

UNIVERSITY OF MILAN

Selection procedure for recruiting associate professors under art.18, paragraph 1 and 4, of Law No.240/2010 for competition sector 02/B2 - Fisica Teorica della Materia _____, (scientific-disciplinary sector FIS/03 - Fisica della Materia_) at the Department of FISICA "ALDO PONTREMOLI" Dell'Università Degli Studi di Milano _____, (announcement published in Official Gazette No. 35 of_04/05/2021_) - Competition code 4584

[Pier Luigi Cudazzo]

CURRICULUM VITAE

PERSONAL DATA (DO NOT WRITE YOUR PERSONAL ADDRESS AND LANDLINE OR MOBILE PHONE NUMBER)

Surname	Cudazzo
Name	Pier Luigi
Date of Birth	[20, 09, 1978]

INSERT YOUR CURRICULUM VITAE (up to 30 pages)

CURRENT POSITION (Since March 2018)

Senior Researcher at the Faculté des Sciences, de la Technologie et de la Communication University of Luxembourg (Research group of Prof. Ludger Wirtz) (Luxembourg);
Member of European Theoretical Spectroscopy Facility (ETSF) (www.etsf.eu).

PREVIOUS POSITIONS

June 2017-February 2018

Post-doc at the LSI École Polytechnique Palaiseau (France) on ERC grant SEED

June 2015-May 2017

Post-doc at the LSI École Polytechnique Palaiseau (France) with a Marie Curie fellowship

October 2014-May 2015

Post-doc at the LSI École Polytechnique Palaiseau (France) on ERC grant SEED

January 2009-September 2014

Post-doc at the Nano-Bio Spectroscopy Group, Universidad del Pais Vasco, San Sebastian (Spain)

TITLES

DEGREE TITLE

14/06/2004: "Laurea in Fisica" at Università degli studi dell'Aquila (Italy) with 110/110 cum laude as final score, defending a dissertation in Condensed matter theory: "Theoretical study of the structure and electronic properties of group IV adsorbates on Si(111) surface"

PhD TITLE

12/05/2008: Dottorato di Ricerca in Fisica at Università degli studi dell'Aquila (Italy), defending the dissertation in condensed matter theory: "Superconducting properties of Hydrogen under pressure".

OTHER TITLES

10/04/2017: "Abilitazione Scientifica Nazionale" (ASN): National Scientific Qualification for associate professors in the sector 02/B2.

LANGUAGES

Italian (mother tongue), English (fluent), Spanish (advanced), French (advanced).

PROGRAMMING SKILLS AND NUMERICAL TOOLS

Programming languages:

Fortran, Python, Linux

Numerical Codes:

Quantum Espresso (<http://www.pwscf.org>), Abinit (<http://www.abinit.org>), VASP (<https://www.vasp.at>), YAMBO (<http://www.yambo-code.org>), EXC (<http://www.bethe-salpeter.org>), Octopus (<http://www.tddft.org>)

TEACHING ACTIVITY**COURSES AND MODULES**

2005-2006: Undergraduated course of "Computational Methods" for the degree course in Chemistry (Prof. A. Continenza) at Università Degli Studi dell'Aquila (L'Aquila, Italy) (6 hours as voluntary contribution);

2006-2007: Undergraduated course of "Computational Methods" for the degree course in Chemistry (Prof. A. Continenza) at Università Degli Studi dell'Aquila (L'Aquila, Italy) (6 hours as voluntary contribution);

2006-2007: Lectures on "Density Functional Theory" for the master course of "Molecular Physics" (Master in Physics Prof A. Continenza) at Università Degli Studi dell'Aquila (L'Aquila, Italy) (4 hours as voluntary contribution);

2007-2008: Lectures on "Density Functional Theory" for the master course of "Molecular Physics" (Master in Physics Prof A. Continenza) at Università Degli Studi dell'Aquila

(L'Aquila, Italy) (4 hours as voluntary contribution);

2006-2007: Lectures entitled "Introduction to Superconductivity" for the master course of "Solid State Physics" (Master in Physics Prof A. Continenza) at Università Degli Studi dell'Aquila (L'Aquila, Italy) (5 hours as voluntary contribution);

2007-2008: Lectures entitled "Introduction to Superconductivity" for the master course of "Solid State Physics" (Master in Physics Prof A. Continenza) at Università Degli Studi dell'Aquila (L'Aquila, Italy) (5 hours as voluntary contribution);

2006-2007: Lectures on "Molecular Symmetry and Group Theory" for the master course of "Molecular Physics" (Master in Physics Prof A. Continenza) at Università Degli Studi dell'Aquila (L'Aquila, Italy) (5 hours as voluntary contribution);

2007-2008: Lectures on "Molecular Symmetry and Group Theory" for the master course of "Molecular Physics" (Master in Physics Prof A. Continenza) at Università Degli Studi dell'Aquila (L'Aquila, Italy) (5 hours as voluntary contribution);

2015-2016 Lectures on "Theoretical Spectroscopy" at the LSI École Polytechnique (8 hours);

2016-2017 Lectures on "Theoretical Spectroscopy" at the LSI École Polytechnique (8 hours);

