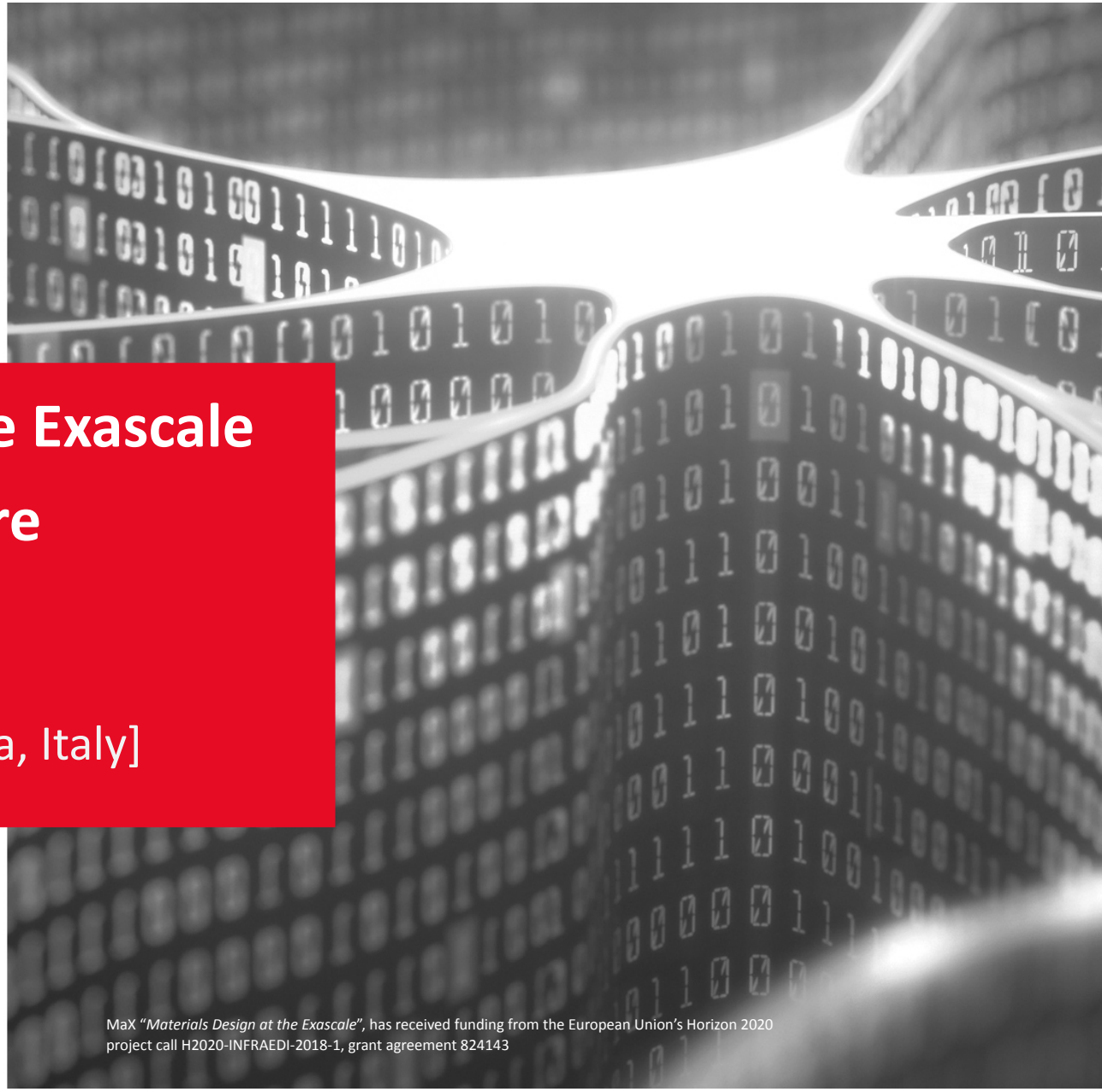
MaX DRIVING THE EXASCALE TRANSITION

MaX: Materials Design at the Exascale

[Advacing electronic structure community codes in HPC]

Andrea Ferretti [CNR-NANO, Modena, Italy]



