MAX DRIVING THE EXASCALE TRANSITION

QUANTUM ESPRESSO towards the exascale

Stefano Baroni
Scuola Internazionale di Studi Superiori ed Avanzati, Trieste

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

what is QUANTUM ESPRESSO

QUANTUM ESPRESSO is the prime open-source suite of codes for quantum mechanical materials modelling, based on DFT, plane waves, and pseudo-potentials

what is QUANTUM ESPRESSO

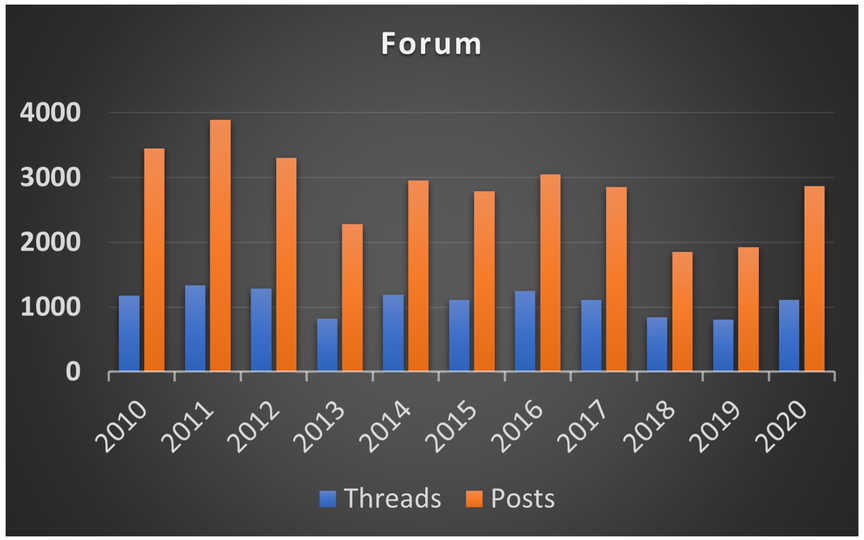
QUANTUM ESPRESSO is the prime open-source suite of codes for quantum mechanical materials modelling, based on DFT, plane waves, and pseudo-potentials

the defining features of QUANTUM ESPRESSO are:

- **innovation —** QE is the workbench of many methodological innovations in electronic-structure theory (CP, DFPT, tdDFPT, …)
- **portability —** QE is available on many different hardware architectures and operating systems
- **performance —** QE is extremely effective on a broad array of systems, ranging from laptops to supercomputers

