MAX DRIVING THE EXASCALE TRANSITION

# Accelerating GW and many-body perturbation theory on GPUs: hunting for excitonic insulators using Yambo

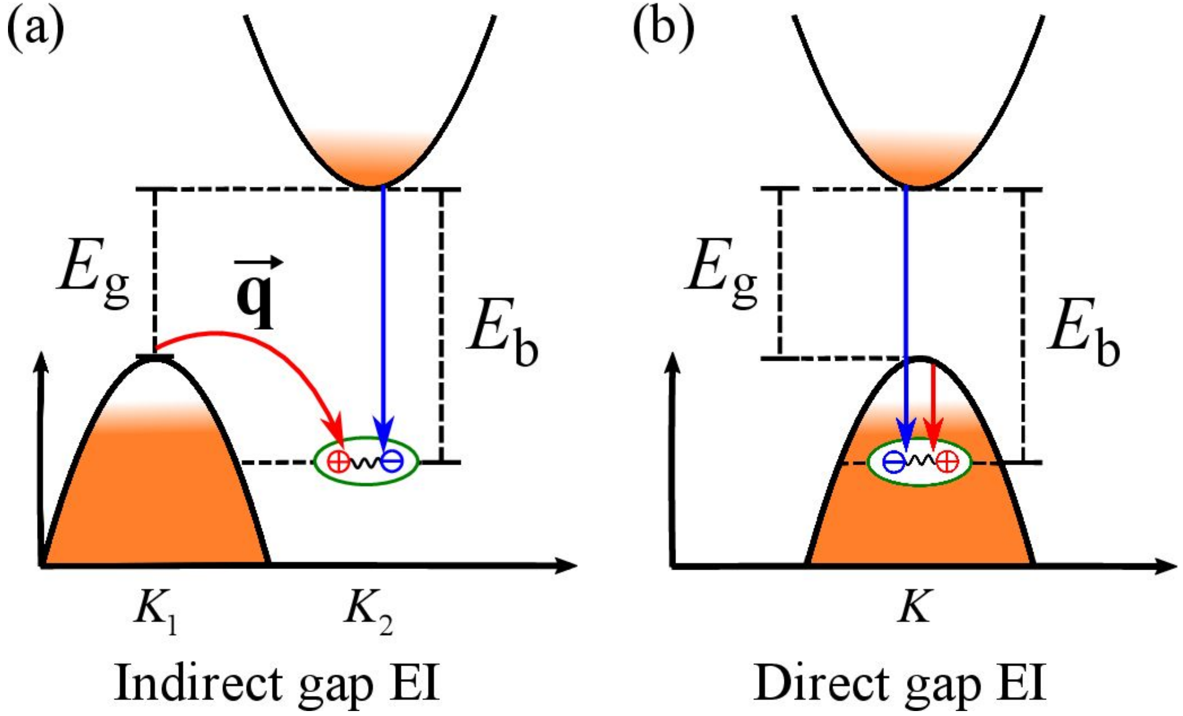
Daniele Varsano, Andrea Ferretti, Elisa Molinari and Massimo Rontani

CNR-Nano, Modena Italy

EuroHPC summit, March 24th, 2021

MaX "*Materials Design at the Exascale*", has received funding from the European Union's Horizon 2020 project call H2020-INFRAEDI-2018-1, grant agreement 824143

# Excitonic insulator: an exotic phase of matter




Z. Jiang et al. Phys. Rev. B **98**, 081408(R) (2018)

**Exciton**: quasiparticle formed by a bound electron-hole pair

**Spontaneous condensation of excitons**, hosted in a narrow-gap semiconductor or a semimetal: a long sought phenomenon analogous to the condensation of Cooper pairs in a superconductor.

As the exciton condensate **a new phase is formed: the 'excitonic insulator' (EI)**. It shares similarities with the superconductor ground state, it may exhibit macroscopic quantum coherence and exotic low-energy excitations.