2018-2019: Course of "Solid State Physics" (Bachelor in Physics) at the University of Luxembourg (18 hours);

2019-2020: Course of "Solid State Physics" (Bachelor in Physics) at the University of Luxembourg (18 hours);

2018-2019: Course of "Quantum Mechanics" (Bachelor in Physics) at the University of Luxembourg (18 hours);

2019-2020: Course of "Quantum Mechanics" (Bachelor in Physics) at the University of Luxembourg (18 hours);

ADDITIONAL TEACHING AND STUDENT SERVICE ACTIVITIES

SUPERVISION OF MASTER AND PHD THESIS

2010-2011: Master thesis in Nanosciences of Jeiran Jokar (Universidad del País Vasco, San Sebastian Spain): "Optical properties of pentacene and picene";

2016-2017: PhD thesis in Condensed Matter Physics of Jaakko Koskela (University of Helsinki): "Spectroscopic properties of materials using electronic-structure calculations";

2018-2019: PhD thesis in Condensed Matter Physics of Fulvio Paleari (University of Luxembourg): "First-principles approaches to the description of indirect absorption and luminescence spectroscopy: exciton-phonon coupling in hexagonal boron nitride";

From 2019 PhD thesis in Condensed Matter Physics of Amir Hossein (University of

Luxembourg): "Resonant Raman and time-dependent spectroscopy: applications to perovskites and 2D materials".

SUPERVISION OF POST DOC RESEARCH ACTIVITIES

2018-2020: Post-doc research activity of Dr. Matteo Barborini (University of Luxembourg): Electronic instability in one dimensional systems;

2018-2019: Post-doc research activity of Dr. Engin Torun (University of Luxembourg): Excitonic effects in multilayer transition metal dichalcogenides;

2016-2017: Post-doc research activity of Dr. Giorgia Fugallo (LSI École Polytechnique Palaiseau France): Optical properties of Transition Metal Dichalcogenides;

2013-2014: Post-doc research activity of Dr. Lede Xian (Universidad del País Vasco, San Sebastian Spain): Photocarrier doping in VO₂

2013-2014: Post-doc research activity of Dr. Huseyin Sener Sen (Universidad del País Vasco, San Sebastian Spain): Ab Initio Modeling of Plasmons in Metal-Semiconductor Bilayer Transition Metal Dichalcogenide Heterostructure

INVITED SEMINARS

October 2017: University of Luxembourg, Luxembourg. "Excitonic effects in solids from first principles";

November 2016: Laboratoire de Physique Théorique, Université Paul Sabatier, Toulouse, France. "Plasmon and exciton dispersion in two dimensions";

November 2015: Laboratoire de Physique des Solides (LPS), Université Paris-Sud, Orsay, France. "Plasmon and exciton dispersion in two dimensions";

July 2008: Freie Universität, Berlin, Germany. "Superconductivity and spin-fluctuations";

June 2008: Peter Grünberg Institute (PGI), Jülich, Germany. "Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen";

February 2008: International School for Advanced Studies (SISSA), Trieste, Italy. "Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen"

SCIENTIFIC RESEARCH ACTIVITY

RESEARCH INTERESTS

My present research activity is within theoretical spectroscopy, where we use first principles theoretical tools to simulate, analyze and predict experimental spectra of different materials

involving low-dimensional systems, molecular crystals, charge-density-wave (CDW) systems and strongly correlated materials.

My academic background in condensed matter physics and material science covers several fields ranging from superconductivity, electron-phonon interaction and phase transitions to the electronic and optical properties of matter. The wide variety of issues addressed led me to reach a strong expertise in several and different first-principles theoretical approaches and computational tools that involve Density Functional Theory (DFT) (Quantum Espresso <http://www.pwscf.org>, Abinit <http://www.abinit.org>) with its extension to the superconducting phase (BdG Code) and time-dependent phenomena (TDDFT) (Octopus <http://www.tddft.org>) as well as many-body perturbation theory (MBPT) (YAMBO <http://www.yambo-code.org>, EXC <http://www.bethe-salpeter.org>). Through the application of these methods to real materials and the analysis of the results I was able to infer general pictures of complex phenomena as for example: (i) the physical mechanisms that induce superconductivity in hydrogen and hydrogen-based compounds under pressure; (ii) the mechanisms of the charge transfer in the excited states of molecular crystals; (iii) the physical mechanisms governing exciton dispersion in molecular crystals and two-dimensional systems.

In addition to the applications of these methods, I dedicated a great effort to the development of new theoretical tools in the framework of both DFT and MBPT. This is a long term investment that does not provide immediate results, but it is fundamental to investigate, understand and predict new physical phenomena.

Moreover, during most of my research activity I worked in close collaboration with experimentalists providing interpretations to the experimental spectra and guiding new experiments.