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

CNRNANO
ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE

exascale is now

MAX DRIVING THE EXASCALE TRANSITION

the exascale challenge
in high performance computing

- 10^18 flops/s
- 10^18 Bytes
- abrupt technology changes
- **action is needed** for full exploitation
- **heterogeneous** machines (multiple HW and SW stacks)

EuroHPC Joint Undertaking

MareNostrum V

US DOE

Frontier (@ORNL): HDE+AMD
=> 1100 PFlops

Leonardo: Atos + NVIDIA A100
(CUDA backend) => 250 PFlops

LUMI: CRAY + AMD cards
(ROCm, HIP) => 550 PFlops

ab initio materials modelling

MAX DRIVING THE EXASCALE TRANSITION

quantum mechanics based
atomistic modelling of materials
+
interfacing with **multiscale** approaches

Electronic Structure Methods

- highly accurate (predictive)
- computationally demanding
- **a case for HPC**

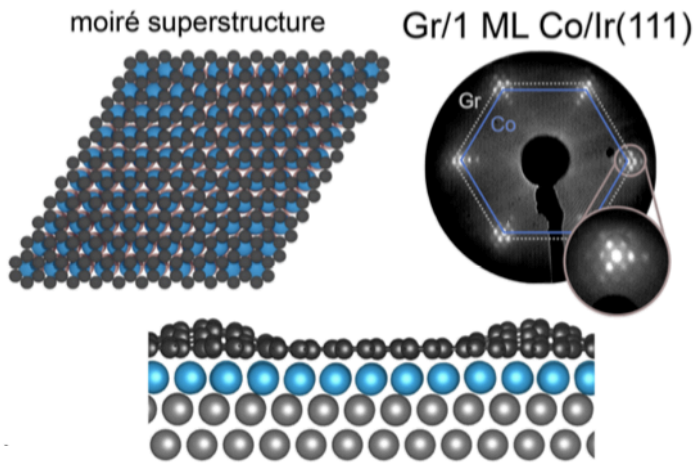
the **exascale** opportunity:

Higher accuracy

High throughput screening

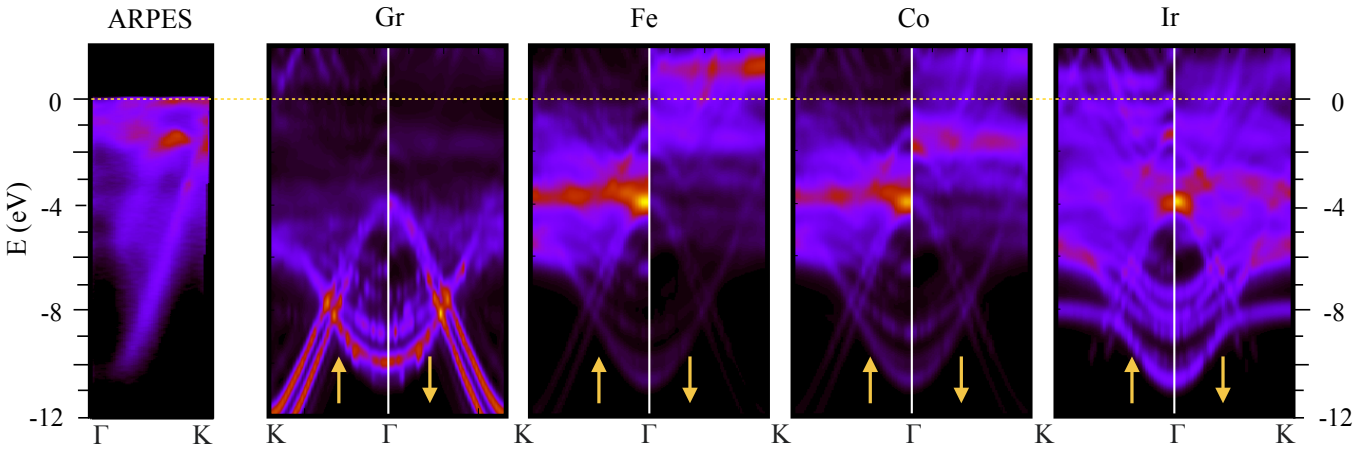
Improved modelling (complexity)

exascale opportunity: **complexity**



- Graphene / Transition Metal / Ir (111)
- **clear experimental evidence** for moire' pattern (**lattice mismatch**) and **Gr corrugation**
- 10x10 Graphene, 9x9 Iridium => 605 atoms / unit cell
- **Precise treatment of the structure** is crucial for modelling