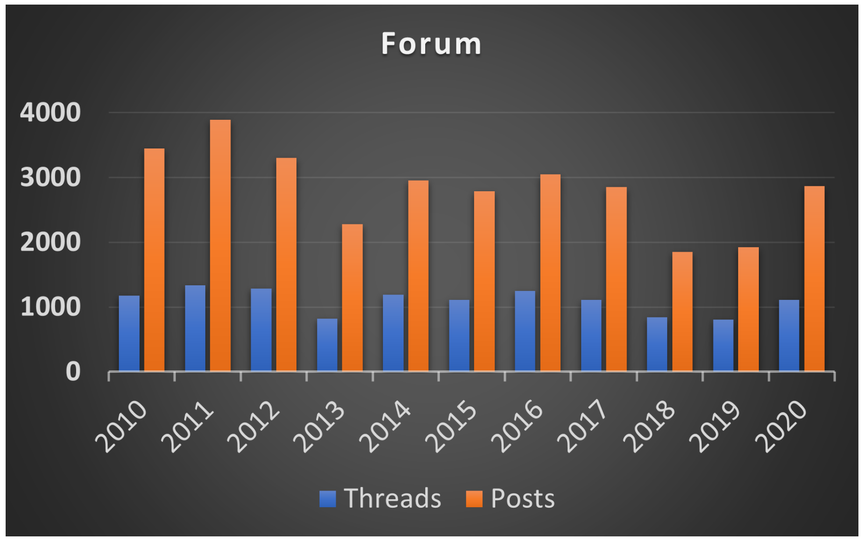
QUANTUM ESPRESSO: the impact

1,800+ active users



QUANTUM ESPRESSO: the impact

1,800+ active users

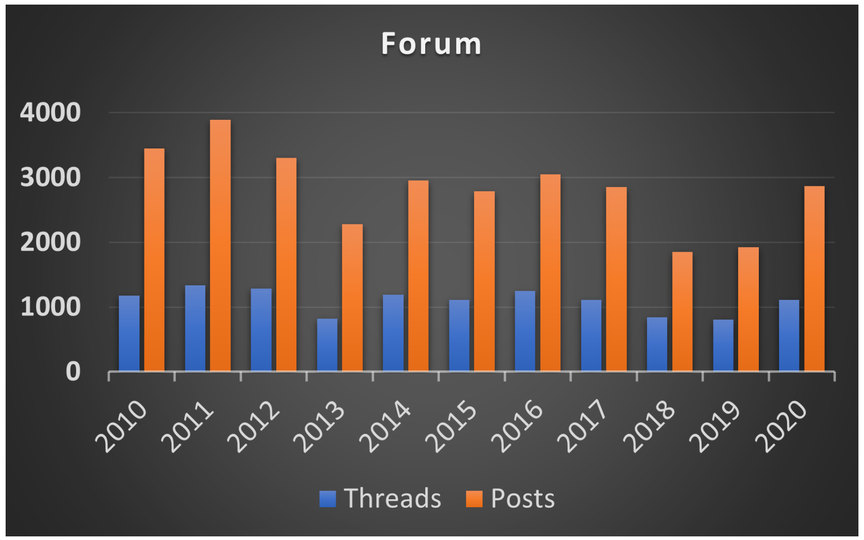


2,000+ citations/year

DRIVING THE EXASCALE TRANSITION

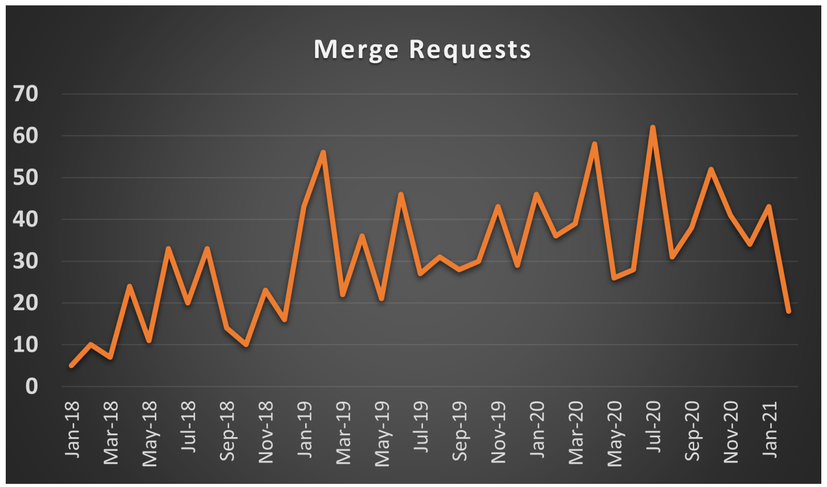
QUANTUM ESPRESSO: the impact

1,800+ active users



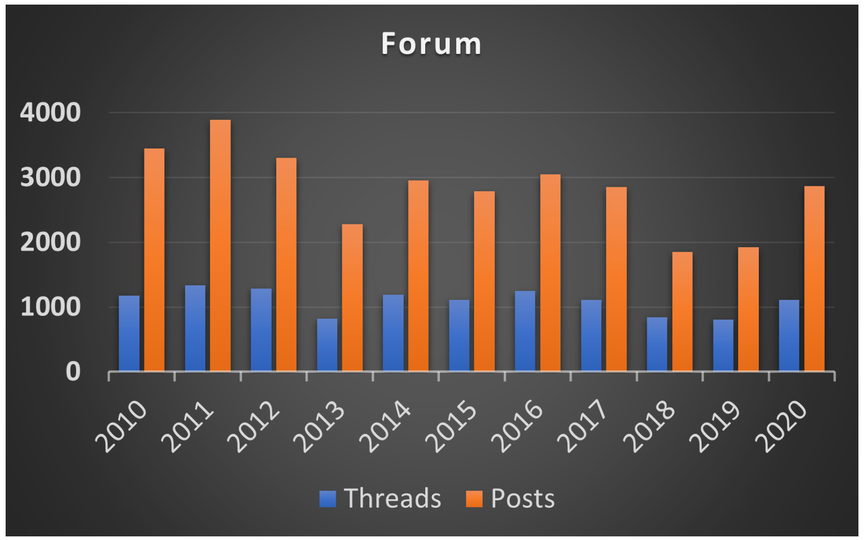
2,000+ citations/year

50+ active developers, ≈50 merges/month on git



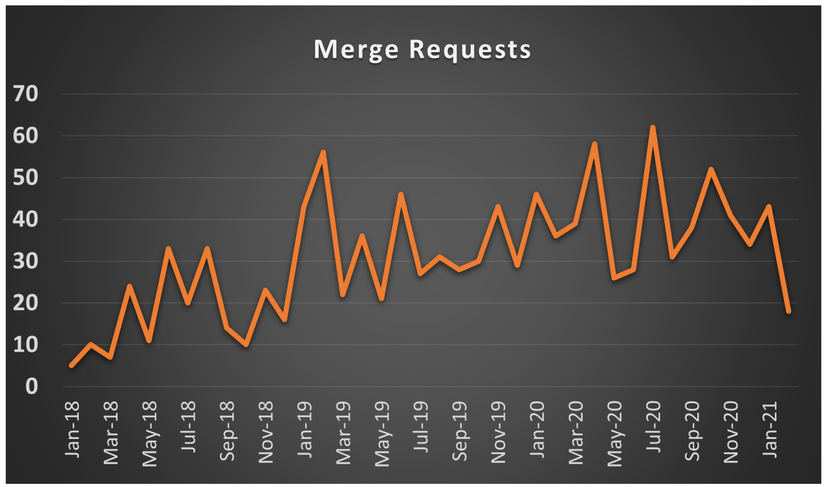
QUANTUM ESPRESSO: the impact

1,800+ active users

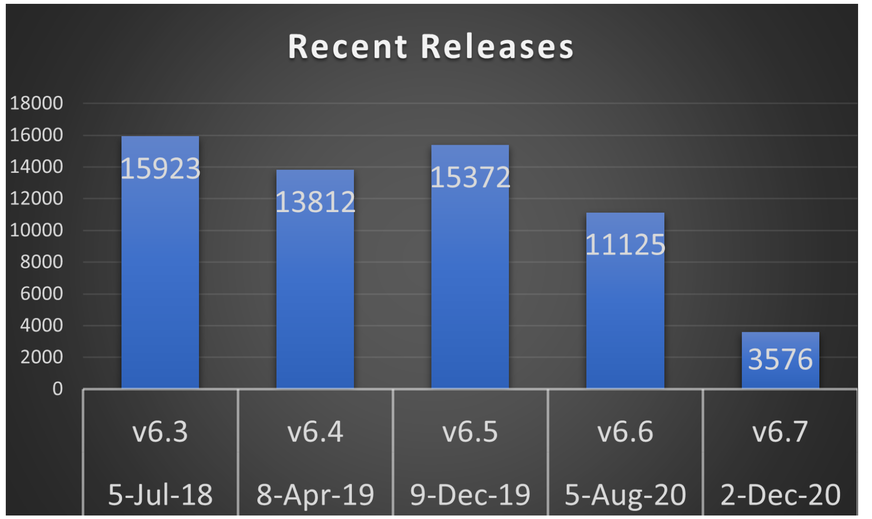


2,000+ citations/year

50+ active developers, ≈50 merges/month on git

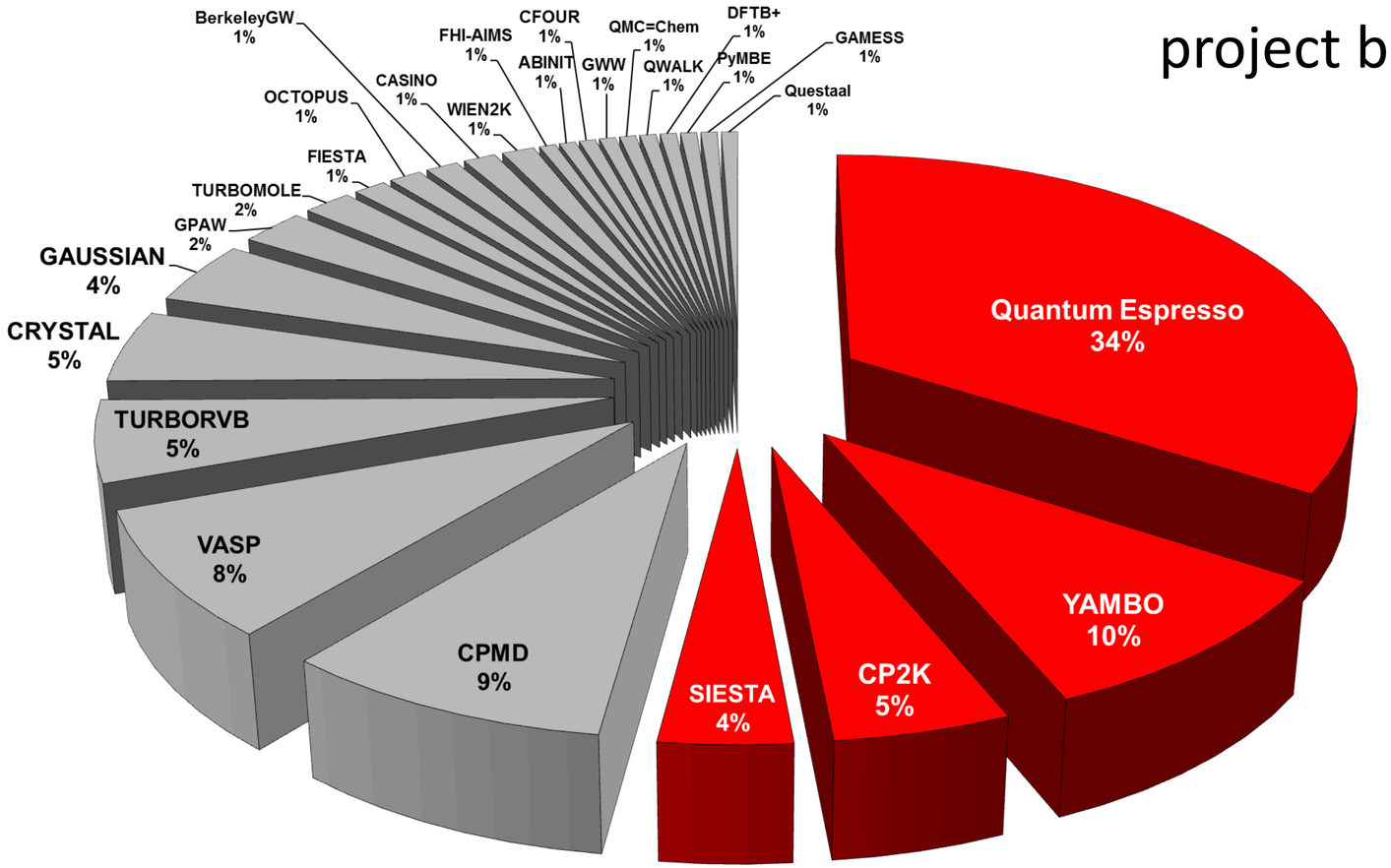


10-15,000 downloads/release

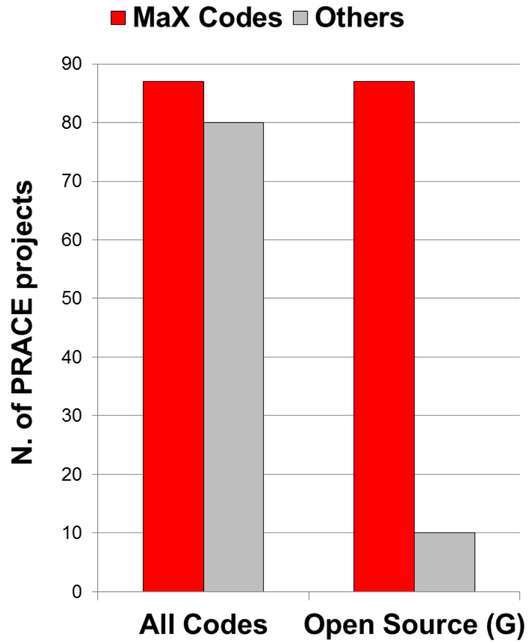


DRIVING THE EXASCALE TRANSITION

