Curriculum Vitae - PhD Alberto Guandalini

RESEARCH INTERESTS

Alberto Guandalini (AG) works in the field of condensed matter and molecular physics. His studies are focused in the methodological and implementation development of ab initio simulations at the DFT level and beyond (many body perturbation theory), for the calculation of the electronic and optical properties of different kind of materials (solids, molecules and low dimensional systems).

AG is a developer of the many-body perturbation theory code Yambo (http://www.yambo-code.org).

SCIENTIFIC CAREER

Post Doc at CNR-Nano, Modena, March 2020 - November 2022

- Project: "MaX Materials design at the eXascale"
- Scientific tutor: Andrea Ferretti
- Other collaborators: Daniele Varsano, Pino D'Amico, Claudia Cardoso, Davide Sangalli

EDUCATION

 \mbox{PhD} student in Physics and Nanosciences, Physics, XXXII cycle, started in November 2016, finish in January 2020

- Title: Charged and nonlinear neutral excitations in low-dimensional and molecular systems by means of density-functional approaches
- Supervisors: Prof. Alice Ruini, Dr. Stefano Pittalis, Dr. Carlo Andrea Rozzi
- University of Modena and Reggio Emilia, Italy
- In collaboration with CNR-NANO, Modena, Italy

PUBLICATIONS

- A. Guandalini, P. D'Amico, A. Ferretti, and D. Varsano, "Efficient GW calculations in two dimensional materials through a stochastic integration of the screening potential", Pre-print available
- A. Guandalini, A. Ruini, E. Räsänen, C. A. Rozzi, and S. Pittalis, "Density functional approach to the band gaps of finite and periodic two-dimensional systems", *Phys. Rev. B*, 104, 085110, 2021
- A. Guandalini, C. Cocchi, S. Pittalis, A. Ruini, C. A. Rozzi, "Nonlinear light absorption in many-electron systems excited by an instantaneous electric field: a non-perturbative approach", *Phys. Chem. Chem. Phys.*, **23**, 10059, 2021
- A. Guandalini, C. A. Rozzi, E. Räsänen, and S. Pittalis, "Fundamental gaps of quantum dots on the cheap", *Phys. Rev. B*, **99**, 125140, 2019

Computational skills

• Programming:

- Proficiency: Fortran 90, High Performance Computing (HPC), Parallel computing (MPI and OpenMP), Python, Bash scripting.
- ♦ Basics: C++.

• Scientific:

- ♦ Proficiency: Yambo, Quantum Espresso, Octopus.
- ♦ Basics: Berkeley GW, NWChem.
- Common: Latex, Office
- OS: Linux, Windows

EXPERIENCES ABROAD

• PhD visiting student at Humboldt University Berlin, Physics Department, in Professor Caterina Cocchi's group, studying nonlinear optical properties of macrocyclic molecules within density functional

approaches.

January-March (3 months) 2019, awarded fundings "HPC-Europa3" and "DAAD short term grant"

INVITED TALKS

• Ab-initio Many-Body Methods and Simulations with the Yambo Code. 4-8 April 2022 Trieste, Italy

Title: "GW approximation in 2D materials"

ATTENDED SCHOOLS, WORKSHOPS AND CONFERENCES • 17 th ETSF Young researcher's meeting. 6-10 September 2021

Cagliari, Italy

Talk: "Efficient GW calculations in 2D systems through the interpolation of the screened potential"

• APS March meeting 2021. 15-19 March 2021

Online event

Talk: "Efficient GW calculations in 2D systems through the interpolation of the screened potential"

• 20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods. 23-25 February 2021

Online event

Poster: "Efficient GW calculations in 2D through the interpolation of the screened potential"

• Yambo developers meeting 2020. 4-18 Dicember 2020

Online event

Talk: "Accelerating convergences in 2D materials"

• Computational School on Electronic Excitations in Novel Materials Using the Yambo Code. 27-31 January 2020

Trieste, Italy

• NanoMeeting 2018. 30-31 October 2018

Pisa, Italy

Poster "Fundamental gap of quantum dots on the cheap"

• Materials.it 2018. 19-23 October 2018

Bologna, Italy

 $\label{thm:constraint} \begin{tabular}{ll} Talk "Energy gaps of low-dimensional many-electron systems from Kohn-Sham quantities: exchange-only approximations" \\ \end{tabular}$

• 8th Time-Dependent Density-Functional Theory: Prospect and Application (Summer school+workshop). 19-31 August 2018

Benasque, Spain

Poster "Fundamental gap of quantum dots on the cheap"

• DPG Spring Meeting. 11-16 March 2018

Berlin, Germany

Talk "Energy gaps of low-dimensional many-electron systems from Kohn-Sham quantities: exchange-only approximations"

• Introduction to parallel computing with MPI and OpenMP. 22-24 February 2017 CINECA, Bologna, Italy

Awards

• Second prize for the poster presented at the 8th Time-Dependent Density-Functional Theory: Prospect and Application 19-31 August 2018

Title: "Fundamental gap of quantum dots on the cheap"

Benasque, Spain

Teaching

• Teaching assistant for the course "Physics III" (electrodynamics and waves) for three years. September-December 2015/2017/2018

Lecturer: Prof. Stefano Frabboni UNIMORE, Modena, Italy

Language skills • Italian Mothertongue

• English C1