We are assisting to a renewed interest in EI realization from both theoretical and experimental side (see e.g. Kogar, A. et al. *Science* **358**, 1314–1317 (2017).) A direct observation of the EI phase remains elusive.

LV Keldysh, YV Kopaev Sov. Phys. Sol. State 6,2219 (1965)
J des Cloizeaux J. Phys. Chem. Solids 26, 259 (1965).
D Jèrome, TM Rice, W Kohn, Phys. Rev.158, 462 (1967)

MAX DRIVING THE EXASCALE TRANSITION

# Prediction on EI realizations by First principle calculations

State-of-the-art methods (post-DFT) to compute the main quantities to establish EI phase

Band structures and energy gap via **GW method**

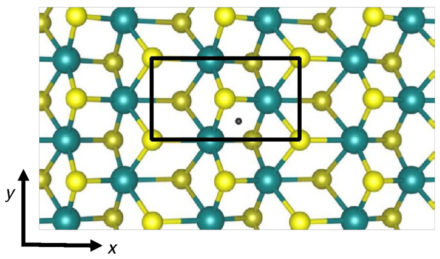
Excitation energy (binding energy of the exciton) by solving the **Bethe Salpeter equations**

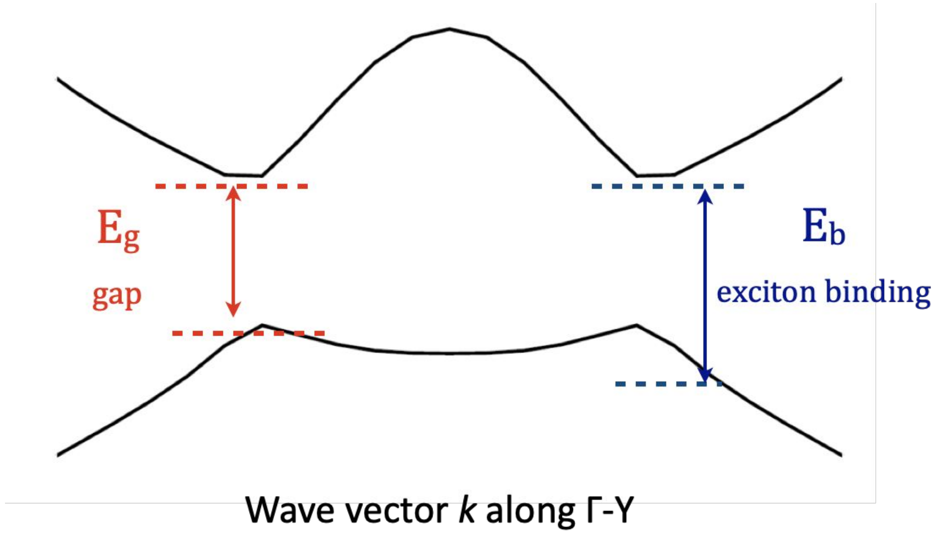
Binding energy strongly dependent to the **electronic screening** calculated at RPA level

**Challenging problem:** key quantities controlling the instability (energy gaps and exciton binding energies—involve many-body corrections beyond density functional theory (DFT) that are of the order of a few meV.