QUANTUM ESPRESSO: the impact



PRACE materials & chemistry project breakup per code



DRIVING THE EXASCALE TRANSITION

QUANTUM ESPRESSO on the marketplace

custom-built solutions

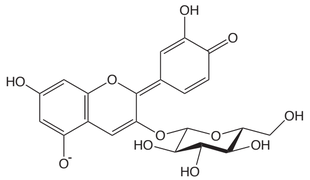
MARS

chocolate

north america

QUANTUM ESPRESSO on the marketplace

custom-built solutions

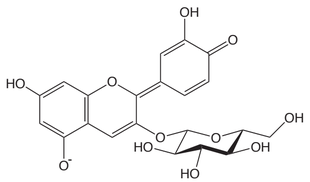


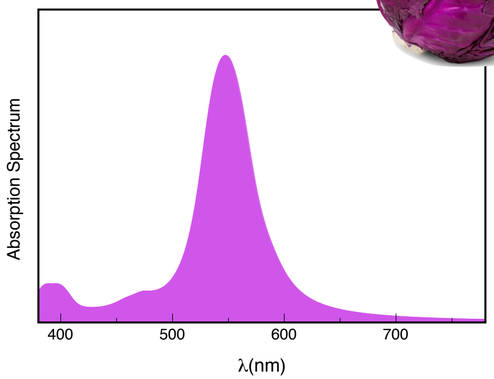
MARS
chocolate
north america

QUANTUM ESPRESSO on the marketplace

custom-built solutions

MARS chocolate north america

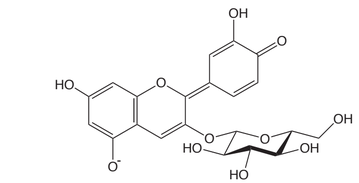


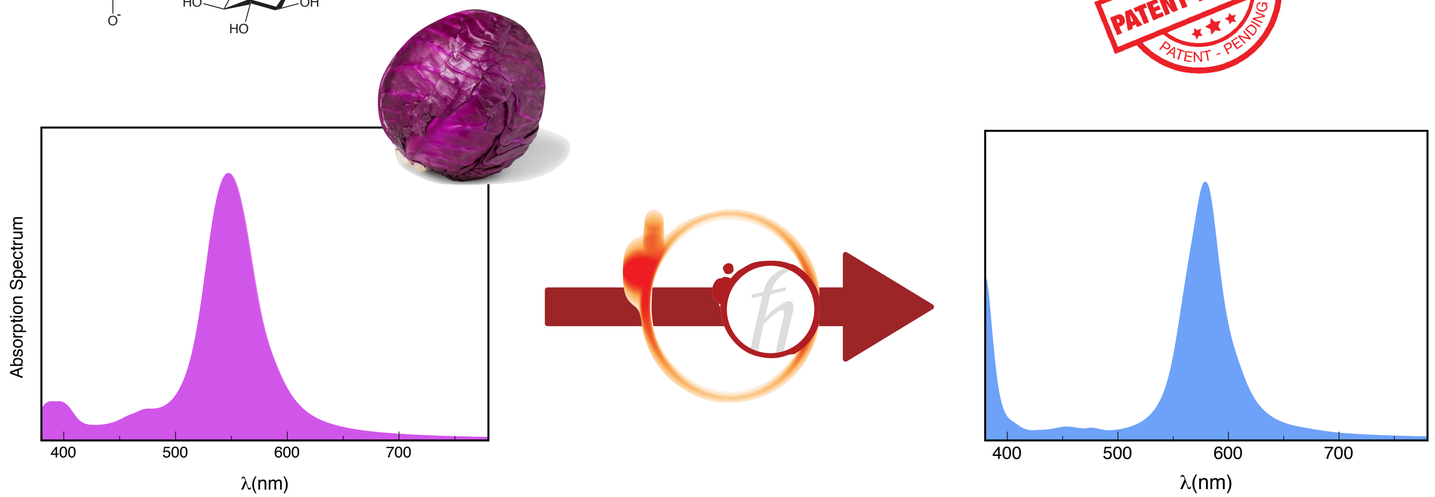


QUANTUM ESPRESSO on the marketplace

custom-built solutions

MARS chocolate north america





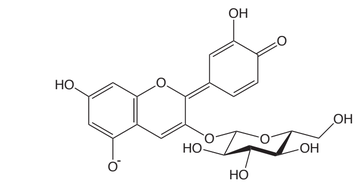
PATENT - PENDING
PATENT-PENDING
PATENT - PENDING