Altogether, the expertise that I have acquired spans several aspects and several fields of condensed matter physics:

Development of new theoretical approaches and implementation of new algorithms in computer codes;

Superconductivity and electron phonon interaction;

Optical properties of complex materials;

Collaboration with experimentalists:

MAIN ACHIEVEMENTS

Development of new theoretical approaches and implementation of new algorithms in computer codes

During my PhD studies at the University of L'Aquila (Italy) I formulated the theory of the isotopic effect in the framework of superconducting DFT (SCDFT) that is the extension of the DFT to the superconducting state. The isotopic effect is the dependence of the superconducting critical temperature on the average isotopic mass. Historically, its discovery was fundamental to understand the superconducting mechanism. Indeed it suggested the idea that an effective interaction between electrons arising from their interaction with crystal lattice vibrations (phonons) was of primary importance in bringing about the condensation. In general, the measure of the isotopic coefficient gives information about the role played by the electron-phonon interaction and represents a fundamental parameter to distinguish between conventional and unconventional superconductivity. I implemented the SCDFT evaluation of the isotopic coefficient as a post-processing of the Bogoliubov-DeGennes (BDG) code used for the solution of the superconducting gap equation, in order to obtain the ab-initio prediction of the isotopic effect of real materials without any semi-empirical parameter.

Moreover still within SCDFT I derived an ab-initio and parameter-free effective electron-electron interaction that goes beyond the screened random phase approximation and accounts for superconducting pairing driven by spin fluctuations. The construction is based on MBPT and relies on the approximation of the exchange-correlation part of the electronic self-energy within TDDFT. This effective interaction is included in an exchange-correlation kernel for SCDFT in order to achieve a completely parameter free superconducting gap equation.

Finally, during my post-doc at the Laboratoire Des Solides Irradiés (LSI) at the Ecole Polytechnique, I worked with a Marie Curie fellowship in collaboration with Dr. Lucia Reining on the development of a new method for the evaluation of the two-particle Green's function. The final aim is to include dynamical effects which are neglected in the standard Bethe-Salpeter equation (BSE), in order to describe multiple excitations. In the new approach, contrarily to the standard BSE where the two-particle Green's function is obtained from the solution of a Dyson-like equation, we start from an integro-differential equation equivalent to the Baym-Kadanoff equation for the single-particle Green's function. I demonstrated that, using suitable approximations, this equation can be solved and allows including dynamical effects induced by electronic correlation in a way that can be implemented as a post processing of standard BSE based codes. Moreover I further generalized the method in order to include the effect of lattice vibration. Presently, I am extending this promising new approach to deal with out-of-equilibrium systems. The final goal is the study of exciton dynamics for applications in excitonics.

Superconductivity and electron-phonon interaction

During the PhD my research activity was dedicated to the study of superconductivity in the framework of SCDFT. I focused on superconductivity in light metals, in particular on hydrogen under high pressure.

The renewed interest in metallic hydrogen (possibly achievable at high pressures) is due to its expected high critical temperature, given the small mass of the ions, the absence of an electronic core that screens the electron-ion interaction and the possible increase of the electron-phonon coupling constant as the density of the system raises e.g. simple metals under high pressure.

Using Density functional perturbation theory (DFPT) I performed a detailed analysis of the electron-phonon interaction in presence of an applied pressure identifying the most important phonon modes and electronic states involved in the electron-phonon coupling in this system. This was a fundamental step for understanding superconductivity, being the electron-phonon coupling one of the main ingredient in SCDFT. Then I investigated the superconducting phase performing ab-initio calculations based on SCDFT.

The study has been able to single out the features which drive the system towards superconductivity at very high temperature: mainly, a rich and complex Fermi surface, strongly coupled phonon modes driving the intra- or inter-molecular charge transfer, anisotropy and the presence of superconducting multigaps.

Being the peculiarity of compressed molecular hydrogen common to other molecular systems under pressure namely hydrides (SiH_4 , CH_4 , SnH_4 ...) that reach a metallic phase at pressure achievable experimentally, the work contributed to open a new path in the research field of superconductivity. An example is represented by SiH_4 or by the recent discovery of superconductivity induced by electron-phonon coupling at the unprecedented temperature of 203 K in sulfur hydride.

Optical properties of complex materials

During my post-doc at the Nanobio Spectroscopy Group in San Sebastian (Spain) and at the LSI my research activity focused on the study of electronic and optical properties of

complex systems. I treated a very broad range of materials and spectroscopies with different theoretical approaches: from low-dimensional systems to molecular solids, charge-density wave systems, and strongly correlated materials. In the following the main research achievements are summarized.

Low-dimensional systems: Using state-of-the-art MBPT, I studied the optical properties of graphane (hydrogenated graphene) and I investigated the excitonic effects in this system. Starting from my ab-initio results, I provided a theory of the macroscopic screening in two-dimensional (2D) systems which has strong implications for describing gap-impurity levels and also the exciton binding energy in the effective mass approximation that is often used to model excitons. Through this study I was able to infer a general picture to explain the huge binding energy of excitons in low-dimensional materials. The theory has been recently used to describe the effective interaction between particles in 2D transition metal dichalcogenides (TMD) in order to model excitons and charged excitons (trions). This allowed explaining several experimental findings as for example the huge exciton and trion binding energy and the non-Rydberg excitonic series observed in optical spectra. Moreover, at the LSI, through the solution of the BSE at finite momentum transfer I investigated for the first time the exciton dispersion in 2D crystals. From the study of three prototypical 2D systems, namely graphane, hBN and phosphorene, I inferred a general picture of the physical mechanisms governing the exciton dispersion in 2D. In particular, I demonstrated that, due to the confinement of the electronic charge on a layer, at low momentum transfer the exciton energy is characterized by a linear dispersion relation which is a feature common to all 2D systems. In addition I demonstrated that in 2D systems the exciton band structure, which can be accessed experimentally, provides a powerful way to identify the exciton character and its degree of localization.

