnique, Palaiseau (France)
Efficient formulation for the exchange and correlation kernel of time-dependent density-functional theory for extended systems. Supervisor: Dr. Francesco Sottile

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

2021-22 **Scuola Media Ruzante,** Padova (Italy)
Middle school maths and science teacher.

2015-17 **Scuola Media Ruzante,** Padova (Italy)
Middle school maths and science teacher.

2011-12 **Xgroup SPA,** San Pietro in Viminario (Italy)
Full-time R&D employee, responsible for the solar cell manufacturing company's research projects concerning 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

INSTITUTIONAL ACTIVITIES

2023-present Member of the "Commissione per l'orientamento" of the Bachelor in Material Science course, University of Bologna.

2024-present Member of the "Commissione Assicurazione della Qualità" of the Bachelor in Physics course, University of Bologna.

2024-present Member of the "Gruppo di Lavoro Pari Opportunità e Inclusione" of the Physics and Astronomy Department, University of Bologna.

2024 Member of the "Commissione passaggio anno del dottorato in Nanoscienze", University of Bologna (11/10/2024).

2024 Member of the "Commissione per gli esami finali del dottorato di ricerca in Fisica", University of Roma Tor Vergata (05/07/2024).

2024 Member of the "Commission for the discussion of the doctoral thesis in Physics", University of Padova (16/04/2024).

2008-11 Member of the European Theoretical Spectroscopy Facility (funded under FP7-INFRASTRUCTURES Grant agreement ID: 211956) "Improving Communication, Dissemination, and Widening Understanding" implementation team.

COORDINATION OF RESEARCH ACTIVITIES, PROJECTS AND CPU-TIME GRANTS

2023 -present Coordination of Tribchem developer team. Tribchem is an open-source software devoted to the first principle calculation of tribological properties of solid-solid interfaces. (See https://triboteam.gitlab.io/tribchem/)

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/GPU-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 porphyrin films."Assigned budget: 2.500.000 CPU h @fermi.cineca.it

METHODOLOGICAL DEVELOPMENTS, CODE IMPLEMENTATION AND OPTIMIZATION

Large part of my research work is and has been devoted to methodological developments and implementations in open-source publicly distributed codes (under GPL licence) such as Quantum Espresso, WaveT-TDPLAS, and Tribchem. This work is documented in publications n. 41, 38, 32, and 31 (see the publication list below). Between 2014 and 2020 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). Currently I am coordinating the developer team of Tribchem.

2022-present Coordination of Tribchem (https://gitlab.com/triboteam/tribchem) developer team. Tribchem is a software specifically designed to perform automated studies of solid-solid interfaces.

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

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

2014-20 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/)

PARTICIPATION TO RESEARCH PROJECTS/NETWORKS

2024-present European Theoretical Spectroscopy Facility (ETSF) Research Team Leader

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

2021-22 Team member of the international project H2020 ProID

2018-21 Team member of the international project H2020 ERC “TAME Plasmons - A Theoretical chemistry approach to time-resolved molecular plasmonics”

2014-15 Team member of the national project FIRB “Flashit - Analisi dei fenomeni ultraveloci fotoindotti alla scala nanometrica: una approccio teorico sperimentale”

2010-11 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)

WORKSHOPS AND CONFERENCES ORGANISATION

2015
Conference “Excitations in Realistic Materials using Yambo on Massively Parallel Architectures”,

Place/Date CECAM-HQ-EPFL, Lausanne, Switzerland 13-17 April
Role Member of the organising committee

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

2010
Conference "15th ETSF Workshop on Electronic Excitations - New Frontiers in Theoretical Spectroscopy and Quantum Transport"
Place/Date Berlin, Germany, October 12-15
Role Member of the organising committee

2006
Conference "3rd Nanoquanta Young Researchers Meeting"

Place/Date Rome, Italy, May 3-5
Role Member of the organising committee

INVITED TALKS AT INTERNATIONAL CONFERENCES AND WORKSHOPS

2025
Talk title "Novel Mechanisms in Plasmonic Photocatalysis revealed by a multiscale GW-BSE/continuum approach"
Conference Metamaterials, Photonic Crystals and Plasmonics (META) 2025
Date/Place July 22-25, 2025, Malaga, Spain

2025
Talk title "Automating Calculations for Advancing Solid Interfaces and Tribology"

Conference PASC 2025 - Fair by design HPC-driven research minisymposium
Date/Place June 16-18, 2025, Brugg, Switzerland

