MAX DRIVING THE EXASCALE TRANSITION

Yambo ©

Description

Yambo is an open-source code implementing first-principles methods based on Green's function theory to describe excited-state properties of realistic materials. These methods include the GW approximation, the Bethe Salpeter equation, real-time NEGF, electron and exciton phonon. Yambo calculations require a previously computed electronic structure, and for this reason it is interfaced with other density functional theory (DFT) codes, including Quantum ESPRESSO and ABINIT.

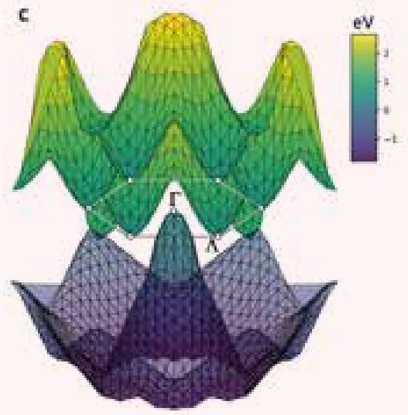
Level of theory

- Many-body perturbation theory (MBPT), incl. GW, BSE
- Electron-phonon coupling (ELPH)
- Real-time non-equilibrium Green's function (NEGF)
- Time Dependent DFT (TDDFT)

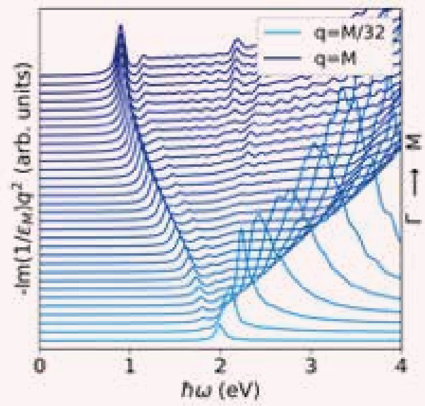
Features

- Electronic properties: quasi-particle energies, line-widths, and renormalization factors
- Linear optical properties, capturing the physics of excitons, plasmons, and magnons
- Temperature dependent electronic and optical properties via electron-phonon coupling
- Non-equilibrium and Non-linear optical properties via NEGF real-time simulations
- Calculation of 2D and 1D systems
- Advanced post-processing tools to analyse the simulation flow of data

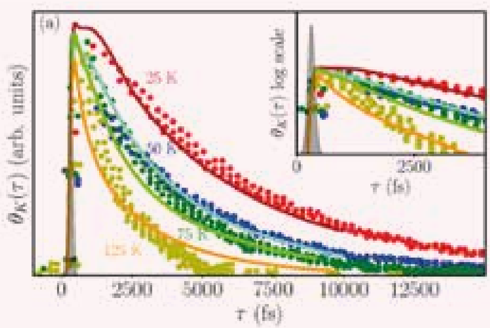
Case studies



Quasiparticle band structure of bulk MoS2 at ultra-high pressure [Ataei et al. Pnas (2021)]



Excitonic EELS spectra at finite momenta of monolayer C3N [Bonacci et al. Phys rev. Mat (2022)]



Intervalley relaxation dynamics of monolayer WSe2 via ELPH scattering [Molina-Sánchez et al. Nano Lett. (2017)]

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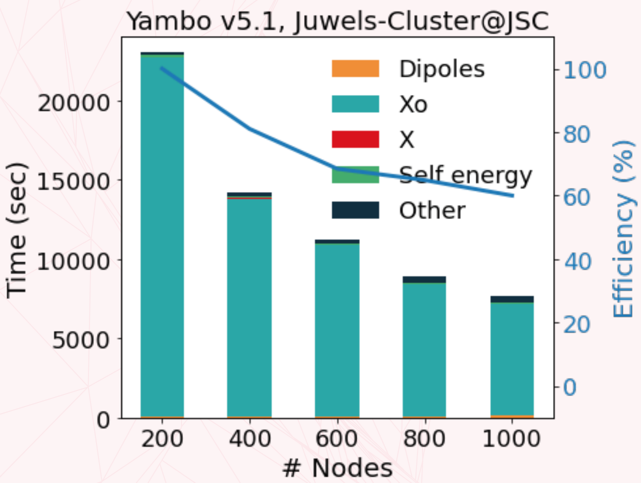
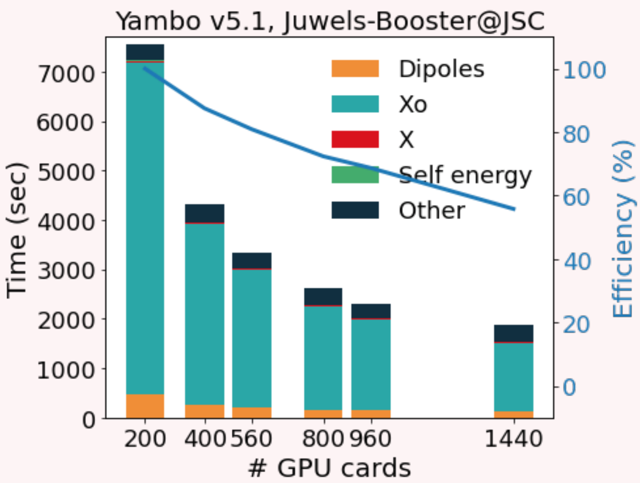
Parallelization and HPC performance

Yambo has a user-friendly command-line interface, flexible I/O procedures, and, concerning high performance computing (HPC), it is parallelised by using a hybrid MPI plus OpenMP approach, well integrated with support of GPGPU-based heterogeneous architectures. This makes it possible to distribute the workload to a large number of parallel levels. In practice, depending on the kind of calculation, all the variables to be used (k/q grids, bands, quasi-particles, G-vectors, etc) are distributed along the different levels of parallelisation.

Yambo has proved to be efficient in large-scale simulations (tens of thousands of MPI tasks combined with OpenMP parallelism) for most of its calculation environments. The GPU porting supports CUDA-Fortran as well as other programming models (OpenACC and OpenMP5 under development). Yambo has been demonstrated to run efficiently on a number of HPC architectures, including homogeneous clusters (e.g., based on Intel, AMD, IBM Power and ARM chips), as well as heterogeneous GPU-accelerated machines (currently based on NVIDIA cards).





Support

Forum

Tutorials

Hands-on schools on yearly basis

Open repository with benchmark data

References

- *A. Marini, C. Hogan, M. Grüning, and D. Varsano, yambo: An ab initio tool for excited state calculations, Comput. Phys. Commun.* ***180****, 1392 (2009).*
- *D. Sangalli, A. Ferretti, H. Miranda, C. Attaccalite, I. Marri, E. Cannuccia, P. Melo, M. Marsili, F. Paleari, et al., Many-body perturbation theory calculations using the yambo code, J. Phys.: Condens. Matter* ***31****, 325902 (2019).*