

Quasiparticle Band Structures and Excitons in Novel Materials using the Yambo Code

Daniele Varsano (Modartor) CNR-Nano

Speakers: Andrea Marini (CNR), Maurizia Palummo (TOV), Myrta Gruning (U. Belfast), A. Ferretti (CNR)

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- > This is the third of a series of MaX webinars on the most recent developments of the MaX flagship codes
 - > Past webinars on **Quantum Espresso** and the **Aiida** platform
 - > Next MaX webinars: HPC libraries for **CP2K** and other electronic structure codes scheduled for June 24
 - > **Siesta** code September 22
- > <http://www.max-centre.eu/news/max-webinars>

Key focus in MaX:

Materials science from first principle toward exascale

- > Software architecture towards exascale
- > Performance portability
- > Code evolution: exploiting algorithmic advances enabled by the exascale transition

Extremely relevant for **excited states** calculations, this will allow e.g.

- affordability of large systems
- Better precision in term of convergence

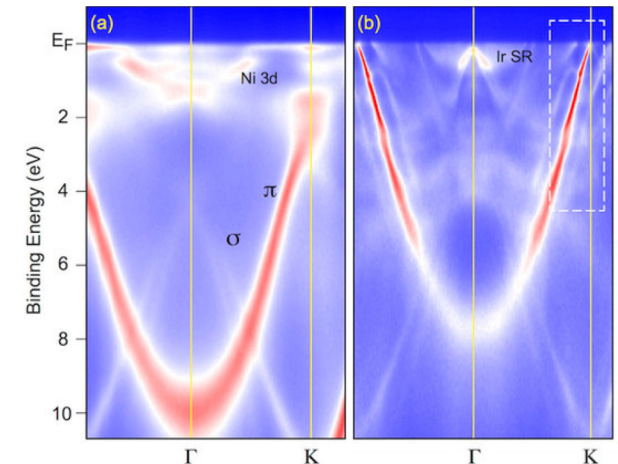
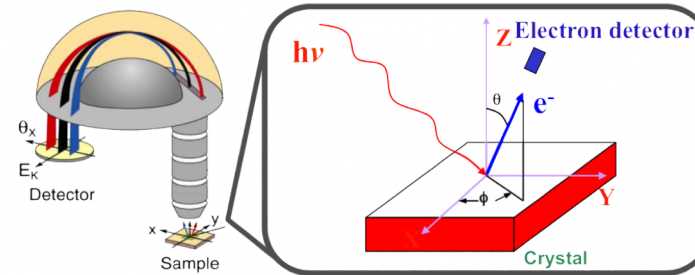


<http://www.yambo-code.org>

YAMBO a fortran code implementing Many-Body Perturbation Theory (MBPT) methods (such as GW and BSE) and (TDDFT).

Accurate predictions of properties as:

- band structure of semiconductors
- band alignments
- defect quasi-particle energies
- High Harmonic generation
- optics and out-of-equilibrium properties of materials.



Today's presentation and presenters



<http://www.yambo-code.org>



Code intro, Yambo Educational and User support

Dr. Andrea Marini (CNR-ISM)

15:05-15:20 CEST



Quasi-particles and excitons using Yambo

Prof. Maurizia Palumbo (University of Rome Tor Vergata)

15:20-15:40 CEST

Today's presentation and presenters



In Real Time: nonlinear optical spectroscopy
Dr. Myrta Grüning (Queen's University Belfast)
15:40-16:00 CEST



Yambo at HPC: running in parallel on GPUs
Dr. Andrea Ferretti (CNR-Nano)
16:00-16:20 CEST



DRIVING THE EXASCALE TRANSITION

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THANKS