

Simone Grillo

Institution: University of Rome “Tor Vergata” * *Department:* Physics

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Place of birth: Frascati (RM), Italy * *Date of birth:* 21-10-1995

I am currently a PhD student in Physics at the University of Rome “Tor Vergata”, specializing in theoretical and computational Condensed Matter Physics. The focus of my research is to exploit computational and theoretical approaches for the study of materials ranging from 3D to 0D. The main topic of my PhD is the calculations of the electronic and optical properties of 2D Tellurium-based materials, using Density Functional Theory and Many-Body Perturbation Theory.

Disciplines: Solid State Physics · Condensed Matter Physics · Material Science

Skills & Expertise: Ab Initio Calculations · Density Functional Theory · Many-Body Perturbation Theory · Bethe-Salpether Equation

Education

PhD Student in Physics

University of Rome “Tor Vergata”

Supervisors: Prof. Olivia Pulci, Prof. Maurizia Palummo

November 2021 - Ongoing

Master’s Degree in Physics (Condensed Matter)

University of Rome “Tor Vergata”

Graduated with honors (110/110 cum laude)

Supervisors: Prof. Olivia Pulci, Prof. Maurizia Palummo

Thesis title: From bulk tellurium to 2D tellurene: an ab-initio study

October 2018 - May 2021

Bachelor’s Degree in Physics

University of Rome “Tor Vergata”

Supervisors: Prof. Olivia Pulci, Prof. Maurizia Palummo

Thesis title: Theoretical study on the effect of B and P codoping on a SiGe core-shell nanocrystal

October 2014 - October 2018

High School Diploma

Liceo Scientifico “Edoardo Amaldi”

September 2009 - June 2014

Teaching Experience

Hands-on lessons on Quantum ESPRESSO integrate suite

Quantum Theory of Matter Lectures (by Prof. Olivia Pulci)

Master’s Degree in Physics, University of Rome “Tor Vergata”

- 4 hours (2022)

- 10 hours (2023)

Research Experience

MSCA-RISE DiSeTCom Project (G.A. ID: 823728) Visiting Scholar at Exeter University

21 November - 8 December 2022

Collaboration with Prof. M. Portnoi and Prof. F. Ogryn at Exeter University and MaxLLG Ltd. (UK).

MSCA-RISE DiSeTCom Project (G.A. ID: 823728) Visiting Scholar at Exeter University

6 March - 18 March 2022

Collaboration with Prof. M. Portnoi and Prof. F. Ogryn at Exeter University and MaxLLG Ltd. (UK).

Talks

19th ETSF Young Researchers' Meeting 2023

11 June - 16 June 2023

Contributed talk: "Non-Trivial Excitonic Fingerprints and Optical Anisotropy of 2D Tellurium".
Zaragoza (Spain).

EMRS Spring Meeting 2023

29 May - 2 June 2023

Contributed talk: "Ground and Excited State Properties of Meta-Stable Allotropic Forms of 2D Tellurium from First Principles Approaches".
Strasbourg (France).

GDR HOWDI Annual Meeting 2023

8 May - 12 May 2023

Contributed talk: "Non-Trivial Excitonic Fingerprints and Optical Anisotropy of 2D Tellurium".
Porquerolles island (France).

Nanoscience & Nanotechnology Conference 2022

13 December - 14 December 2022

Contributed talk: "Evolution of the Electronic and Optical Properties of Meta-Stable Allotropic Forms of 2D Tellurium for Increasing Number of Layers".
LNF, Frascati (Italy).

Conferences & Schools

International School of Solid State Physics (EPIOPTICS-16 & XENES-4)

3 July - 9 July 2022

Poster presentation, Best student award winner. Erice (Italy).

25th ETSF Workshop on Electronic Excitations

13 June - 17 June 2022

Poster presentation. Leuven (Belgium).

GDR HOWDI Annual Meeting 2022

9 May - 13 May 2022

Poster presentation. Dourdan (France).