- Avvisati et al, Nano Lett. **18**, 2268 (2018)
- Calloni et al, J. Chem. Phys. **153**, 214703 (2020)
- Cardoso et al, Phys. Rev. Mat. **5**, 014405 (2021)
- Pacile' et al, Appl. Phys. Lett. **118**, 121602 (2021)

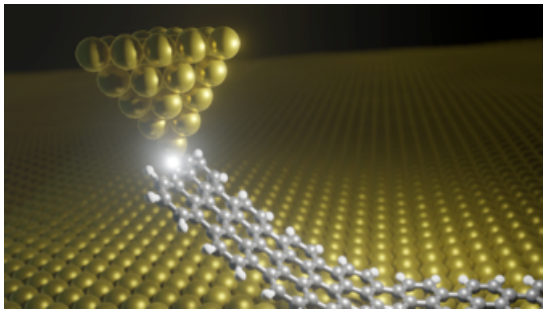


exascale opportunity: **accuracy**

NANO LETTERS
Letter
Cite This: Nano Lett. 2018, 18, 175−181
pubs.acs.org/NanoLett

Bright Electroluminescence from Single Graphene Nanoribbon Junctions

Michael C. Chong,[†] Nasima Afshar-Imani,[†] Fabrice Scheurer,[†] Claudia Cardoso,[‡] Andrea Ferretti,[‡] Deborah Prezzi,[*,‡] and Guillaume Schull[*,†]



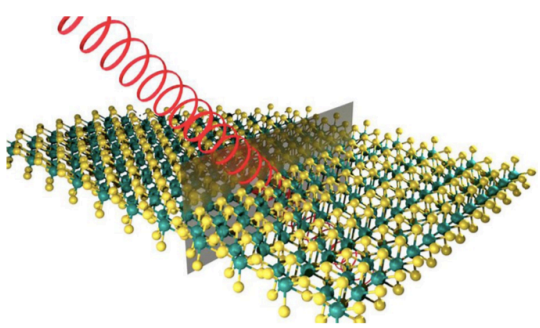
- clear experimental evidence of tip-induced **photoluminescence** from **suspended ribbons**
- tip needs to be in chemical contact with the ribbon (C-term.)
- excitation energy significantly smaller than extended GNR => **GNR termination**

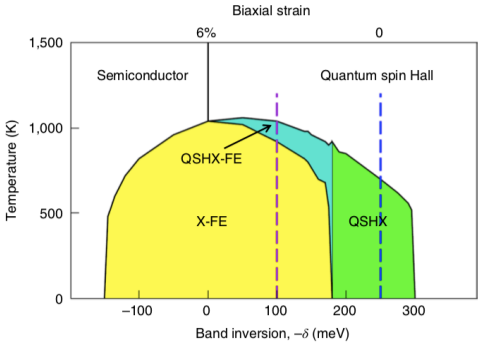
- Use of **manybody perturbation theory methods (MBPT)** (GW and BSE) to describe spsectroscopy

