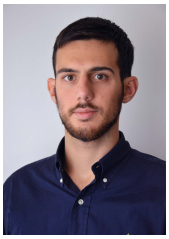
Giacomo Sesti, Ph.D.

Modena, Italy



Education

11/2018-01/2022 — PhD in Physics and NanoSciences at Università degli Studi di Modena e Reggio Emilia
Thesis Title: **Excitonic Insulator in Narrow-Gap Carbon Nanotubes**, supervisors: E. Molinari and M. Rontani (CNR-NANO)
Phd thesis available at *https://www.iris.unimore.it/handle/11380/1271910*
Exams and courses include: lboratory of computational quantum mechanics, theoretical optical spectroscopy, course on Material Science codes on innovative HPC architectures: from electronic structure to spectra with Quantum ESPRESSO and Yambo, MUSIQ E-schools - Ultrafast optics and spectroscopy, ICTP Yambo School 2022.

10/2015-10/2017 — Master degree in Physics at Università degli Studi di Modena e Reggio Emilia
(Final Grade 110 e Lode)
Thesis Title: **Time-Evolution of Magnetic Vector Fields through Disorder-Averaged Green Functions in Layered Antiferromagnets**, supervisors: C.M. Bertoni and M. Titov (Radboud University Nijmegen)
Master thesis available on request at *https://morethesis.unimore.it/theses/available/etd-10042017-102332/*
From August 2016 to July 2017, I visited Radboud University in Nijmegen.

9/2012-9/2015 — Bachelor degree in Physics at Università degli Studi di Modena e Reggio Emilia
(Final Grade 110 e Lode)
Thesis Title: **Trasporto di Carica Coerente in Stati di Edge: Separazione degli Stati mediante Profili di Potenziale**, supervisors: P. Bordone and A. Beggi at MonteCarlo Laboratory.

9/2007-7/2012 — Diploma Liceo Scientifico, Final Grade 98/100
Liceo Alessandro Tassoni, Modena

Previous positions

04/2022-04/2025 — Post-doctoral fellow at CNR NANO and Università degli Studi di MODENA e REGGIO EMILIA, respectively, under the supervision of Prof. Elisa Molinari and Dr. Andrea Ferretti.

01/2018-12/2018 — Undergraduate fellowship at CNR NANO Modena, under the supervision of Dr. Massimo Rontani

01/2017-07/2017 — Visiting (Master Thesis Research) within the Theory of Condensed Matter group at Radboud University Nijmegen, supervisor prof. M. Titov.

Research projects

First Principles treatment of Screening in Metallic Systems

- I developed a new computationally efficient method to accurately treat metallic systems in first-principles many-body calculations. Many-Body Perturbation Theory calculations in the GW approximation are a reliable scheme for computing quasi-particle (QP) band structures of materials. Although QP corrections are typically smaller in metallic systems than in semiconductors, they are critical for accurate spectroscopic descriptions, especially in low-dimensions. The computational cost of GW in metals poses challenges for the need to characterize the screened potential both in frequency and k-space. In particular, the long-wavelength limit of intraband transitions is correctly described using dense k-space grids at the cost of a severe computational slow down. A workaround commonly used consists in introducing a Drude term at the plasmon energy, which however may be unknown.
  During the grant, I developed and implemented in the Yambo code the new W-av technique for metals. This allows for an accurate evaluation of the screened potential in both simple and complicated 3D and 2D metals, without requiring additional parameters. I reproduce QP calculations of 3D and 2D metals with reduced k-point grids, providing a more efficient approach to the study of metallic systems.
  As an application, I performed first principles simulations of electron energy loss (EELS) in doped graphene. I was able to account for intraband effects in the EELS scattering by using the W-av approach for metals. Graphene was studied at different levels of intrinsic doping with the aim to compare with experimental EELS measurements. Specifically, the experimental measurements are performed on n doped graphene placed over a Germanium substrate. The extrinsic n doping is achieved through alkaline deposition. Although this part of the work is still in progress, the theoretical/experimental comparison shows encouraging results thus far.