Molecular crystals: Using MBPT I investigated the electronic and optical properties of aromatic molecular crystals (picene, pentacene, tetracene, coronene, etc.). The work, which has been performed in collaboration with the experimental group of Prof. Martin Knupfer (IFW Dresden, Germany), has been focused on excitons as well as collective excitations namely plasmons. The results allowed a deep understanding of the nature of the neutral excitations in this class of materials revealing also the microscopic mechanisms governing their dispersion as a function of momentum transfer. Moreover, from the solution of the BSE, I provided a model for the description of the excitonic effect and exciton dispersion in terms of the excitations of the isolated molecules inferring a general picture of the microscopic mechanisms that give rise to the formation of charge-transfer excitons in molecular crystals. These results have strong implications for both fundamental studies and technological applications.

Layered systems: During the last year of my post-doc at the LSI in the Ecole Polytechnique (Palaiseau, France) I have been the lead scientist in a research work focused on the excitonic effects in bulk layered systems that is part of the PhD thesis of Jaakko Koskela (University of Helsinki, Finland). Within this work, combining my previous experience on 2D materials and molecular systems with ab-initio BSE calculations in bulk hBN, I generalized the model hamiltonian that I used in previous works to describe excitonic effects in molecular crystals to the case of layered systems, which are other prototypical van der Waals materials. In this way a general picture of the exciton physics in terms of the properties of the single layer has been obtained. This result allowed explaining several interesting properties related to the exciton dispersion, the relation between exciton and plasmon excitations, the mechanism of inter-layer charge transfer excitons. Beside molecular crystals and layered materials, the model can be extended to other van der Waals systems involving compounds with lower dimensionality such as clusters of 0D

quantum-dots or 1D quantum wires.

This model was also successfully used to analyze in detail the results of the BSE calculations that Giorgia Fugallo (another post-doc in the group) did in the last years on MoS₂ in collaboration with Francesco Sottile and Matteo Gatti. Finally, this achievement stimulated new research projects on multilayer heterostructures involving transition metal dichalcogenides.

Charge-density-wave (CDW) systems: In the last years of my post-doc at the Nanobio Spectroscopy Group my research activities was devoted to the electronic properties of bulk metallic transition metal dichalcogenides (TMD) which are typical materials displaying CDW instability. In particular my work was focused on the understanding of the physical mechanisms responsible for the unusual negative plasmon dispersion observed experimentally and its link with the CDW instability. Through first principles TDDFT simulations of the loss function in four prototypical TMD belonging to the 2H family (NbSe₂, NbS₂, TaS₂ and TaSe₂), I demonstrated that, contrarily to the previous interpretations based on model calculations, the negative plasmon dispersion is not related to the CDW instability but is an effect related to the particular band structure and represents a peculiarity of this class of materials. The ab initio calculations predicted that also NbS₂ displays a negative plasmon dispersion even though it doesn't have a CDW phase transition. In order to test this prediction, a new EELS experiment was carried out by the group of M. Knupfer (IFW Dresden), who also had authored the first experiment. The results definitely corroborate my interpretation, demonstrating the great capabilities of the first-principles approach that I have employed in this investigation. Moreover, in this research project theory was clearly crucial in making the bridge between two different experimental techniques, namely EELS and inelastic X ray scattering (IXS), and two corresponding experimental groups, that of M. Knupfer and that of S. Huotari (University of Helsinki). This bridging role of theory also stimulated a new similar collaboration between the two experimental groups and the LSI group (as a part of the postdoc of G. Fugallo with F. Sottile and M. Gatti) on the exciton and plasmon dispersion of MoS₂.

MAJOR COLLABORATIONS

Collaboration with theoreticians:

Prof. Angel Rubio, Universidad del Pais Vasco (UPV), San Sebastian (Spain):
electronic and optical properties of complex materials as low-dimensional systems (transition metal dichalcogenides, graphene-based systems), molecular crystals, strongly correlated materials (VO₂);

Prof. E.K.U. Gross, Max Planck Institute of Microstructure Physics, Halle (Germany):
superconductivity in hydrogen and hydrogen compounds under pressure and development of new theoretical tools in the framework of Superconducting Density Functional Theory (SCDFT);

Dr. Lucia Reining, LSI École Polytechnique, Palaiseau (France):
development of new theoretical tools in the framework of MBPT for the evaluation of the charge-charge response function beyond state-of-the-art Bethe-Salpeter equation;

Dr Matteo Gatti and Dr. Francesco Sottile, LSI École Polytechnique, Palaiseau (France):

excitonic effects and exciton dispersion in two-dimensional systems.