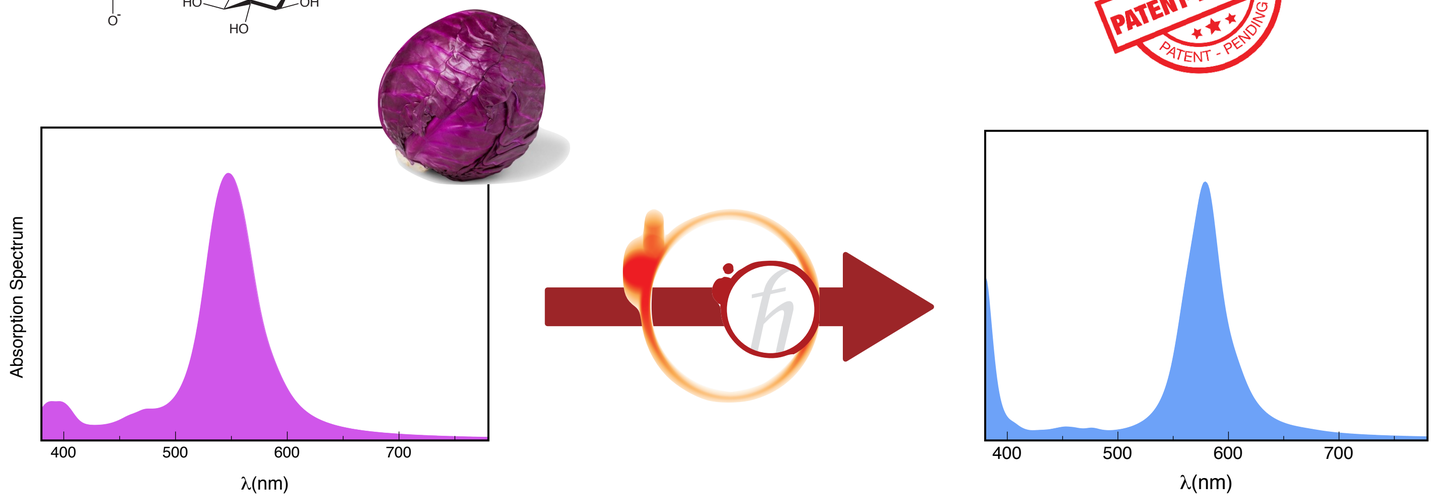
DRIVING THE EXASCALE TRANSITION

QUANTUM ESPRESSO on the marketplace

custom-built solutions

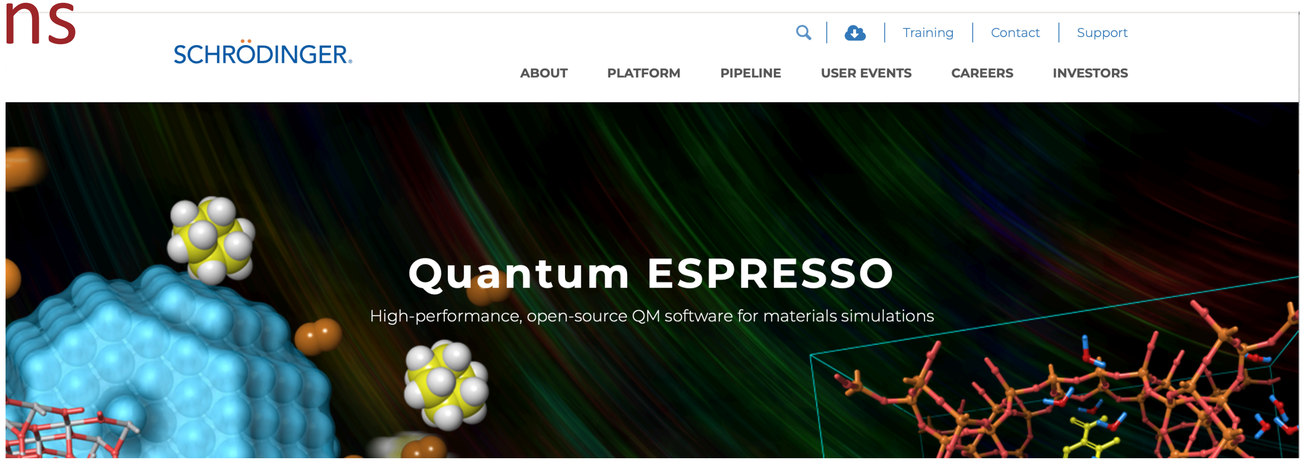
MARS chocolate north america



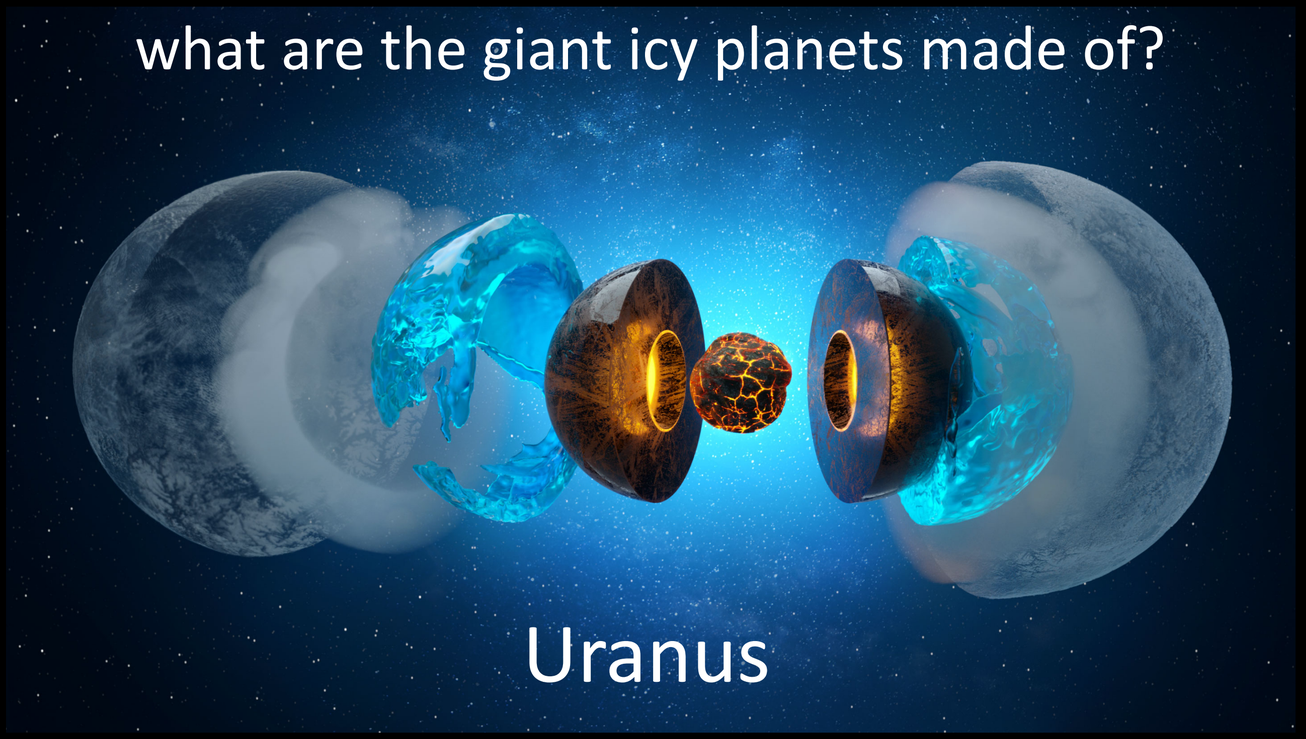


