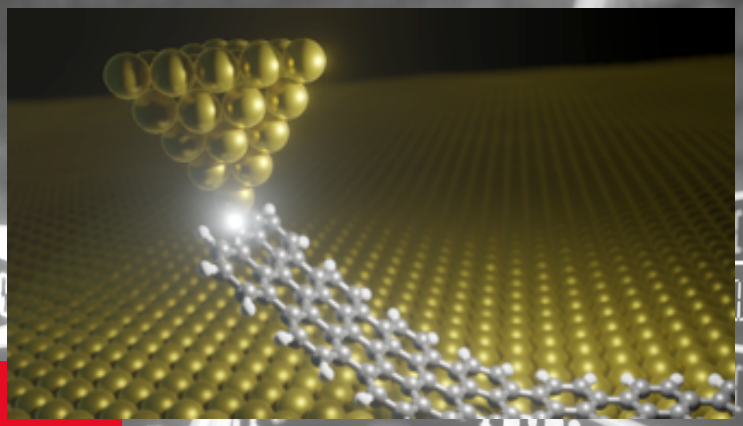
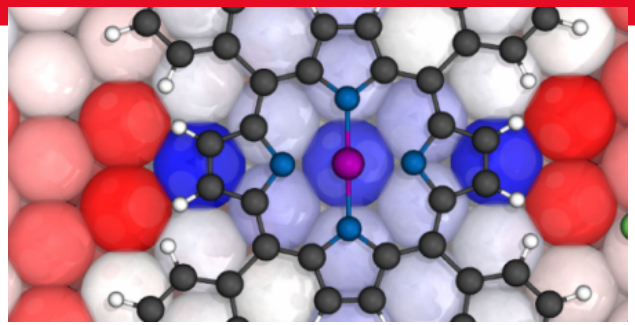
MAX DRIVING THE EXASCALE TRANSITION



Computational Materials Design at the Exascale:

Porting community codes, challenges and success cases

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

materials modelling

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

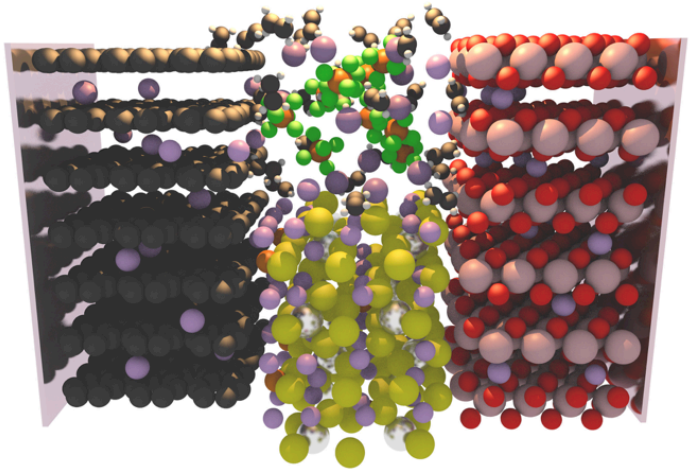
Electronic Structure Methods

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

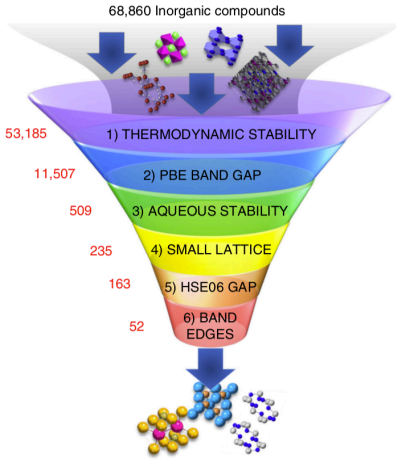
MAX

the **exascale** opportunity:

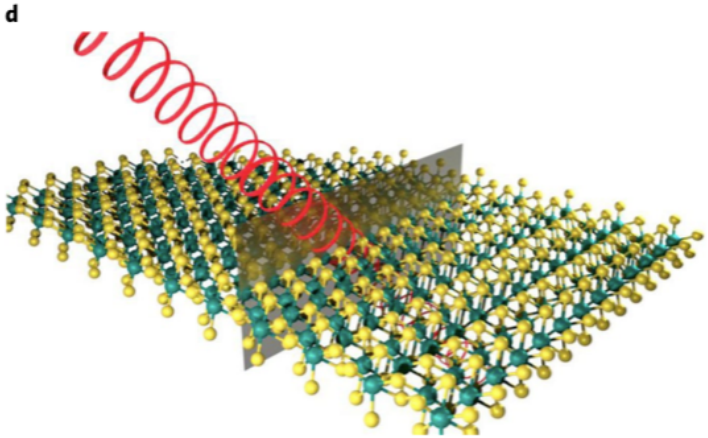
complexity



high-throughput screening



accuracy &
adv. properties



exascale is approaching

MAX DRIVING THE EXASCALE TRANSITION

the exascale challenge
in high performance computing

EuroHPC Joint Undertaking

- 10^18 flop/s
- 10^18 Bytes
- abrupt technology changes
- **action is needed** for full exploitation
- **multiple** HW and SW stacks
- memory hierarchies

MareNostrum V

Currently:

Jewels Booster:
NVIDIA A100, 71 PFl
Marconi100:
NVIDIA V100, 29 PFl
PizDaint:
NVIDIA P100, 27 PFl

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

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

programme

MAX DRIVING THE EXASCALE TRANSITION

Agenda:

- **Andrea Ferretti (CNR Nano):** *Welcome*
- **Nicola Marzari (EPFL):** *Materials design at the intersection of high-throughput and high-performance-computing*
- **Stefano Baroni (SISSA):** *Challenges and success towards the exascale: the perspective of Quantum ESPRESSO, a large community code'*
- **Joost VandeVondele (ETHZ):** *Software engineering towards exascale: domain specific libraries, communication optimality, and machine learning*
- **Daniele Varsano (CNR Nano):** *Accelerating GW and many-body perturbation theory using GPUs: yambo hunting for excitonic insulators*
- **Uliana Alekseeva (FZ Juelich):** *Parallelization and optimization of the FLEUR code: new possibilities for all-electron Density Functional Theory*
- **Pablo Ordejón (ICN2):** *HPC-enabled very large scale quantum simulations in materials with SIESTA*
- **Live** *Q&A*

Enjoy !

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