Prof. Francesco Mauri, University La Sapienza, Rome (Italy) and Prof. Matteo Calandra, University of Trento (Italy):

Electronic correlations and electron-phonon coupling in CDW systems.

Collaboration with experimentalists:

Prof. Martin Knupfer, IFW Dresden, Germany:

Electron Energy Loss Spectroscopy in transition metal dichalcogenides and molecular crystals;

Dr. Simo Huotari, University of Helsinki:

Inelastic X-rays Scattering in transition metal dichalcogenides and hBN

FELLOWSHIPS AND AWARDS

June 2015: Marie Curie Fellowship at the École Polytechnique with the project entitled: "Dynamical effects on neutral excitations". The objective of the project is the inclusion of dynamical effects in the evaluation of the charge-charge response function beyond the state-of-the-art Bethe-Salpeter equation. The final goal is the description of multiple excitations in the framework of many-body perturbation theory;

November 2012 High-Performance Computing-Europa2 fellowship (3000 euro) for short-term visit at the host group at the Laboratoire des Solides Irradiés (LSI) of the Ecole Polytechnique (Palaiseau, France) to study the exciton dispersion in molecular crystals;

July 2008 Regional fellowship "Assegni regionali per attività di ricerca e alta formazione" for short-term visit at the Freie Universität (Berlin, Germany) (research group of Prof. E.K.U. Gross) to study the effect of the spin-fluctuations on the superconducting phase transition;

2005-2007 PhD fellowship from Università degli studi dell'Aquila (Italy).

ORGANIZATION AND COORDINATION OF RESEARCH ACTIVITIES

Principal investigator in the following projects:

HPC Europa2 "Exciton dispersion in molecular crystals", 20/11/2012-20/12/2012. Group: Dr. Francesco Sottile and Dr. Matteo Gatti (Laboratoire des Solides Irradiés (LSI) of the Ecole Polytechnique, Palaiseau, France);

ESRF project "Plasmon dispersion in layered transition metal dichalcogenides". May 2013, one week of beam-time at the ESRF, Grenoble (France). Group: Dr. Matteo Gatti (LSI Ecole Polytechnique, Palaiseau, France), Dr Simo Huotari (University of Helsinki, Finland);

Marie Curie project "Dynamical effects on neutral excitations" (DENE), 01/06/2015-

31/05/2017. Group: Dr. Lucia Reining (Laboratoire des Solides Irradiés (LSI) of the Ecole Polytechnique, Palaiseau, France).

Leading scientist in scientific collaborations not necessarily related to funded projects as demonstrated by being last author (i.e., the senior scientist) in the related papers:

"Excitons in van der Waals materials: from monolayer to bulk hexagonal boron nitride". Phys. Rev. B 95, 035125 (2017). Result of a collaboration with the Ecole Polytechnique and the University of Helsinki involving 5 scientists;

"Phonon assisted photoluminescence from many body perturbation theory". (Article in preparation). Result of a collaboration with the University of Luxembourg involving 2 scientists;

"Excitonic-insulator instability and Peierls distortion in one-dimensional semimetals". (Article in preparation). Result of a collaboration with the University of Luxembourg and Università La Sapienza (Rome, Italy) involving 4 scientists;

"Excitonic effects in multilayer transition metal dichalcogenides". (Article in preparation). Result of a collaboration with the University of Luxembourg involving 3 scientists.

PARTICIPATION TO FUNDED PROJECTS

ANR 2019: "Anharmonic and exchange interactions in phonon spectra", principal investigator: Prof. Ludger Wirtz (University of Luxembourg, Luxembourg);

ERC 2013-2017: "Seizing electron energies and dynamics: a seed for the future" (SEED), principal investigator: Dr. Lucia Reining (Ecole Polytechnique, Palaiseau, France);

Ministerio de la Ciencia y Innovacion (MICINN) 2011-2013: "Dynamical processes in complex quantum systems: from theoretical developments to energy harvesting and storage" (DYNAPLEX), principal investigator: Prof. Angel Rubio (Universidad del Pais Vasco, San Sebastian, Spain);

Gobierno Vasco 2007-2012 "Simulacion de Nanoestructuras, Biomoleculas y sistemas complejos de interes tecnologico: tecnicas espectroscopicas. ETSF en Espania (Grupos Consolidados y Alto Rendimiento)", principal investigator: Prof. Angel Rubio (Universidad del Pais Vasco, San Sebastian, Spain);

Ministerio de la Ciencia y Innovacion (MICINN) 2009-2011 "Desarrollo de la Vicepresidencia Cientifica de la European Theoretical Spectroscopy Facility (ETSF) - ACI promociona", principal investigator: Prof. Angel Rubio (Universidad del Pais Vasco, San Sebastian, Spain);

Ministerio de Educacion y Ciencia (MEC) 2007-2010 "Aplicaciones en la frontera de la espectroscopia teorica: nanoestructuras y sistemas complejos" (FANCYNANO), principal investigator: Prof. Angel Rubio (Universidad del Pais Vasco, San Sebastian, Spain);

Diputacion Foral de Gipuzkoa 2009-2009 "Consolidacion de la infraestructura cientifica de la ETSF en San Sebastian Proyecto Red Guipuzcoana de Ciencia y Tecnologia e Innovacion",

principal investigator: Prof. Angel Rubio (Universidad del Pais Vasco, San Sebastian, Spain).