PATENT - PENDING

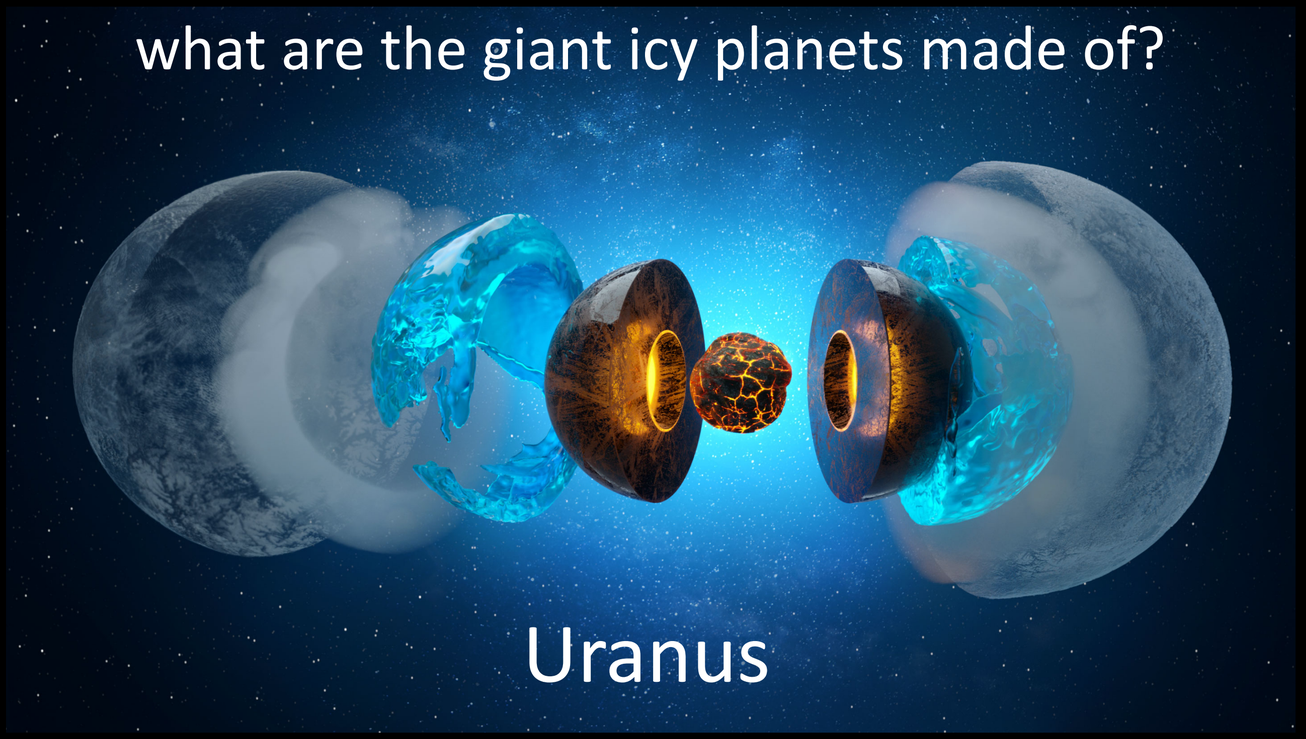
turn-key solutions

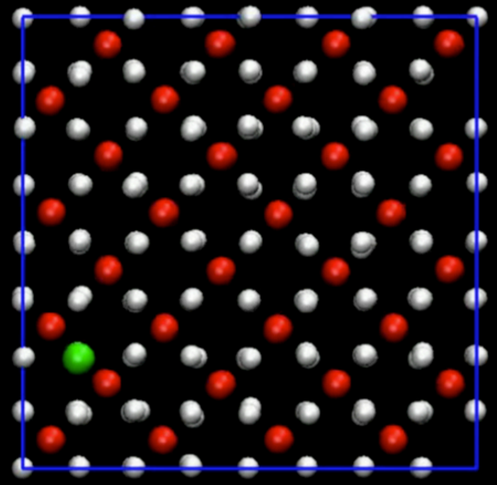


from the supermarket shelf up to the heavens



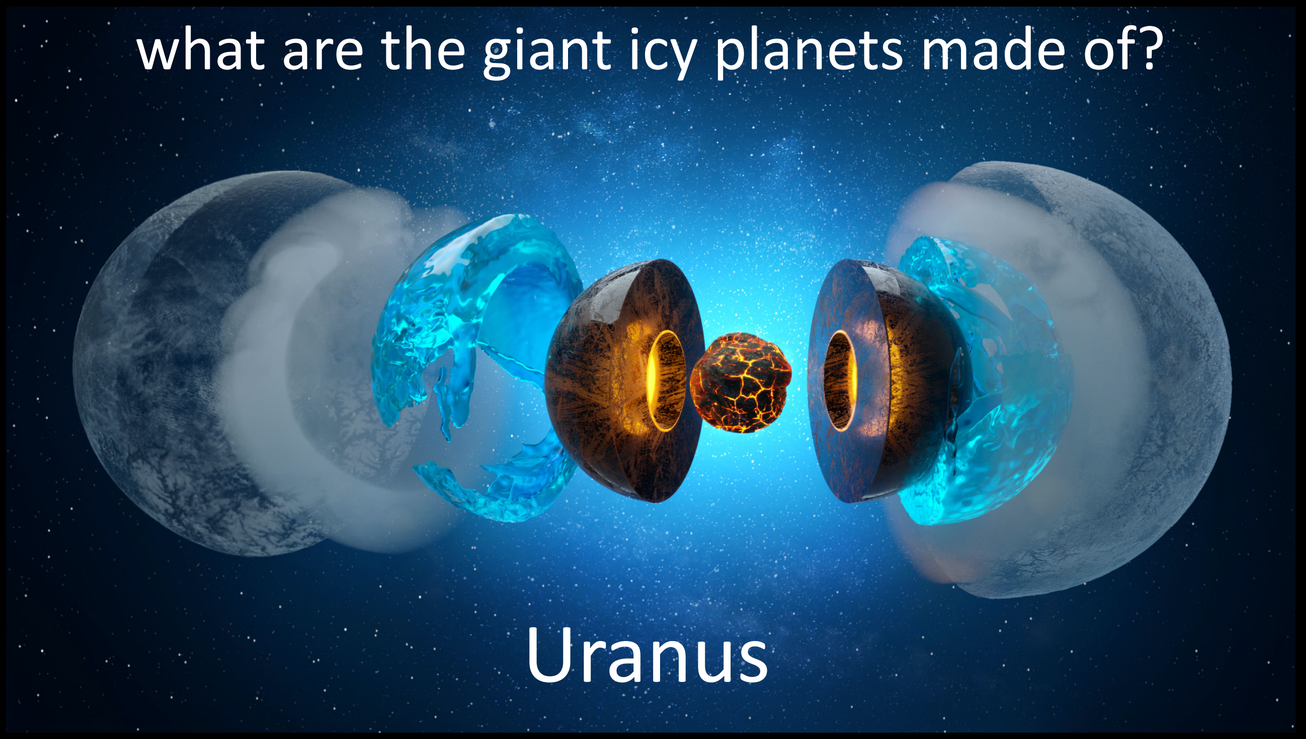
from the supermarket shelf up to the heavens