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]✉

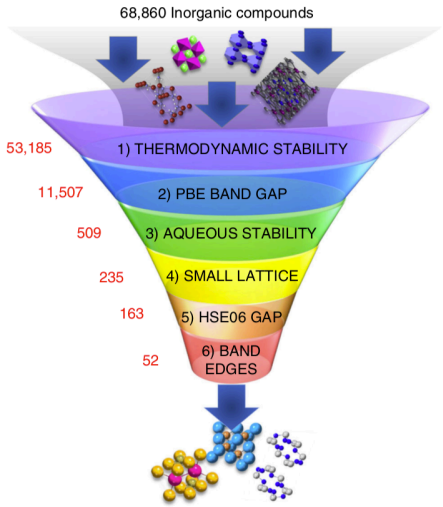




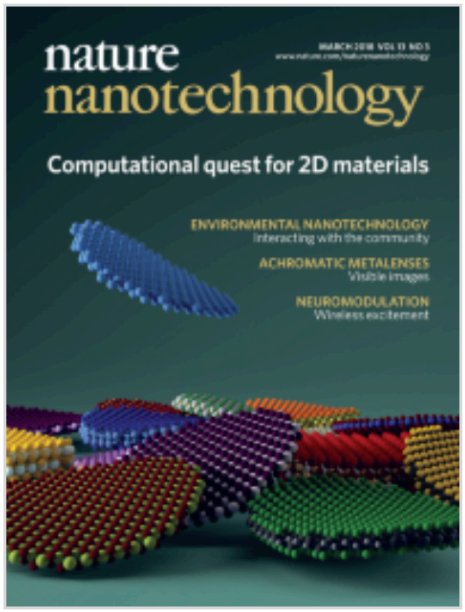
- computational search and detection of the long-sought **excitonic insular phase**
- **MBPT required** to describe the physics of the problem
- **extreme accuracy needed**

high-throughput screening

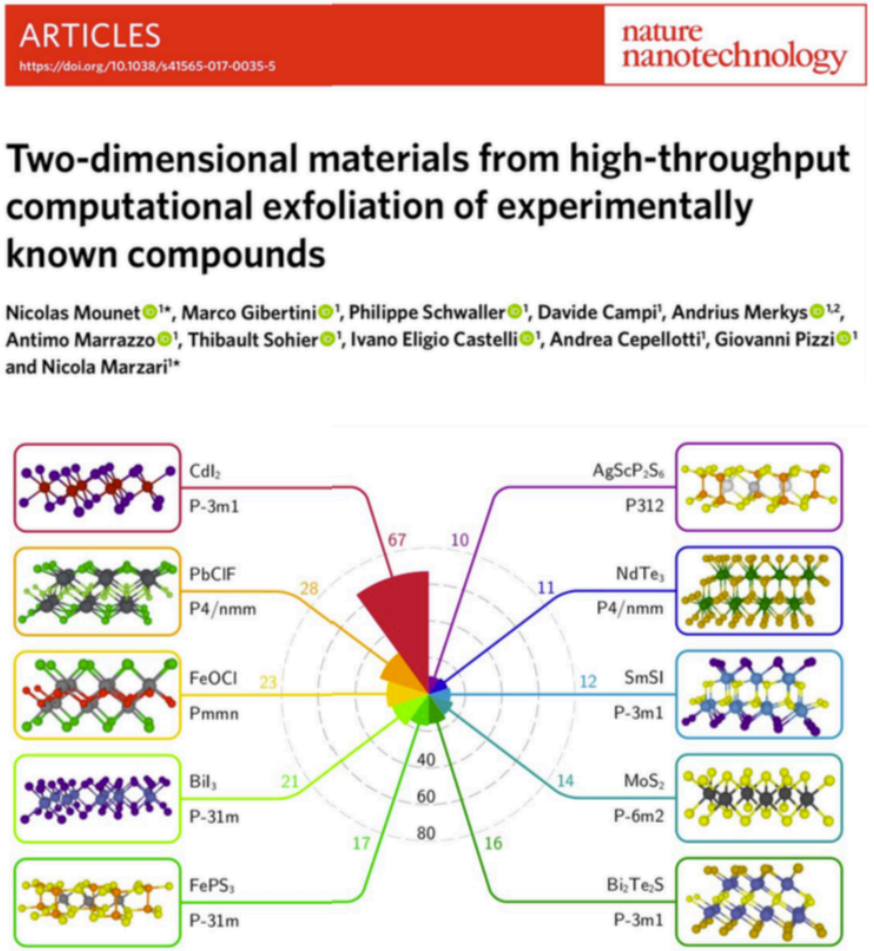
in materials science



Singh et al, Nature Commun **10**, 443 (2019)



Mounet, Gibertini, et al, Nature Nanotech **13** (2018)



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MAX

[**GPUs:** Today and Tomorrow]