EVALUATION OF RESEARCH ACTIVITIES

Reviewer for the following peer-reviewed journals:
Nano Letters, Physical Review Letter, Physical Review B,

OVERVIEW OF THE SCIENTIFIC PRODUCTION

H index: 17 (Source: Web of Science)

N. of total citations: 1436 (Source: Web of Science)

Average citations per item: 49.52 (Source: Web of Science)

Average citations per year: 104.64 (Source: Web of Science)

29 research articles published on international peer-reviewed journals (19 as first author)

7 Invited talks at international conferences

15 Oral presentations and 3 Posters at international conferences

6 Invited seminars at research institutes/Universities

"Abilitazione Scientifica Nazionale" (ASN): National Scientific Qualification for associate professors in the sector 02/B2 from 10/04/2017 to 10/04/2023

SCIENTIFIC PUBLICATIONS

1. Exciton band structure of Molybdenum Disulfide: from monolayer to bulk.
Giorgia Fugallo, Pierluigi Cudazzo, Matteo Gatti and Francesco Sottile.
Electron. Struct. **3**, 014005 (2021);

2. First-principles description of the exciton-phonon interaction: A cumulant approach.
Pierluigi Cudazzo,
Phys. Rev. B **102**, 045136 (2020).

3. Correlation satellites in optical and loss spectra.
Pierluigi Cudazzo, and Lucia Reining.
Phys. Rev. Research **2**, 012032(R) (2020).

4. Direct evaluation of the isotope effect within the framework of density functional theory for superconductors.

Martin Lueders, Pierluigi Cudazzo, Gianni Profeta, Alessandra Continenza, Sandro Massidda, Antonio Sanna, and E.K.U. Gross.

J. Phys. Condens. Matter **31**, 334001 (2019).

5. Collective charge excitations of the two-dimensional electride Ca₂N.

Pierluigi Cudazzo and Matteo Gatti.

Phys. Rev. B **96**, 125131 (2017).

6. Excitons in van der Waals materials: from monolayer to bulk hexagonal boron nitride.

Jaakko Koskela, Giorgia Fugallo, Mikko Hakala, Matteo Gatti, Francesco Sottile, and Pierluigi Cudazzo.

Phys. Rev. B **95**, 035125 (2017).

7. Negative plasmon dispersion in 2H-NbS₂ beyond charge-density-wave interpretation.

Pierluigi Cudazzo, Eric Müller, Carsten Habenicht, Matteo Gatti, Helmuth Berger, Martin Knupfer, Angel Rubio, Simo Huotari.

New Journal of Physics **18**, 103050 (2016).

8. Exciton band structure in two-dimensional materials.

Pierluigi Cudazzo, Lorenzo Sponza, Christine Giorgetti, Lucia Reining, Francesco Sottile, and Matteo Gatti,

Phys. Rev. Lett. **116**, 066803 (2016).

9. Exciton dispersion in molecular solids.

Pierluigi Cudazzo, Francesco Sottile, Angel Rubio, and Matteo Gatti,

J. Phys. Condens. Matter **27**, 113204 (2015).

10. Superconducting pairing mediated by spin-fluctuations from first principles.

F. Essenberger, A. Sanna, A. Linscheid, F. Tandetzky, G. Profeta, P. Cudazzo, and E.K.U. Gross,

Phys. Rev. B **90**, 214504 (2014).

11. Interplay between structure and electronic properties of layered transition-metal dichalcogenides: comparing the loss function of 1T and 2H polymorphs.

Pierluigi Cudazzo, Matteo Gatti, and Angel Rubio,

Phys. Rev. B **90**, 205128 (2014).

12. Instantaneous band gap collapse in photoexcited monoclinic VO₂ due to photocarrier doping.

Daniel Wegkamp, Marc Herzog, Lede Xian, Matteo Gatti, Pierluigi Cudazzo, Christina L. McGahan, Robert E. Marvel, Richard F. Haglund, Jr., Angel Rubio, Martin Wolf, Julia Stähler,

Phys. Rev. Lett. **113**, 216401 (2014).

13. High-energy collective electronic excitations in layered transition-metal dichalcogenides.

Pierluigi Cudazzo, Kari O. Ruotsalainen, Christoph J. Sahle, Ali Al-Zein, Helmuth Berger, Efren Navarro-Moratalla, Simo Huotari, Matteo Gatti, and Angel Rubio,

Phys. Rev. B **90**, 125125 (2014).

14. Local-field effects on the plasmon dispersion of two-dimensional transition metal dichalcogenides.

Pierluigi Cudazzo, Matteo Gatti and Angel Rubio,
New Journal of Physics **15**, 125005 (2013).