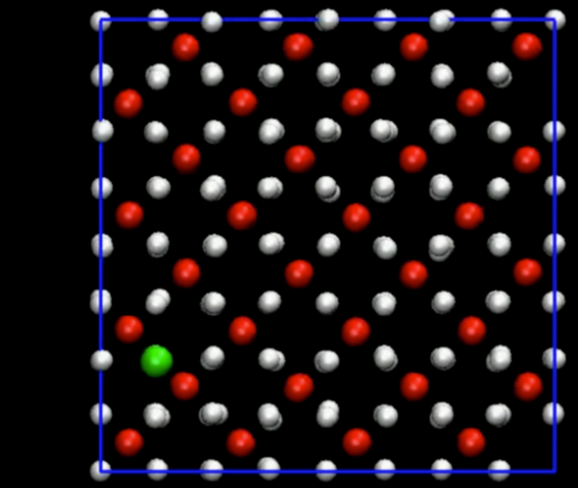


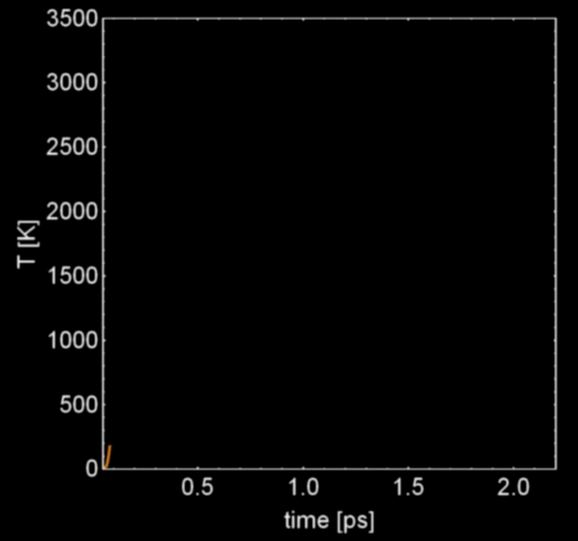


P=175 GPa
ice X

from the supermarket shelf up to the heavens

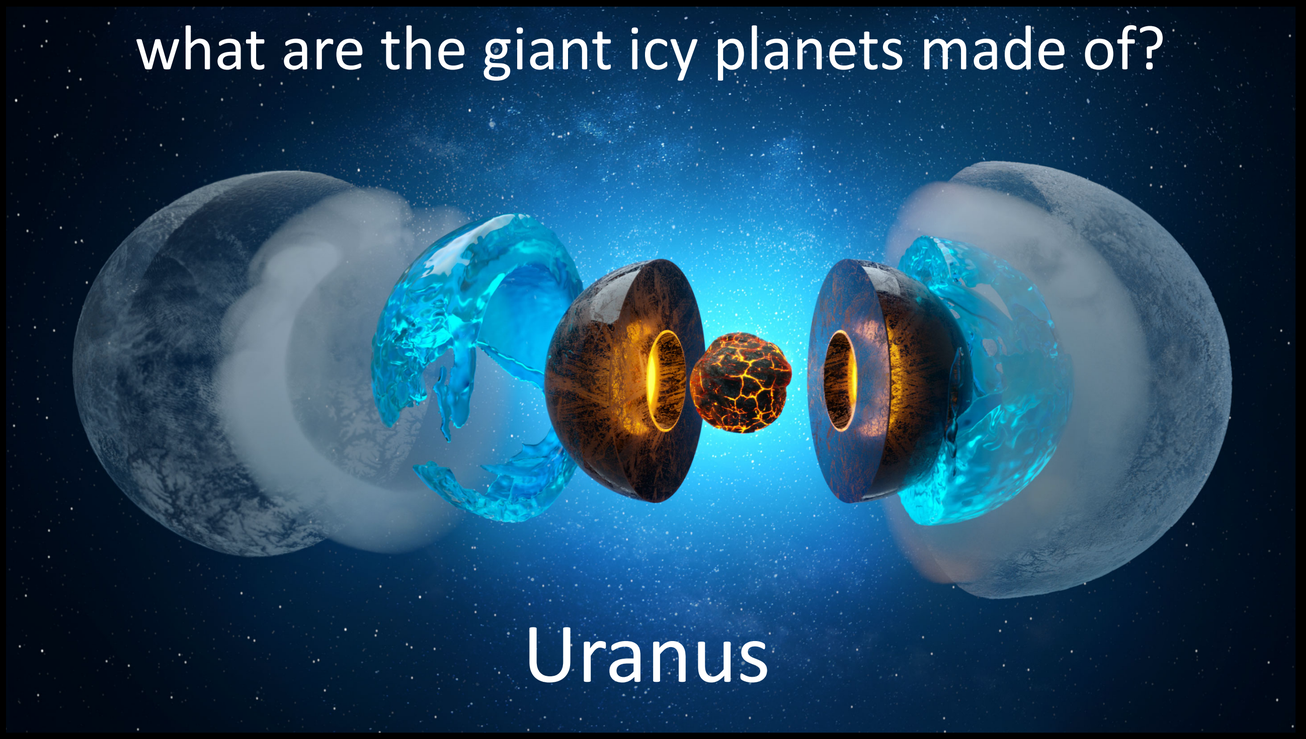


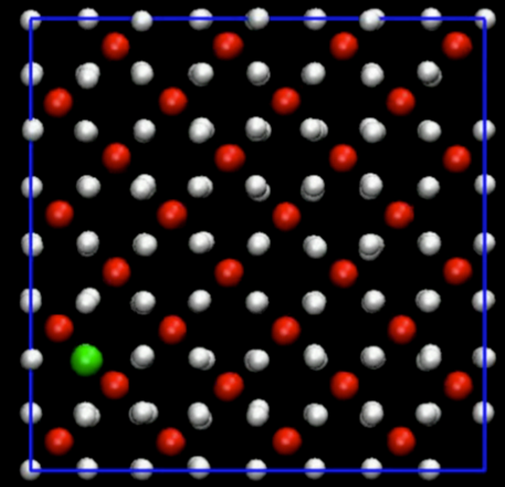


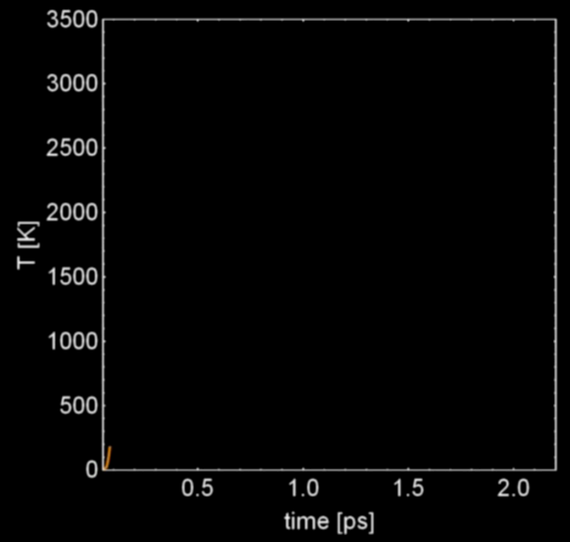


P=175 GPa
ice X

from the supermarket shelf up to the heavens







P=175 GPa
ice X

nature COMMUNICATIONS

ARTICLE

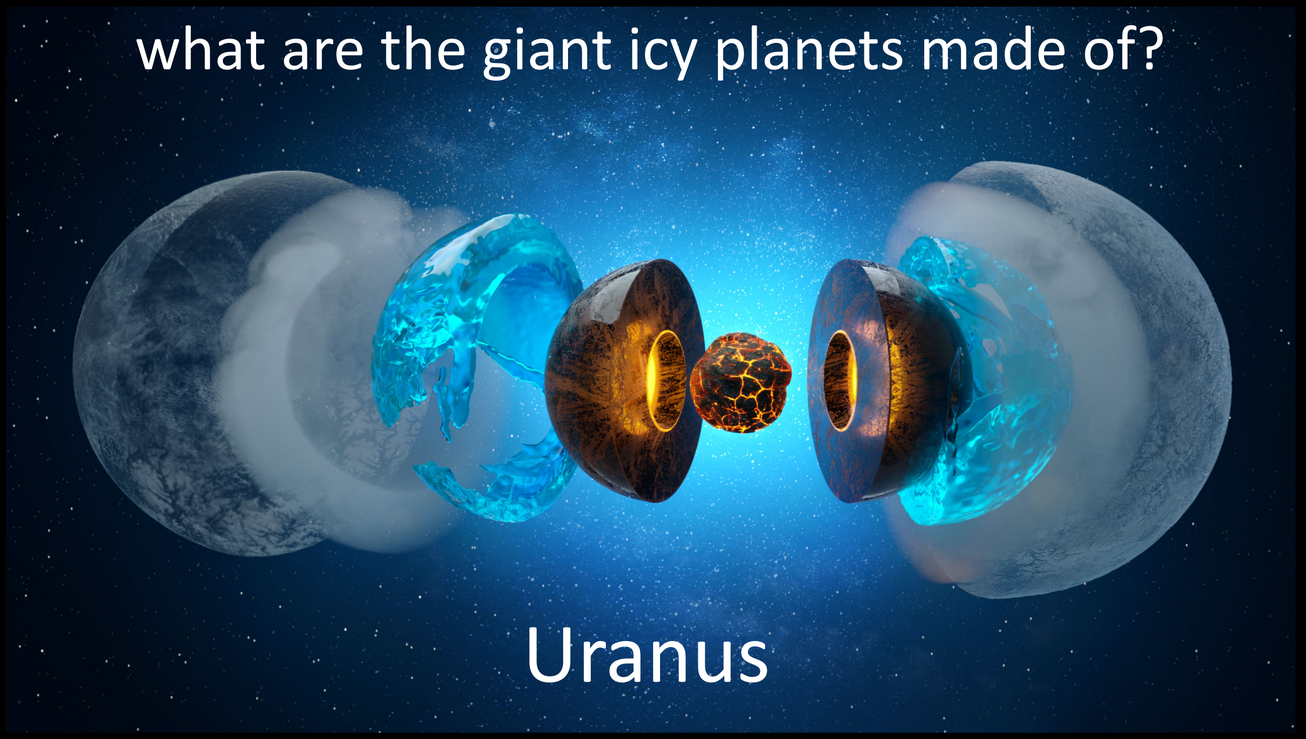
https://doi.org/10.1038/s41467-020-17275-5 OPEN

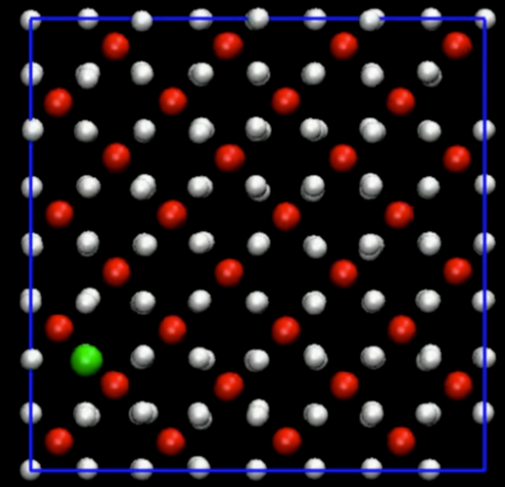
Heat and charge transport in H_2O at ice-giant conditions from ab initio molecular dynamics simulations