Narrow-Gap Carbon Nanotubes as Excitonic Insulators

- I investigated the possibility of a spontaneous excitonic condensation in narrow-gap carbon nanotubes. Excitons could potentially induce instabilities in narrow-gap carbon nanotubes since the excitation energies are small, the binding energy is increased for the small dimensionality, and the system has poor screening. For instance, excitonic instability has been shown to occur in gapless armchair tubes. Nanotubes with narrow gaps show a reduced dielectric screening of the Coulomb interaction compared to armchair tubes due to their semiconducting nature. This allows bound excitons despite the presence of finite single-particle gaps.
  Crucial to the study of excitons was the initial development and computational implementation of a screening theory to model the large electron-hole Coulomb interaction of narrow-gap carbon nanotubes. This theory, validated by first-principles calculations, has been shown to be able to explain the anomalous screening of narrow-gap carbon nanotubes. Using the developed theory of screening, I have calculated the excitonic energies of a wide range of nanotubes and observed the occurrence of an instability in all the nanotubes considered. I have characterised the properties of the excitonic phase, illustrated by phase diagrams. I also show that transport studies of carbon nanotubes with respect to the magnetic field can provide a fingerprint of an excitonic instability.

Master Thesis

- I analysed the time evolution of the characteristic fields of an antiferromagnet, the Néel vector and the magnetization, under the injection of a spin polarised current. As generally a polarised current generates spin torques in a magnetic system, I looked for their expression in an antiferromagnetic model, starting from a microscopic approach. In particular, I computed the spin orbit torque, the spin transfer torque and the Gilbert damping originated by the electron flow. The structure of the torques is found in the case of two model Hamiltonians, in which it is included a Gaussian distributed impurity disorder.

Research projects (continued)

Bachelor Thesis

- I carried out simulations to study the transport of electrons in edge states in contact with a potential mesa. The edge states are highly energetic and extremely coherent states that arise in the region next to a confining potential in the presence of a magnetic field. I show that the edge state splits at the contact with the mesa and the electronic channel propagating over the mesa loses of coherence.

Programming and computational skills

Coding

- Extensive expertise in Fortran coding developed during both my PhD and PostDoc. During my Post-Doc, I also acquired experience of GPU porting within Yambo.
- I have made extensive use of Python, of which I have expertise in data analysis and visualization using Python libraries and classes.
- I also have good ability with the software Mathematica.

First-principle calculations

- Experience in first principle computations at DFT level, specifically with the Quantum Espresso code.
- Professional knowledge of many-body simulations with the Yambo code. Along with that, I have also implemented a new feature in the part of the Yambo code that is dedicated to the calculation of GW self-energies.

Related activities

- I am currently PI of the Leonardo IscraB project IsB30.
- Tutor at the Yambo School 2025. I will supervise the hands-on of the GW tutorial.
- Tutor at MAX CoE/ENCCS Workshop 2024 on Efficient Materials Modelling on HPC with Quantum ESPRESSO, Siesta and Yambo.
- Tutor at the Yambo School 2023, in particular I supervised the hands-on of the GW tutorial

Research Publications

- G. Sesti, D. Varsano, E. Molinari, and M. Rontani, "Anomalous screening in narrow-gap carbon nanotubes," *Phys. Rev. B*, vol. 105, 2022.
- Z. Kandemir, P. D'Amico, G. Sesti, C. Cardoso, C. Milosevic, and C. Sevik, "Optical properties of metallic mxene multilayers through advanced first-principles calculations," *Phys. Rev. Mat.*, vol. 8, 2024.
- G. Sesti, D. Varsano, E. Molinari, and M. Rontani, "Narrow gap carbon nanotubes as candidate excitonic insulators," *Nuovo Cimento C- Colloquia and Communications in Physics*, Accepted for publication, 2025.
- G. Sesti, D. Varsano, E. Molinari, and M. Rontani, "Binding and spontaneous condensation of excitons in narrow-gap carbon nanotubes," in preparation, preprint available (2025).
- G. Sesti, A. Guandalini, A. Ferretti, P. D'Amico, C. Cardoso, M. Rontani, and D. Varsano, "Efficient and accurate ab initio description of the long-range limit of the polarisation in metals," in preparation, preprint available (2025).