MAX
DRIVING
THE EXASCALE
TRANSITION


QUANTUMESPRESSO


CP2K

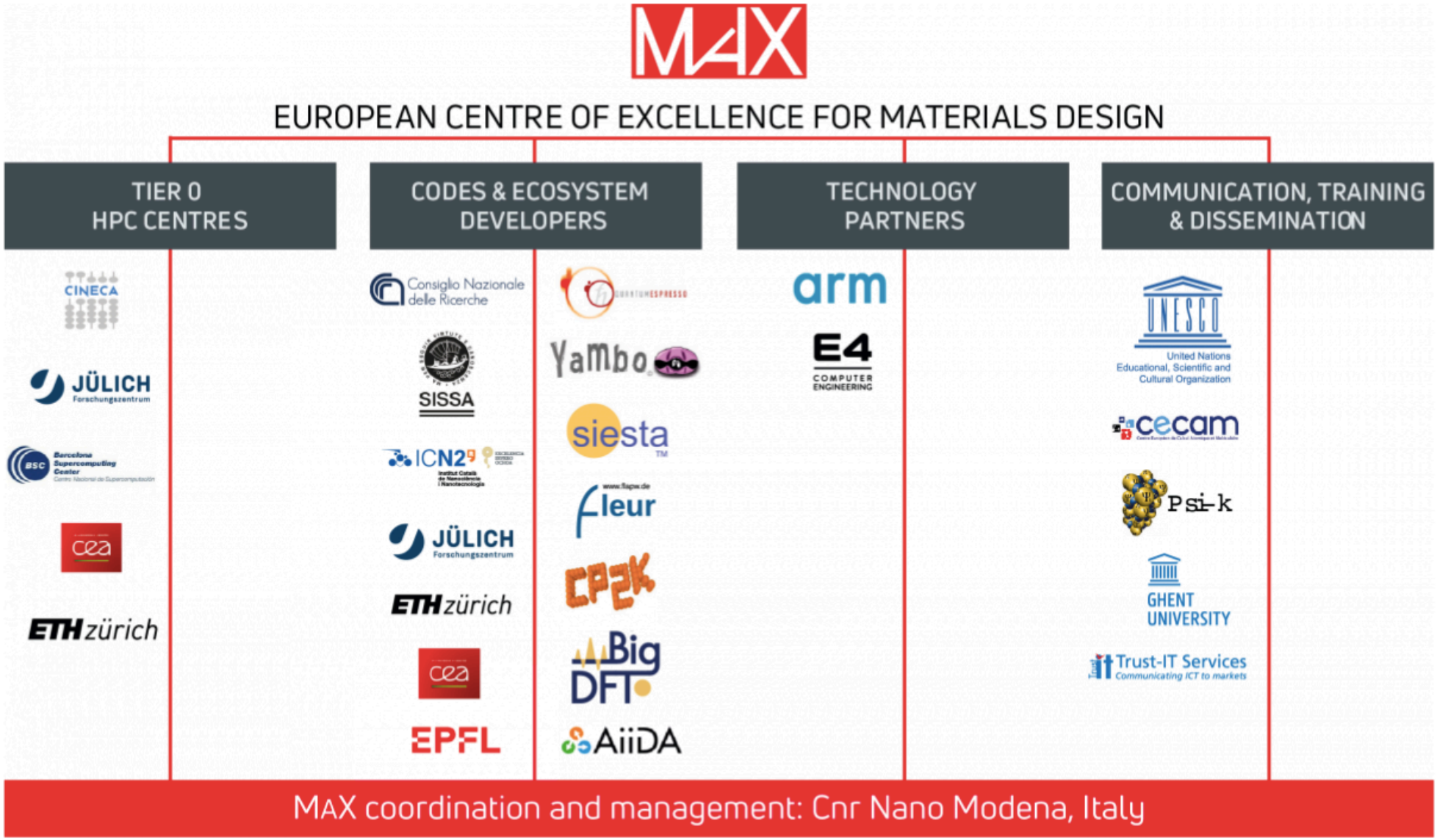

Yambo


siesta


Big
DFT


www.flapw.de
fleur


AiiDA


MAX
EUROPEAN CENTRE OF EXCELLENCE FOR MATERIALS DESIGN
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& DISSEMINATION
UNESCO
United Nations Educational, Scientific and Cultural Organization
cecam
Psi-k
GHENT UNIVERSITY
Trust-IT Services
Communicating ICT to markets
MAX coordination and management: Cnr Nano Modena, Italy