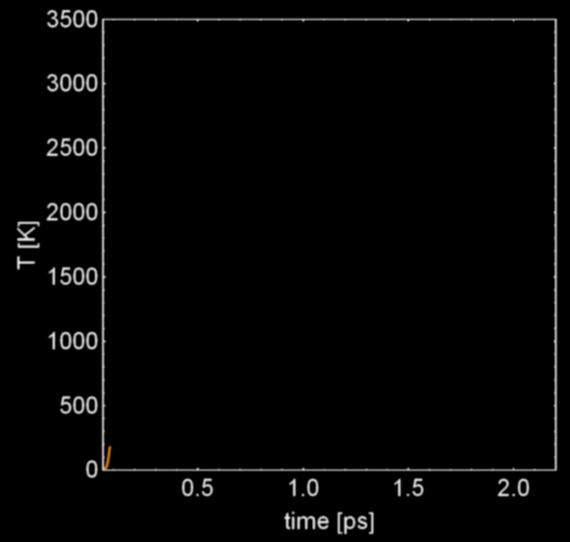
Federico Grasselli[1,4], Lars Stixrude[2] & Stefano Baroni[1,3]✉

DRIVING THE EXASCALE TRANSITION

from the supermarket shelf up to the heavens







P=175 GPa
ice X

nature COMMUNICATIONS

ARTICLE

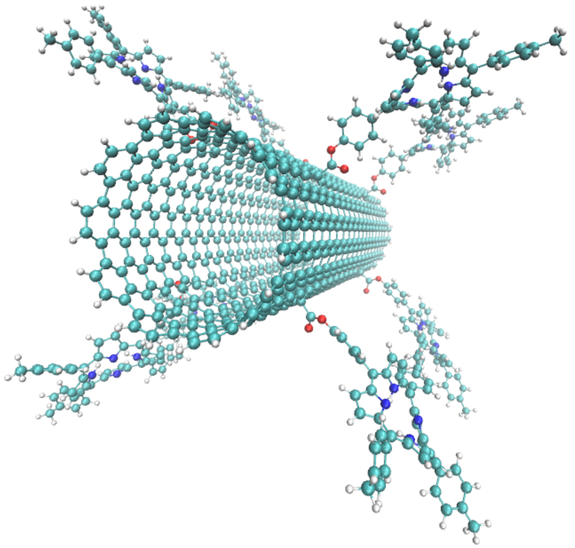
https://doi.org/10.1038/s41467-020-17275-5 OPEN

Heat and charge transport in H_2O at ice-giant conditions from ab initio molecular dynamics simulations

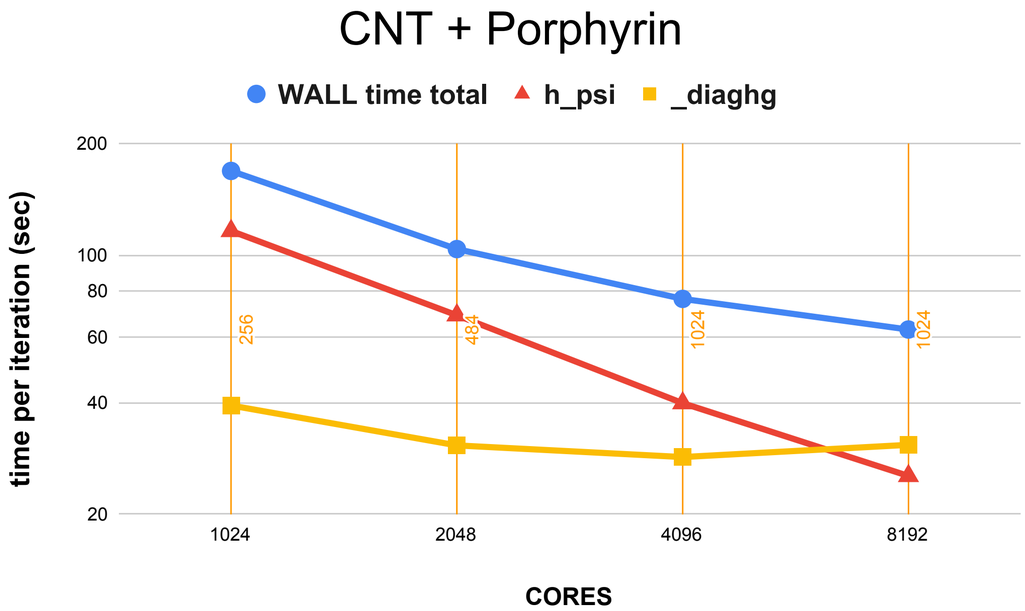
Federico Grasselli[1,4], Lars Stixrude[2] & Stefano Baroni[1,3]✉

