

Yambo developers' meeting:

Program:

Friday 4

09:00 - 09:10 **A. Marini:** Introduction

09:10 - 09:30 **M. Gruning:** Correcting wrong DFT orbital characters considering the off-diagonal elements of the GoWo self-energy

09:30 - 09:50 **M. Bonacci:** The Yambo-Aiida workflow and the GW100 case with GN-PPM model

09:50 - 10:10 **D. A. Leon Valido:** A multipole approach for dielectric screening:

10:10 - 10:30 Break

10:30 - 10:45 **A. Marini:** Test-suite functionality & validation of new developments.

10:45 - 11:05 **D. Varsano:** Organisation of the next Yambo school in virtual format

11:05 - 12:00 Round table

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09:00 - 09:20 **E. Molteni:** Calculating Circular dichroism in Yambo

09:20 - 09:40 **D. Sangalli:** Magnons description in Yambo

09:40 - 10:00 **C. Attaccalite:** Exciton-phonon interactions

10:00 - 10:20 **F. Paleari:** Phonon dynamics description

10:20 - 10:35 Break

10:35 - 10:55 **N. Spallanzani & A. Ferretti:** Yambo porting on GPU machines

10:55 - 11:15 **A. Marini:** Coding good practices: modularization and clearness

11:15 - 12:00 **D. Varsano:** Yambo website, training material, documentation and user's forum

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09:00 - 09:20 **P. D'amico & A. Ferretti:** GW embedded with a Polarizable continuum model

09:20 - 09:40 **M. Marsili:** Spin properties of excitons

09:40 - 10:00 **D. Sangalli:** Technical developments and enhancement of Yambo features

10:00 - 10:20 **D. Varsano & D. Sangalli:** Possible developments of new features coming from user community

10:30 - 10:40 Break

10:40 - 11:10 **F. Paleari:** WhyPy presentation, a python tool to run Yambo smartly

11:10 - 11:30 **A. Guandalini:** Accelerating convergences in 2D materials:

11:30 - 11:50 **F. Affinito:** Short presentation of the Leonardo machine

11:50 - 12:00 Wrap-up