2024
Talk title "Developing tools in computational tribology for the high-throughput modeling of solid-solid interfaces"
Conference CMT@BRIXEN
Date/Place Aug 28-30, Bressanone, Italy

2024 (Keynote Lecture)
Talk title "Theoretical description of photoinduced phenomena: from the basic theory to real-time electronic dynamics in complex systems"
Conference "Ladies' Day" of the DFG research unit FOR 2824 meeting,
Date/Place May 24th INT Karlsruhe, Germany

2022

Talk title "Plasmon enhanced photocatalysis of CO2 methanation within a GW-BSE active space"

Conference CECAM workshop "Green's function methods: the next generation 5"

Date/Place Nov 15-18, Tolosa, France

2021

Talk title "Multiscale modeling of nanoparticle-molecule charge injection"

Conference ERC TAME Plasmons Closing Workshop

Date/Place 22-24 Sept, Virtual meeting

2016

Talk title "First principle insights on MoS2 ultrafast response: the role of photo-induced band gap renormalization"

Conference Ultra-fast phenomena in quantum physics: a challenge for theory & experiment

Date/Place April 11-16, CECAM-HQ-EPFL, Lausanne (Switzerland)

2013

Talk title "Method for an accurate determination of electronic and optical properties of large systems within GW-BSE"

Conference Trends in GW-approaches for Nano-Sciences in Europe

Date/Place July 25-26, Karlsruhe (Germany)

2010

Talk title "The contribution of steps on the optical properties of C(100):H"

Conference Nanoscience and Nanotechnology

Date/Place Sept 20-23, Frascati (Italy)

2010

Talk title "Electronic and optical properties of graphane and related 2-D systems"

Conference European Conference on Surface Science (ECOSS 27)

Date/Place Aug 29-Sept 3, Groningen (Netherlands)

2010

Talk title "Quasi-particle calculations beyond Kohn-Sham and GoWo: self-consistency and vertex corrections"

Conference Epioptics-11

Date/Place June 19-25, Erice (Italy)

2008

Talk title "Theory of optical properties (1): single particle approach applied to ethylene on Si(100)"

Conference: Epioptics-10
Date/Place: June 20-27, Erice (Italy)

LECTURES AND TUTORING AT INTERNATIONAL SCHOOLS

2023

Lecture title: "Introduction to linear response"
School: Ab-initio many-body perturbation theory: from equilibrium to time-resolved spectroscopies and nonlinear optics
Date/Place: Sept 20-23, 2010 Frascati (Italy)

2022

Tutoring session: "Analysis of excitonic spectra, BSE solvers and convergence" hands-on session
School: Ab-initio Many-Body Methods and Simulations with the Yambo Code
Date/Place: 04-08 April 2022, ICTP, Trieste Italy

2015

Lecture title: "Introduction to the BSE"

School: Excitations in Realistic Materials using Yambo on Massively Parallel Architectures
Date/Place: April 13-17, CECAM-HQ-EPFL, Lausanne, Switzerland

2014

Lecture title: "Introduction to GW in QE: the GWW code" + supervisor of the hands on session on GW,
Conference: Summer School on Atomistic Materials Modelling
Date/Place: Pune, India, 30 June-15 July 2014

INVITED SEMINARS

2021

Talk title: "Novel Mechanisms in Plasmonic Photocatalysis revealed by a multiscale GW-BSE/continuum approach"
Date/Place: Sept 24, 2021 ETSF online seminars

2017

Talk title: "Accurate calculations of electronic and optical properties of materials: theory, applications and perspectives"

Date/Place: June 23, 2017 - Dipartimento di Ingegneria civile, ambientale e meccanica - Università degli studi di Trento - Trento - Italy

2013

Talk title: "Accurate first principle calculations of electronic and optical properties of large systems"

Date/Place December 17 2013, S3 CNR-INFM - Modena (Italy)

2013

Talk title "Accurate calculations of optical spectra for large systems"

Date/Place November 22 2013, INFN - Frascati (Italy)

2013

Talk title "First principle calculations of excited properties of materials: the electronic and optical properties of Si, Ge, and SiC 2-dimensional crystals"

Date/Place 15 March 2013 IPCMS, CNRS Strasbourg (France)

2012

Talk title "Many-body effects in Si, Ge and SiC two-dimensional crystals"

Date/Place July 10 2012 University of Würzburg, Physics and Astronomy Faculty, Würzburg (Germany)