- C. Cardoso, Z. Kandemir, P. D'Amico, G. Sesti, K. Şendur, M. V. Milošević, and C. Sevik, "Many-body effects and excitonic corrections in the optical response of 2d metallic mxene," in preparation, preprint available (2025).

Conferences and workshops

- "GW methods in practice; algorithms and approximations used in GW calculations of materials", Yambo School May 2025 Modena, Italy. (Invited lecture)
- "Excitonic Instability in Narrow-gap Carbon Nanotubes", 110° Congresso Nazionale SIF September 2024 Bologna, Italy. (Oral presentation)
- "Excitonic Instability in Narrow-gap Carbon Nanotubes", International Conference on Science and Application of Nanotubes and Low-Dimensiona Materials – NT24 June 2024 Cambridge, MA USA. (Oral presentation)
- "Excitonic Instability in Narrow-gap Carbon Nanotubes", 12th International Conference on Spontaneous Coherence in Excitonic Systems (ICSCE12) June 2024 Dublin, Ireland. (Oral presentation)
- "Excitonic vs Mott Insulator in carbon nanotubes: a proposed experimental test", CMD30 - FisMat September 2023 Milan, Italy. (Oral presentation)
- "Excitonic vs Mott Insulator in carbon nanotubes: a proposed experimental test", Condensed Matter and Quantum Materials July 2022 Bath, UK. (Oral presentation)
- "Excitonic vs Mott Insulator in carbon nanotubes: a proposed experimental test", Young Researchers Meeting September 2021 Cagliari, Italy. (Oral presentation)
- "Excitonic vs Mott Insulator in carbon nanotubes: a proposed experimental test", APS March meeting March 2021 Online event. (Oral presentation)
- "Accurate treatment of metallic screening in many-body calculations from first principles", 22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods January 2025 Trieste, Italy. (Poster presentation)
- "Excitonic insulator phase in narrow-gap carbon nanotubes", CMD30 - FisMat September 2023 Milan, Italy. (Poster presentation)
- "Efficient Integration Scheme for the Screened Interaction in Metals", S3 20 years Workshop June 2023 Modena, Italy. (Poster presentation)
- "Excitonic vs Mott Insulator in carbon nanotubes: a proposed experimental test", CECAM Workshop 'Excitonic and competing orders in low-dimensional materials' July 2021 Online event. (Poster presentation)
- "Excitonic vs Mott Insulator in carbon nanotubes: a proposed experimental test", International Conference on the Science and Application of Nanotubes and Low-dimensional Materials – NT21 June 2021 Online event. (Poster presentation)

Conferences and workshops (continued)

- "Anomalous screening in narrow-gap carbon nanotubes", International School and Workshop on Two-Dimensional Crystals and Photonics September 2019 Tbilisi, Georgia. (Poster presentation)
- "Chirality and Spin-Orbit Effects in the Carbon nanotube Excitonic Insulator Phase Diagram", CNR Nano-meeting October 2018 Pisa, Italy. (Poster presentation)
- "Chirality and Spin-Orbit Effects in the Carbon nanotube Excitonic Insulator Phase Diagram", CE-CAM workshop 'Excitonic insulator: New perspectives in long-range interacting systems' organized by CECAM and EU MaX CoE September 2018 Lausanne, Switzerland. (Poster presentation)
- "Torques in AFM systems", SYMPOSIUM TRENDS IN THEORY of the Dutch Research School of Theoretical Physics, May 2017 Dalfsen, Netherlands. (Poster presentation)

Teaching activity

03/2021-06/2021 — Tutor of the course of "Fisica Generale" in the degree course in Ingegneria del veicolo held by Prof. E. Molinari at Università degli Studi di Modena e Reggio Emilia.

11/2018-12/2018 and 10/2019-12/2019 — Tutor of the course of "Termodinamica statistica" in the degree course in Fisica held by Prof. G. Goldoni at Università degli Studi di Modena e Reggio Emilia.

11/2017-12/2017 — Tutor of the course of "Metodi Matematici per la Fisica" in the degree course in Fisica held by Prof. G. Santoro at Università degli Studi di Modena e Reggio Emilia.