15. Frenkel versus charge-transfer exciton dispersion in molecular crystals.

Pierluigi Cudazzo, Matteo Gatti, Angel Rubio and Francesco Sottile
Phys. Rev. B **88**, 195152 (2013).

16. Loss spectroscopy of molecular solids: combining experiment and theory.

Friedrich Roth, Pierluigi Cudazzo, Benjamin Mahns, Matteo Gatti, Johannes Bauer, Silke Hampel, Markus Nohr, Helmuth Berger, Martin Knupfer, and Angel Rubio,
New Journal of Physics **15**, 125024 (2013).

17. Phonon Softening and Direct to Indirect Bandgap Crossover in Strained Single Layer MoSe₂.

S. Horzum, H. Sahin, S. Cahangirov, P. Cudazzo, A. Rubio, T. Serin, F. M. Peeters,
Phys. Rev. B **87**, 125415 (2013).

18. Excitons in molecular crystals from first principles many body perturbation theory: picene vs. pentacene.

Pierluigi Cudazzo, Matteo Gatti and Angel Rubio,
Phys. Rev. B **86**, 195307 (2012).

19. Plasmon dispersion in layered transition-metal dichalcogenides.

Pierluigi Cudazzo, Matteo Gatti, and Angel Rubio,
Phys. Rev. B **86**, 075121 (2012).

20. Plasmon dispersion in molecular solids: Picene and potassium-doped picene.

Pierluigi Cudazzo, Matteo Gatti, Friedrich Roth, Benjamin Mahns, Martin Knupfer, and Angel Rubio,
Phys. Rev. B **84**, 155118 (2011).

21. Dielectric screening in two-dimensional insulators: Implications for excitonic and impurity states in graphane.

Pierluigi Cudazzo, Ilya V. Tokatly, and Angel Rubio,
Phys. Rev. B **84**, 085406 (2011).

22. Electronic properties of molecular solids: the peculiar case of solid picene.

F. Roth, M. Gatti, P. Cudazzo, M. Grobosch, B. Mahns, B. Bchner, A. Rubio and M. Knupfer,
New Journal of Physics **12**, 103036 (2010).

23. Strong Charge-Transfer Excitonic Effects and Bose-Einstein Exciton Condensate in Graphane.

P. Cudazzo, C. Attaccalite, I.V. Tokatly and A. Rubio,
Phys. Rev. Lett. **104**, 226804 (2010).

24. Electron-phonon interaction and superconductivity in metallic molecular hydrogen. II: Superconductivity under pressure.

P. Cudazzo, G. Profeta and A. Continenza, A. Sanna, S. Massidda, A. Floris and E. K. U. Gross,
Phys. Rev. B **81**, 134506 (2010).

25. Electron-phonon interaction and superconductivity in metallic molecular hydrogen. I: Electronic and dynamical properties under pressure.

P. Cudazzo, G. Profeta and A. Continenza, A. Sanna, S. Massidda, A. Floris and E. K. U. Gross,
Phys. Rev. B **81**, 134505 (2010).

26. Multigap superconductivity in Pb and H under pressure and CaBeSi from ab initio calculations.

C. Bersier, A. Floris, P. Cudazzo, G. Profeta, A. Sanna, F. Bernardini, M. Monni, S. Pittalis, S. Sharma, H. Glawe, A. Continenza, S. Massidda and E.K.U. Gross,
Journ. Phys. Condens. Matter **21**, 164209 (2009).

27. Role of coulomb interaction in the superconducting properties of CaC₆; and H under pressure within the density-functional theory for superconductors.

S. Massidda, F. Bernardini, C. Bersier, A. Continenza, P. Cudazzo, A. Floris, H. Glawe, M. Monni, S. Pittalis, G. Profeta, A. Sanna, S. Sharma and E.K.U. Gross,
Supercond. Sci. Technol. **22**, 034006 (2009)..

28. Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen.

P. Cudazzo, G. Profeta, A. Continenza, A. Sanna, S. Massidda, A. Floris and E. K. U. Gross,
Phys. Rev. Lett. **100**, 257001 (2008). (Editor Suggestion)

29. Low temperature phases of Pb/Si(111) and related surfaces.

P. Cudazzo, G. Profeta and A. Continenza,
Surf. Sci. **602**, 747-754 (2008).

Submitted Articles:

1. Collective charge excitations of quasi one-dimensional Charge Density Wave systems: the case of CuTe.

Pierluigi Cudazzo, and Ludger Wirtz.
Phys. Rev. B (submitted).

Articles in preparation:

1. Phonon assisted photoluminescence from first principles: A cumulant approach.

Fulvio Paleari, Ludger Wirtz and Pierluigi Cudazzo

2. Excitonic-insulator instability and Peierls distortion in one-dimensional semimetals.

Matteo Barborini, Francesco Mauri, Matteo Calandra, Ludger Wirtz, and Pierluigi Cudazzo

3. Exciton dispersion in bi-layer TMD heterostructures.

Engin Torun, Pierluigi Cudazzo, and Ludger Wirtz.