Prediction are possible only with the help of extreme computing

T'-MoS2




Eb > Eg hallmark of exciton instability

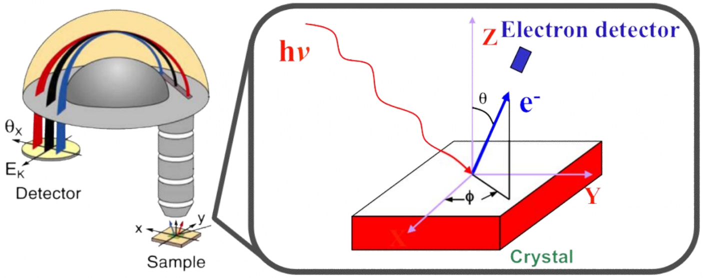
# The Yambo code

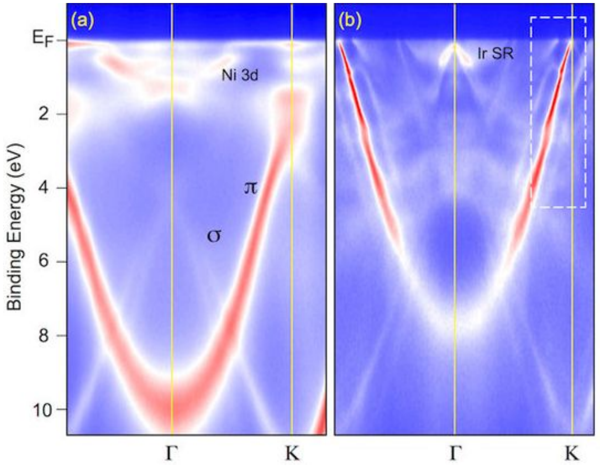
http://www.yambo-code.org

**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.
- Excitonic effects



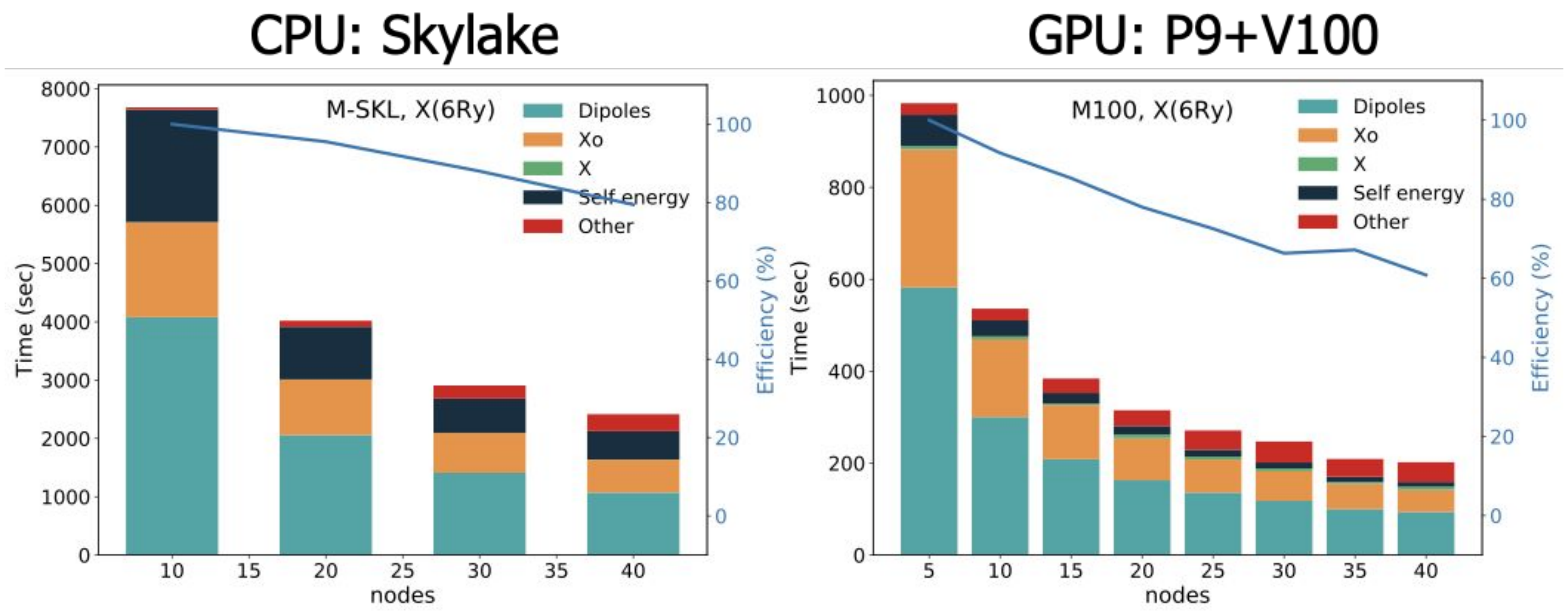




DRIVING THE EXASCALE TRANSITION

# Yambo on GPUs

heterogeneous architectures: MPI + OpenMP + CUDA

Time to solution gain > 10x
Energy to solution >5x




- complete **GW workflow** for a defected TiO2 crystal
- small system, **stress test**
- data obtained on Marconi100,
  4 MPI tasks/node;
  4 V100 GPUs/node

**system size**: 72+1 atoms, 2000 bands, 6 Ry for Xo repr (N=1317); ~290 occ states, 8 kpts.

data available at:
http://www.gitlab.com/max-centre/Benchmarks

DRIVING THE EXASCALE TRANSITION

# An excitonic insulator phase in low D systems: carbon nanotubes

nature COMMUNICATIONS

ARTICLE

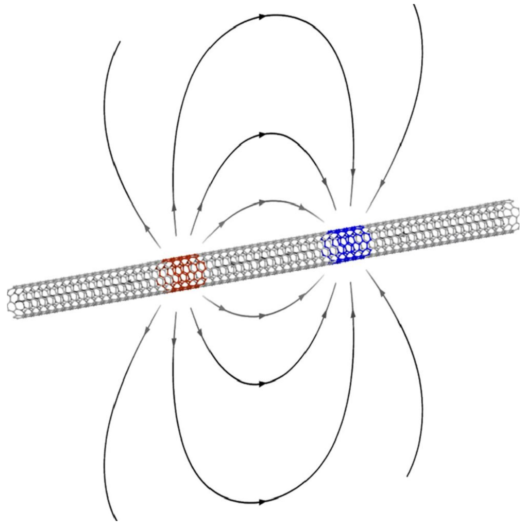
DOI: 10.1038/s41467-017-01660-8 OPEN

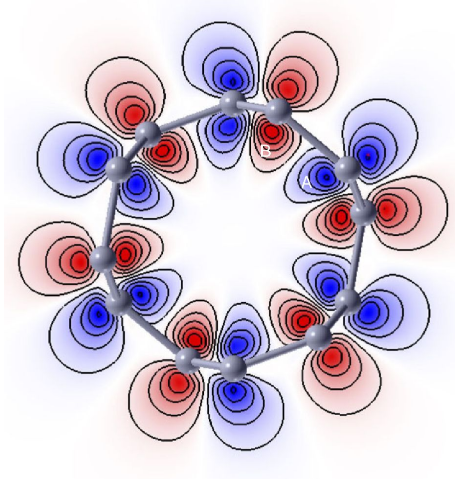
## Carbon nanotubes as excitonic insulators

Daniele Varsano[1], Sandro Sorella[2], Davide Sangalli[3], Matteo Barborini[1,5], Stefano Corni[1,6], Elisa Molinari[1,4] & Massimo Rontani[1]

D. Varsano et al. Nature Communications 8, 1461 (2017)

**PRACE project: TERAX**





Armchair nanotubes realize excitonic insultaor phase

Exciton phase stable up to 40K for the smaller tube

We could rule out other mechanisms of instability proposed in the literature as the Peierls mechanism