- **widely used, open source, community codes in electronic structure**

- **parallel optimization and performance portability are key to keep exploiting HPC resources**
- **All MaX flagship codes released for production with GPU support**

- leverage the convergence of HPC with automated **high throughput computing** and high-performance **data analytics**
- hardware-software **codesign** in practice

- **widely used open source, community codes in electronic structure**

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- **All MaX flagship codes released for production with GPU support**

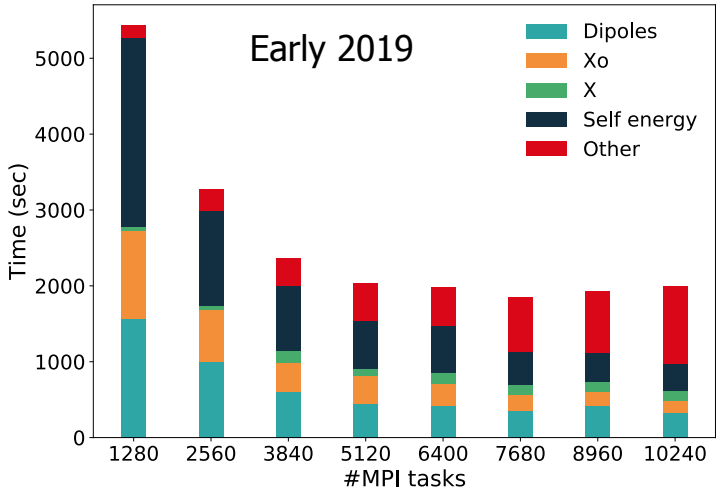
- **large effort on education and training: hands-on schools and hackathons**

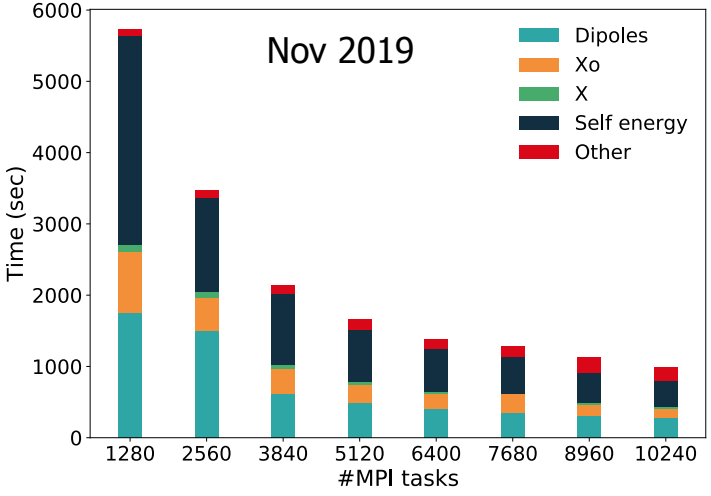
training material available !

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

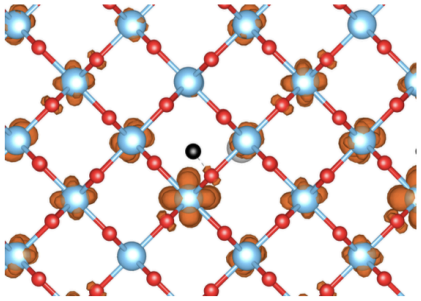
Yambo parallel performance

heterogeneous architectures: **MPI** + OpenMP + CUDA





- **optimisation of MPI+OpenMP** parallelism
- working at scale (bottleneck identification and solution)



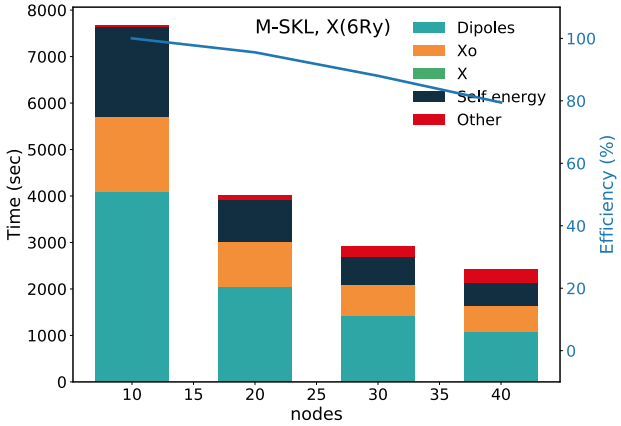
system size: 72+1 atoms, 2000 bands, 6 Ry for Xo repr (N=1317); ~290 occ states, 8 kpts.