DRIVING THE EXASCALE TRANSITION

QUANTUM ESPRESSO towards the exascale

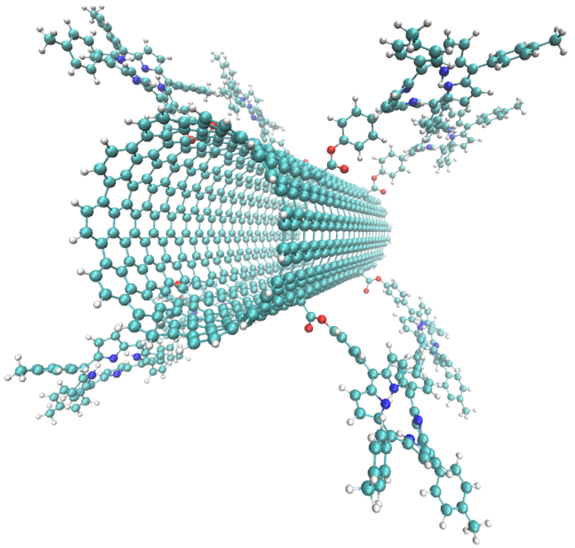


porphyrin@CNT

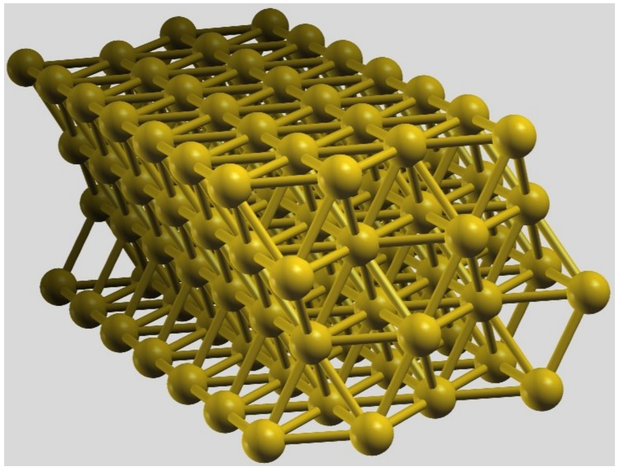


porphyrin@CNT
1,500+ atoms
3,200+ electrons
2.4×10^6 PWs

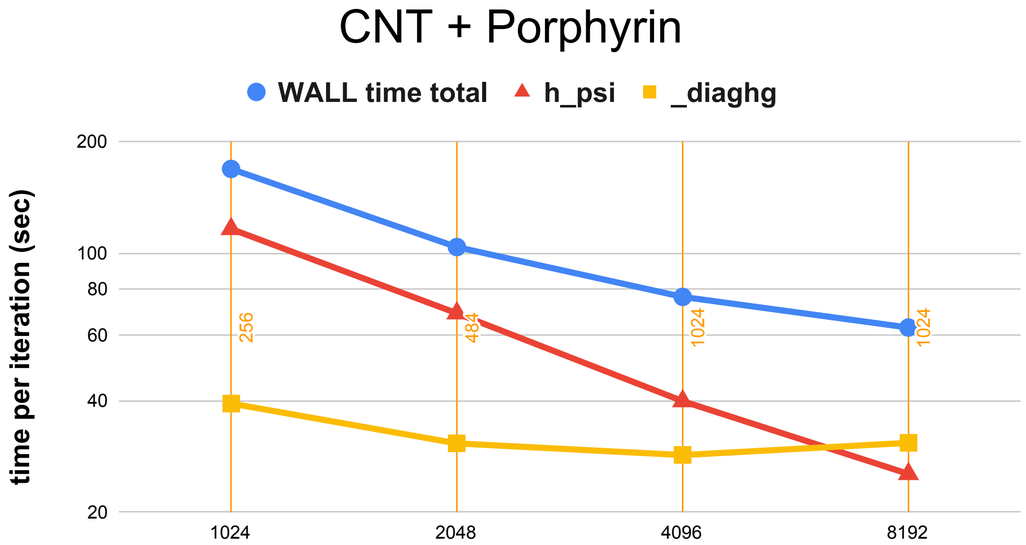
QUANTUM ESPRESSO towards the exascale

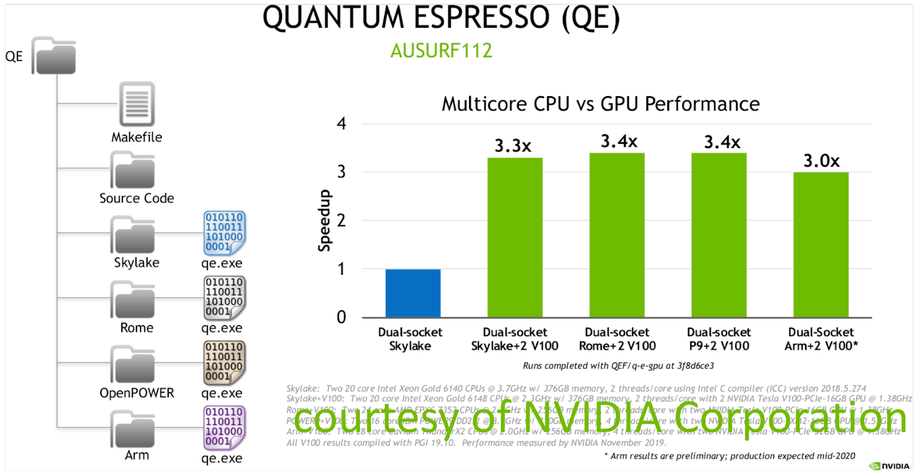


porphyrin@CNT



Au_{112} surface

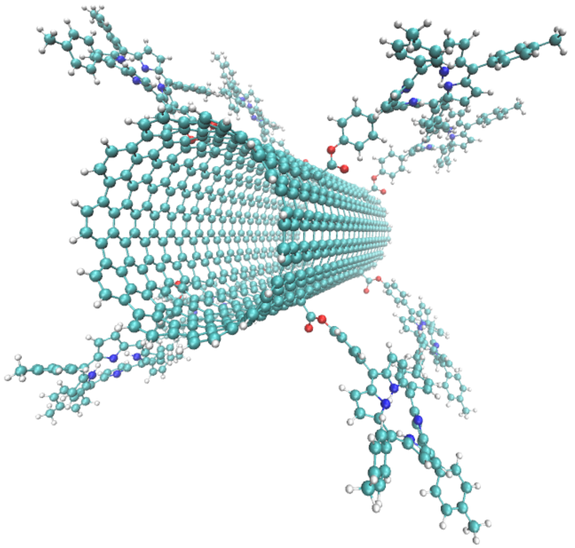




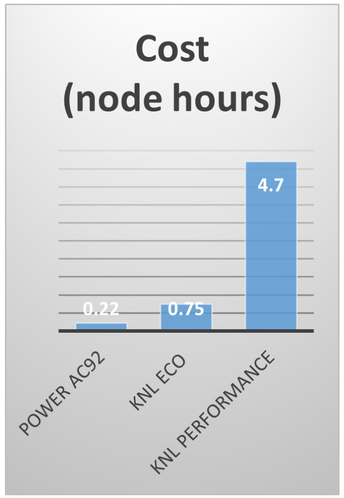
courtesy of NVIDIA Corporation

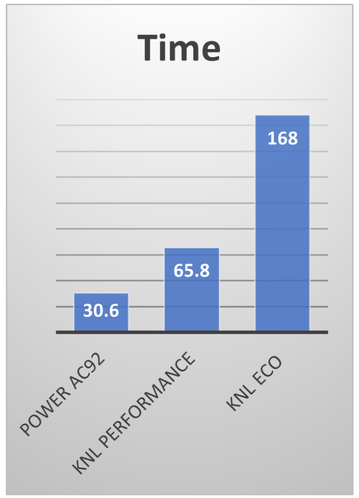
DRIVING THE EXASCALE TRANSITION

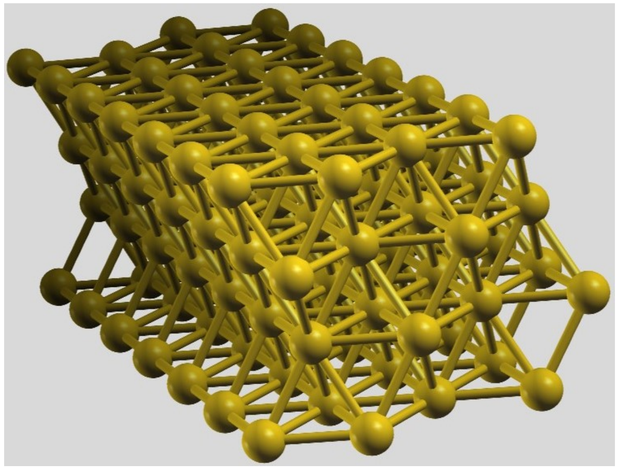
QUANTUM ESPRESSO towards the exascale



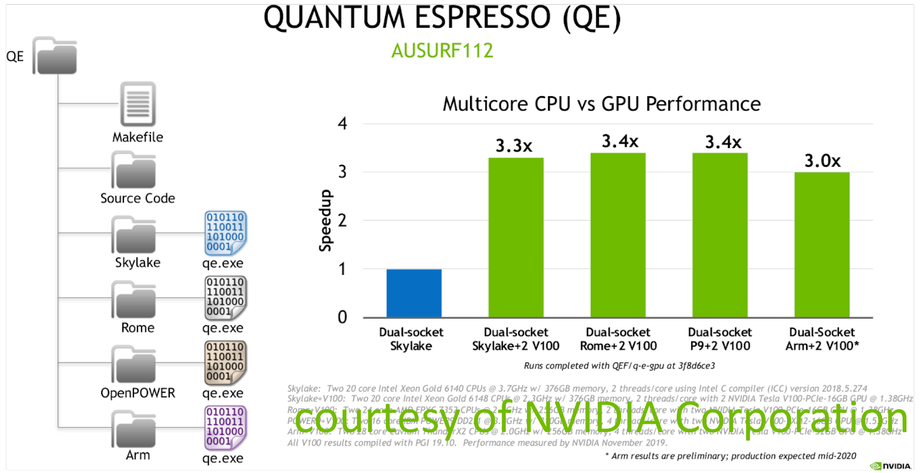
porphyrin@CNT







Au_{112} surface



courtesy of NVIDIA Corporation

DRIVING THE EXASCALE TRANSITION

JOIN THE COMMUNITY NOW!

Follow us on:

company/max-centre/

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

@max_center2

youtube/channel/MaX Centre eXascale

these slides at http://talks.baroni.me

DRIVING THE EXASCALE TRANSITION