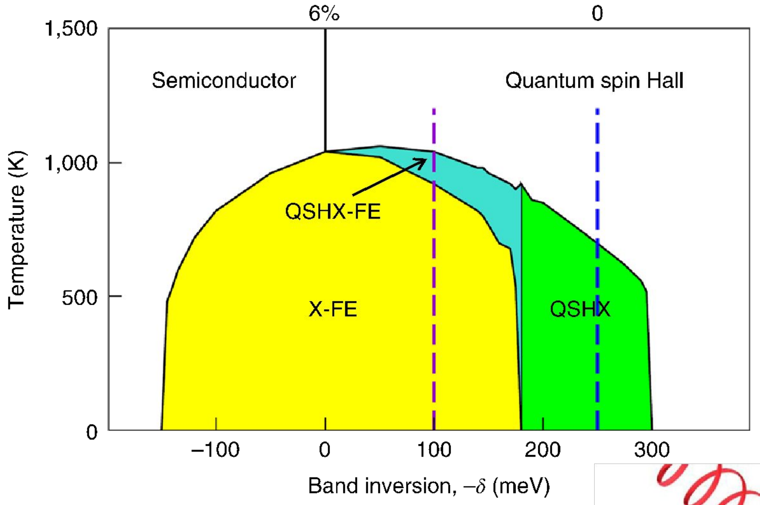
DRIVING THE EXASCALE TRANSITION

# An excitonic insulator phase in low D systems: T'-MoS2

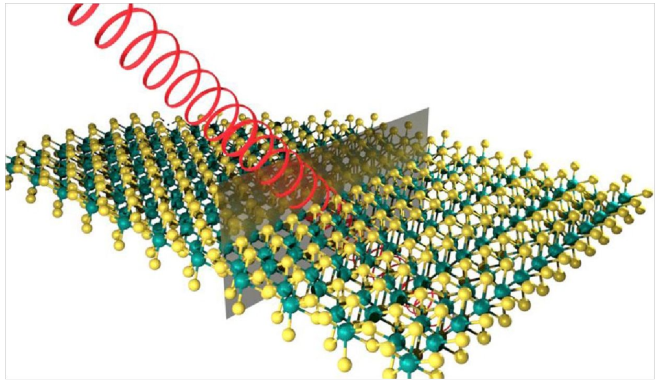
nature nanotechnology
LETTERS
https://doi.org/10.1038/s41565-020-0650-4
Check for updates

## A monolayer transition-metal dichalcogenide as a topological excitonic insulator

Daniele Varsano[1], Maurizia Palummo[2], Elisa Molinari[1,3] and Massimo Rontani[1]




D. Varsano, M. Palummo, E. Molinari and M. Rontani
Nature Nanotechnology 15 , 367 (2020)



PRACE

**PRACE project: EXTEND**

QSH topological insulator: topological and excitonic orders coexist with novel features

A rich phase diagram versus strain and temperature

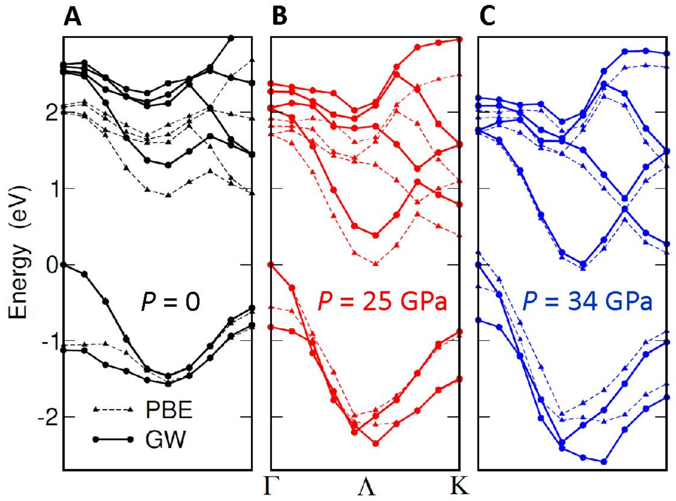
The QSHX phase presents circular dichroism