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

Yambo: performance (GPU)

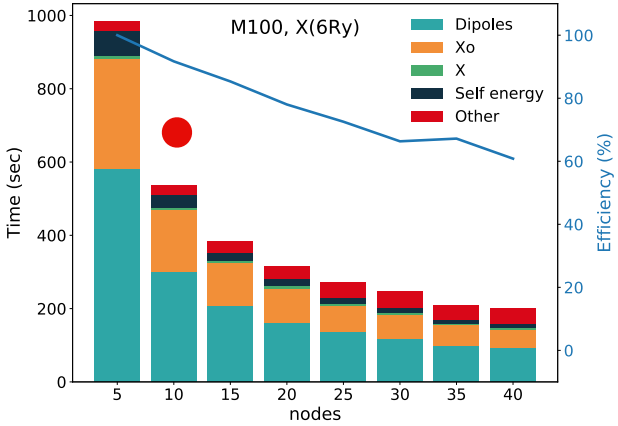
heterogeneous architectures: **MPI** + **OpenMP** + **CUDA**

CPU: **Skylake**



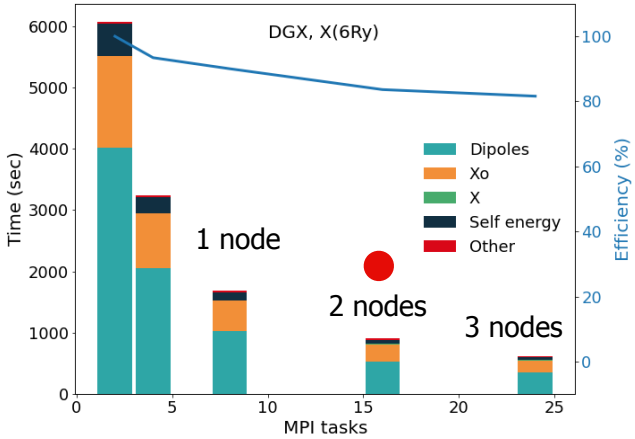
x14 wrt SKL (10 nodes)

GPU: P9+**V100**

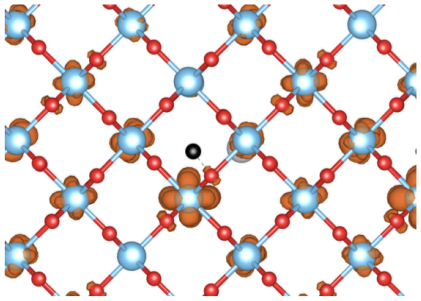


x1.4 wrt V100 (2 nodes)

GPU: AMD-Rome + **A100** (DGX)



- complete **GW workflow** for defected TiO2 (rutile)
- small system, **stress test**
- 1 MPI task/GPU
- data obtained on Marconi100, 4 V100 GPUs/node
- and DGX arch, 8 A100 GPUs/node