PARTICIPATION TO INTERNATIONAL CONFERENCES

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INVITED TALKS AT INTERNATIONAL CONFERENCES:

1. May 2019 Invited Talk at CECAM workshop Green's function methods: the next generation IV, Lausanne, Switzerland.
"Correlation satellites in optical and loss spectra".
2. September 2018 Invited Talk at workshop Excitonic insulator: New perspectives in long-range interacting systems, Lausanne, Switzerland.
"Cumulant expansion of the electronic polarizability: beyond the static Bethe-Salpeter equation".
3. December 2017: Invited Talk at Mini-workshop "REST in Paris": Common problems and solutions in core and valence theoretical spectroscopies, Paris, France.
"Cumulant expansion of the electronic polarizability: beyond the static Bethe-Salpeter equation".
4. September 2016: Invited Talk at Marseille Condensed Matter 2016: Optics and Magnetism, Marseille, France
"Exciton band structure in two-dimensional materials".
5. January 2014: Invited Talk at Benasque 2014: Time-Dependent Density-Functional Theory: Prospects and Applications Benasque, Spain.
"Frenkel versus charge transfer exciton dispersion in molecular crystals".
6. June 2013: Invited Talk at CECAM Workshop Green's function methods: the next generation, Toulouse, France.
"Exciton dispersion in molecular solids".
7. October 2012: Invited Talk at MMM2012-VI International Conference on Multiscale Materials Modeling, Biopolis, Singapore.
"Excitonic Effects in Solids from First Principles".

CONTRIBUTED TALKS AND POSTERS AT INTERNATIONAL CONFERENCES:

1. March 2019: Talk at the APS March Meeting, Boston (USA).
"Correlation satellites in optical and loss spectra".
2. October 2016: Talk at Annual meeting of GDR-I GNT "Graphene and Nanotubes: Science and applications", Saint Pierre d'Oléron (France)
"Exciton band structure in two dimensional materials".
3. June 2016: Talk at JEELS 2016 10eme edition des Journées de l'EELS. Tarragona (Spain).
"Exciton band structure in two dimensional materials".
4. May 2016: Talk at the Roscoff Meeting "The first general meeting of the GDR RES" T, Roscoff (France).
"Plasmon and exciton dispersion in two dimensions".
5. September 2015: Talk at the Discussion Lavoisier "Nouveaux Matériaux bi-dimensionnels: dichalcogénures de métaux de transition et nitrure de bore", Toulouse (France).

"Plasmon and exciton dispersion in two dimensions".

6. September 2015: Poster at the PsiK conference, San Sebastian (Spain).

"Plasmon and exciton dispersion in two dimensions".

7. March 2015: Talk at the DPG Conference, Berlin (Germany).

"Plasmon and exciton dispersion in two dimensions".

8. September 2014: Poster at XIX ETSF Workshop on Electronic Excitations, Saragoza (Spain).

"Interplay between structure and electronic properties of layered transition-metal dichalcogenides: comparing the loss function of 1T and 2H polymorphs".

9. October 2013: Talk at XVIII ETSF Workshop on Electronic Excitations, Luxembourg.

"Exciton dispersion in molecular solids".

10. November 2012: Talk at MORE 2012 Meeting on Optical Response in Extended Systems, Vienna, Austria.

"Plasmon dispersion in layered transition-metal dichalcogenides".

11. October 2012: Talk at XVII ETSF Workshop on Electronic Excitations, Coimbra, Portugal.

"Excitons in molecular solids: picene vs. pentacene".

12. September 2012: Talk at XII international conference ICESS 2012, Saint Malo, France.

"Excitons in molecular solids: picene vs. pentacene".

13. September 2011: Poster XVI ETSF Workshop on Electronic Excitations, Turin, Italy.

"Plasmon dispersion in molecular solids: picene and K3picene".

14. October 2010: Talk at XV ETSF Workshop on Electronic Excitations, Berlin, Germany.

"Strong Charge-Transfer Excitonic Effects and the Bose-Einstein Exciton Condensate in Graphene".

15. June 2010: Talk at VII Nanoquanta-ETSF Young Researchers Meeting, Jyväskylä, Finland.

"Strong Charge-Transfer Excitonic Effects and the Bose-Einstein Exciton Condensate in Graphene".

16. September 2009: Talk at XIV Nanoquanta-ETSF Workshop on Electronic Excitations: Ab-initio Tools for the Characterization of Nanostructures, Evora, Portugal.

"Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen".

17. June 2009: Talk at VI Nanoquanta-ETSF Young Researchers Meeting, Berlin, Germany.

"Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen".

18. January 2005: Poster at the XII International Workshop on Computational Condensed Matter Physics: Total Energy and Force Methods, Trieste, Italy.

"Low temperature phase of Pb on Si(111): an ab-initio investigation".

MANAGEMENT, ORGANIZATIONAL AND SERVICE ACTIVITIES

ORGANIZATION OF CONFERENCES AND SCHOOLS

May 2011: 8th ETSF Young Researchers' Meeting, Naples (Italy)

December 2015: ETSF Workshop 2015, Palaiseau (France)

February 2016 and 2017: Theoretical Spectroscopy Lectures Theory and Codes, Palaiseau (France)

Date

Place