MSCA-RISE DiSeTCom Project (G.A. ID: 823728) Workshop

1 October 2021

Online presentation. University of Eastern Finland (Finland).

17th ETSF Young Researchers' Meeting 2021

6 September - 10 September 2021

Poster presentation

University of Cagliari (Italy)

Virtual School on Electron-Phonon Physics and the EPW Code

14 June - 18 June 2021

University of Texas at Austin (US, online event)

School on Electronic Excitations in Solids and Nanostructures Using the YAMBO Code

8-9, 15-16 April 2021

MAX EU Centre of Excellence (online event)

20th International Workshop on Computational Physics and Materials Science

23 February - 25 February 2021

ICTP, Trieste (Italy, online event)

Introduction to New Accelerated Property Partition of Marconi, for Users and Developers

24 November 2020

CINECA University Consortium (online event)

School on Electronic Excitations in Novel Materials Using the YAMBO Code

27 January - 31 January 2020

ICTP, Trieste (Italy)

Scientific Skills

- Quantum ESPRESSO integrate suite (very good experience)
- YAMBO code (good experience)
- molGW code (basic experience)
- GROMACS software (basic experience)

Informatic Skills

Programming Languages/Tools Python, Fortran95, Linux, Microsoft Office, L^AT_EX

Language Proficiencies

| | |
|----------------|--------------------------------|
| Italian | Mother tongue |
| English | Fluent (certified C1) |
| German | Basic knowledge (certified A2) |
| French | Basic knowledge |

Scientific Projects

- PI of the “SAGACE” CINECA class C ISCRa project on the MARCONI cluster, 2018
- PI of the “SWYFT” CINECA class C ISCRa project on the MARCONI100 cluster, 2021
- PI of the “MT-SENS” CINECA class C ISCRa project on the MARCONI100 cluster, 2021
- Collaborator of the “TUTTO” CINECA class B ISCRa project on the MARCONI100 cluster, 2021
- Collaborator of the “STRANO” CINECA class B ISCRa project on the MARCONI100 cluster, 2022
- PI of the “TeB2LowD” CINECA class C ISCRa project on the MARCONI100 cluster, 2022
- Collaborator of the “ANODE” CINECA class B ISCRa project on the MARCONI100 cluster, 2023
- Collaborator of the “NHCOSURF” CINECA class B ISCRa project on the GALILEO100 cluster, 2023
- PI of the “WeDiTe” CINECA class B ISCRa project on the LEONARDO cluster, 2023

- Participant of the MSCA-RISE “DiSeTCom” project (G.A ID: 823728)
- Participant of the Time2Quest INFN project
- Participant of the 2020 PRIN “PHOTO” project (Prot. 2020RPEPNH)
- Collaborator of the 2022 PRIN “IRIDE” project (Prot. 2022T2ZJZF)

Publications

1. Bechstedt, F., **Grillo, S.**, Pulci, O., and Gori, P. (2021). Thermal properties of Dirac fermions in Xenon: Model studies. *Physical Review B*, 104(16), 165420.
2. **Grillo, S.**, Pulci, O., and Marri, I. (2022). Evolution of the Electronic and Optical Properties of Meta-Stable Allotropic Forms of 2D Tellurium for Increasing Number of Layers. *Nanomaterials*, 12(14), 2503.
3. Marri, I., **Grillo, S.**, Amato, M., Ossicini, S., and Pulci, O. (2023). Interplay of Quantum Confinement and Strain Effects in Type I to Type II Transition in GeSi Core-Shell Nanocrystals. *The Journal of Physical Chemistry C*, 127(2), 1209-1219.

4. Mendoza, B. S., **Grillo, S.**, Juárez-Reyes, L., and Fregoso, B. M. (2023). Pure spin current injection of single-layer monochalcogenides. *Materials Research Express*, 10(3), 035003.

Membership

Istituto Nazionale di Fisica Nucleare (INFN) *2021 - Ongoing*

European Theoretical Spectroscopy Facility (ETSF) *2021 - Ongoing*