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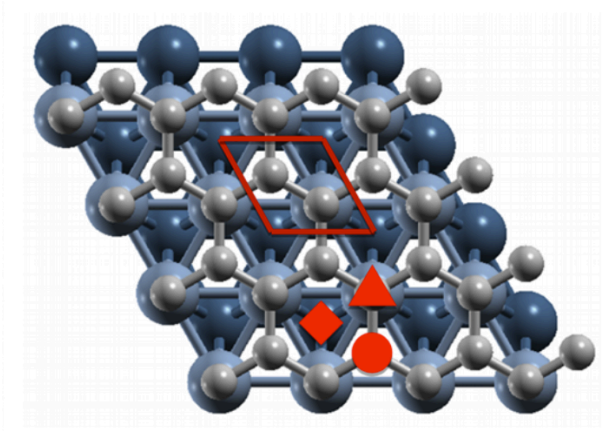
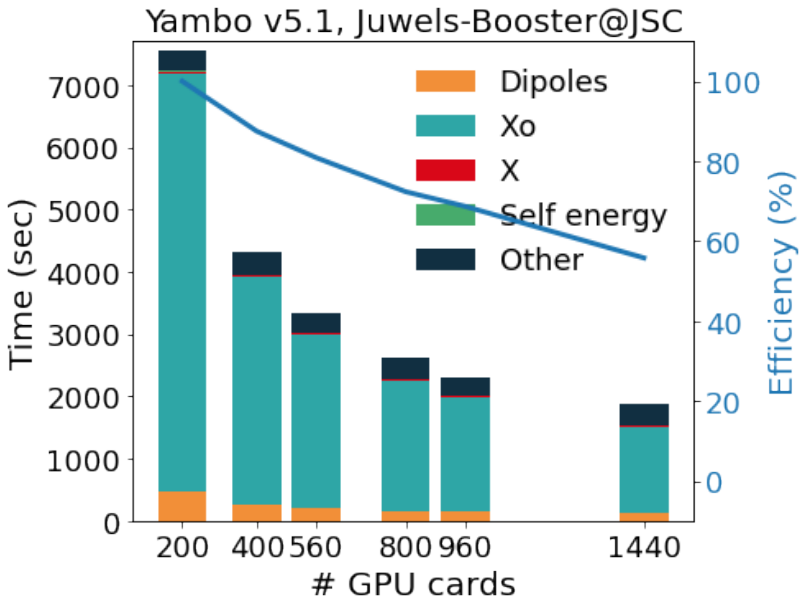
Yambo: performance (GPU)

Juwels-Booster: 4 Nvidia A100 / node

runs: up to 360 J-B nodes about 40% of the whole machine (960 nodes)

GW study of
Graphene @ Co(0001) interface





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electronic structure

nature materials

INSIGHT | REVIEW ARTICLE

https://doi.org/10.1038/s41563-021-01013-3

Check for updates

Electronic-structure methods for materials design

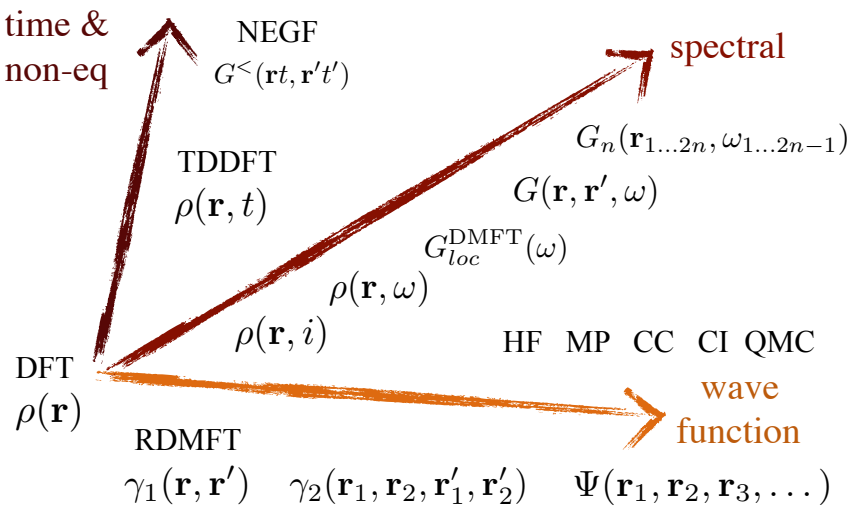
Nicola Marzari[1]✉, Andrea Ferretti[2] and Chris Wolverton[3]

Density functional theory (DFT):

- applications ranging from **materials modelling, to quantum chemistry and drug design**
- compatible with **high performance computing** and **high-throughput screening**

beyond DFT:

- **multiple hierarchies** can be climbed
  - wavefunction-based methods
  - **many-body perturbation theory and spectral methods**
  - time-dependent and non-equilibrium methods



Thanks !

@max_center2

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