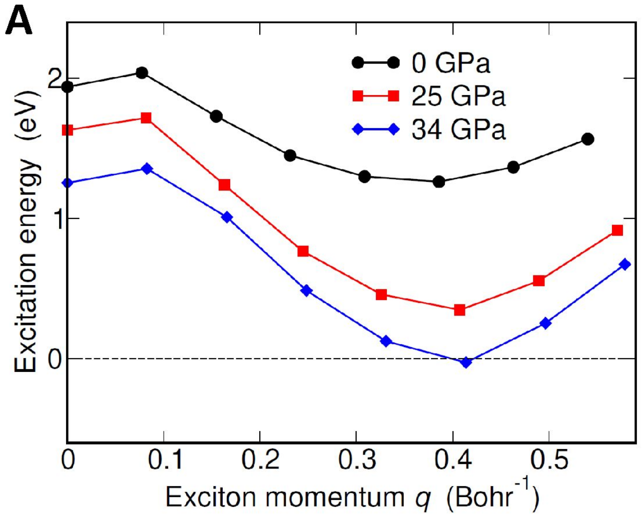
MAX DRIVING THE EXASCALE TRANSITION

# An excitonic insulator phase driven by pressure in bulk MoS2

Evidence of ideal excitonic insulator in bulk MoS2 under pressure
S. S. Ataei, D. Varsano, E. Molinari and M. Rontani
Proc. Natl. Acad. Sci. (2021) in press

Preprint available at: https://arxiv.org/abs/2011.02380



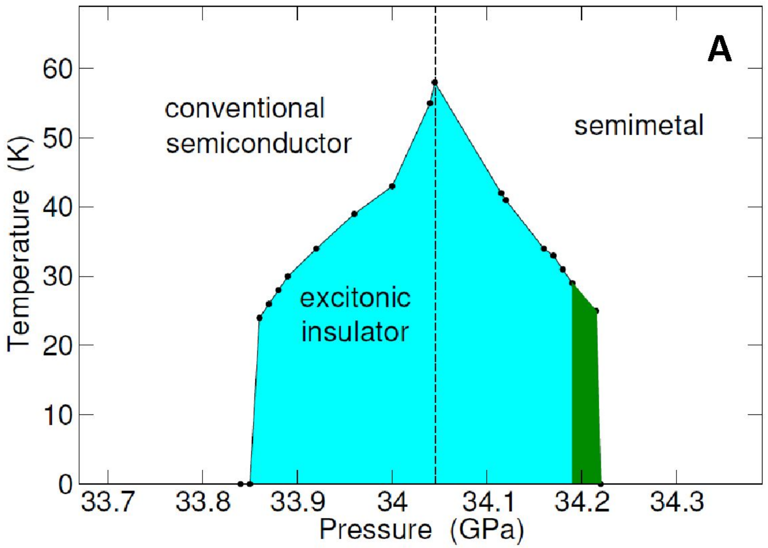




CINECA

**ISCRA project: ExcPress**

Indirect band gap semiconductor showing at high pressure condensation of excitons at finite momentum.

A real excitonic insulator phase sets in between the semiconducting and semimetallic phase




we identify a Raman feature that was previously observed experimentally as a fingerprint of the EI formation

MAX DRIVING THE EXASCALE TRANSITION

# Conclusion and acknowledgments

First principle evidence of EI phase in three systems of different dimensionality and conditions.

The resulting correlated phase was characterized in terms of the broken symmetry inherited by the exciton condensation.

The porting of the codes on GPU machines and their performance was an imprescindible step due to the accuracy needed to investigate this new state of matter by first principle correlated methods.


MAX DRIVING THE EXASCALE TRANSITION

H2020 Centre of Excellence MaX: Materials Design at the Exascale http://max-centre.eu

PRIN MIUR

PRIN 2017 EXC-INS

PRACE CINECA

Partnership for Advanced Computing in Europe

Yambo ©

QUANTUMESPRESSO

All the community of developers of Yambo and QE

MAX

DRIVING THE EXASCALE TRANSITION

**Follow us on:**

**company/max-centre/**

**@max_center2**

**http://www.max-centre.eu/**

# THANKS