TEACHING

2024-25
Class Scienza dei Materiali 1, Modulo 1 (40 h)
Where University of Bologna
Corso di laurea in Scienza dei Materiali

2024-25
Class Fisica della Materia, Modulo 2 (36 h)
Where University of Bologna
Corso di laurea in Fisica

2023-24
Class Fenomeni Termici, Modulo 2 (16 h)
Where University of Bologna
Corso di laurea in Fisica

2023-24
Class Scienza dei Materiali 1, Modulo 1 (40 h)
Where University of Bologna
Corso di laurea in Scienza dei Materiali

2022-23
Class Fenomeni Termici, Modulo 2 (12 h)
Where University of Bologna
Corso di laurea in Fisica

2022-23
Class Fisica, Modulo 3 (36 h)
Where University of Bologna
Corso di laurea in Scienze Biologiche

2013-14
Class Classical Mechanics Lab (24h - Attività formative di supporto - tutoring)
Where University of Padova

Corso di laurea di Ingegneria dell'Informazione

2013-14
Class Electromagnetism Lab (24h - Attività formative di supporto - tutoring)
Where University of Padova
Corsi di laurea di Ingegneria dell'Informazione e dell'Energia

2012-13
Class Classical Mechanics Lab (24h - Attività formative di supporto - tutoring)
Where University of Padova
Corsi di laurea di Ingegneria Biomedica, dell'Informazione, Elettronica e Informatica.

2012-13 Electromagnetism Lab (24h - Attività formative di supporto - tutoring)
Class University of Padova
Where Corsi di laurea di Ingegneria dell'Ambiente e Territorio, Civile, dell'Energia, Meccanica e Aerospaziale

2012-13
Lessons DFT hands-on tutorial (6h)
Class Solid State Physics
Where University of Rome 'Tor Vergata' (Italy)
Corso di Laurea Magistrale di Scienze e Tecnologia dei Materiali

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

2006-07
Lessons Atomic and structure form factor (4 h)
Class Class: Solid state theory
Where University of Rome 'Tor Vergata'
Corso di Laurea Magistrale in Fisica

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

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THESIS CO/SUPERVISION

Name Elisa Damiani (PhD Thesis), ongoing
Topic Multiscale tribology simulation of materials for a sustainable mobility.
Role Supervisor

Name Mohamed Elmahi Mohamed Ahmed (Master Thesis), ongoing
Topic High-throughput screening of 2D-materials/metal interfaces.
Role Co-supervisor

Name Lucrezia Berghenti (Master Thesis), 2024
Topic First-principle study of high-entropy alloys: from bulks to surfaces.
Role Co-supervisor

Name Elisa Damiani Master Thesis (Master Thesis), 2023
Topic Tuning adhesion by chemical modifications: Diamond/Copper interfaces as a case study
towards a high throughput approach.
Role Co-supervisor

THIRD MISSION AND COMMUNITY ENGAGEMENT

2024 Main organizer of the event “Alla Scoperta dei Premi Nobel nella Scienza dei Materiali: dai fullereni al grafene” 25 Nov 2024.
Target audience: high school teachers and students.

2023 Main organizer of the event “Alla Scoperta dei Premi Nobel nella Scienza dei Materiali: i Quantum Dot” 23 Jan 2024.
Target audience: high school teachers and students.

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.

PUBLICATIONS

(To date bibliometric indices from SCOPUS: h-index 19; total citations 7504)

50 C. Goletti, F. Bechstedt, G. Bussetti, L. Ley , M. Marsili, O. Pulci, and P. Chiaradia *“Comment on ``Diamond (111) surface reconstruction and epitaxial graphene interface''* , accepted for publication in Phys. Rev. B (2025)

49. M. Vanzan and M. Marsili[+] *“Theoretical approaches for the description of plasmon generated hot carriers phenomena”* npj Computational Materials10 (1), 222 (2024) [+] corresponding author

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48. G. Dall'Osto, M. Vanzan, S. Corni, M. Marsili, and E. Coccia *"Stochastic Schrödinger equation for hot-carrier dynamics in plasmonic systems"* Journal of Chemical Physics 161 (12) (2024)

47. E. Damiani, M. Marsili, and M.C. Righi *"Tuning the adhesion of diamond/copper interfaces through surface chemical modifications and reconstruction"* Carbon 230, 119555 (2024)

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)
* the two authors contributed equally to the work; + corresponding author

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 *"Hybrid theoretical models for molecular nanoplasmonics"* 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)

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