# Ab-initio Many-Body Methods and Simulations with the Yambo Code

## 4 - 8 April 2022 An ICTP Hybrid Meeting Trieste, Italy

The Computational School on *Ab-initio Many-Body Methods* and *Simulations with the Yambo Code* will introduce many-body perturbation theory (MBPT) approaches and specifically to *firstprinciples* excited-state simulations using the YAMBO code.

The target participants are graduate students, postdocs, and researchers who are interested in learning or in improving their knowledge and skills to calculate electronic and optical properties of an efficient, beyond the well-known DFT limitations and using an efficient, highly parallelized and accurate many-body computational tool.

Both theoretical and technical lectures will be offered as well as dedicated hands-on sessions where students will learn how to use the code for materials of current research interest and how to optimize its use in a parallel environment. Several post-processing tools for the analysis of the results will be also introduced and practically applied.

General topics will include self-energy and quasiparticles concepts, the GW approximation, and the Bethe-Salpeter equation, all placed in the context of and linked with experimental measurements (photoemission, absorption, photoluminescence).

At variance with previous editions, this school will present some advanced lectures such as: new algorithms developed to deal with electron-phonon interactions, real time evolution of equations of motion, time dependent polarization in terms of the Berry phase, and computation of non-linear optical properties.

The specific usage in massively parallel environments equipped with modern accelerated video cards (GPU's) will be introduced.

Participants are required to have a pre-existing background in DFT and

Further information: http://indico.ictp.it/event/9780/ smr3694@ictp.it

#### **Directors:**

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## Local Organiser:

N. SERIANI, ICTP, Italy

### **Lecturers:**

- C. ATTACCALITE, CNRS, Aix-Marseille University, France
- A. FERRETTI, CNR-NANO, Italy
- M. GRUNING, Queen's University Belfast, UK
- A. GUANDALINI, CNR-NANO, Italy
- D. A. LEON VALIDO, CNR-NANO, Italy
- A. MARINI, CNR-ISM, Italy
- P. MELO, University of Utrecht, Netherlands
- B. MONSERRAT, University of Cambridge, UK
- F. PALEARI, CNR-NANO, Italy
- M. PALUMMO, Università di Roma Tor Vergata, Italy
- S. RAFAELY-ABRAMSON, Weizmann Institute, Israel
- L. REINING, École Polytechnique, France
- D. SANGALLI, CNR-ISM, Italy

in running DFT simulations.

Due to the pandemic, the school is designed to allow participants to join part in person and part online.

P. SHEVERDYAEVA, CNR-ISM, Italy D. VARSANO, CNR-NANO, Italy

# How to apply:

Online application: http://indico.ictp.it/event/9780/

Female scientists are encouraged to apply.

#### Grants:

A limited number of grants are available to support the attendance of selected participants, with priority given to participants from developing countries. There is no registration fee.

#### **Deadline:** 8 March 2022

Applications needing financial support and/or visa

## 20 March 2022

All other applications







The Abdus Salam International Centre for Theoretical Physics



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