



# 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



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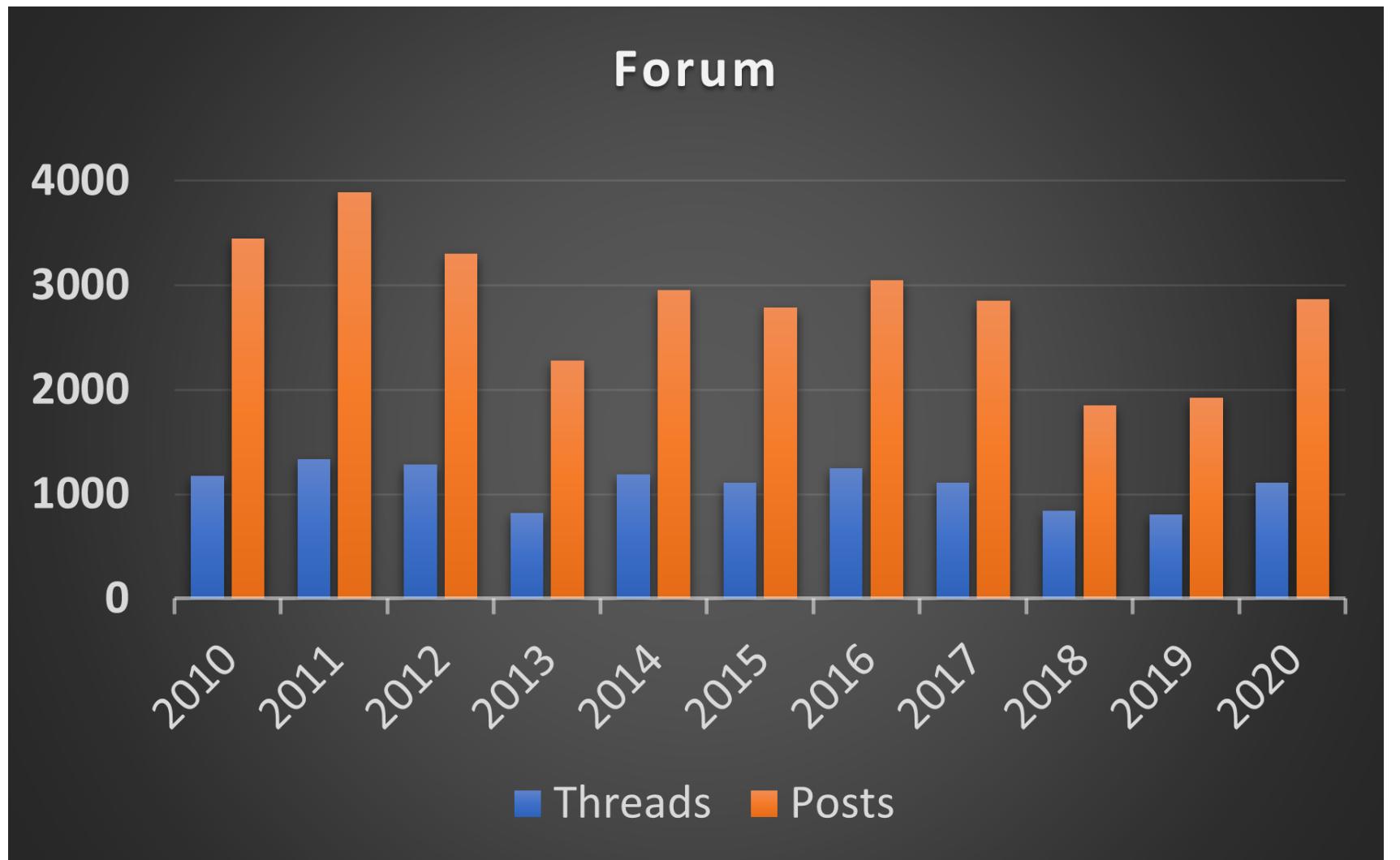
the defining features of  
QUANTUM ESPRESSO are:

- **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



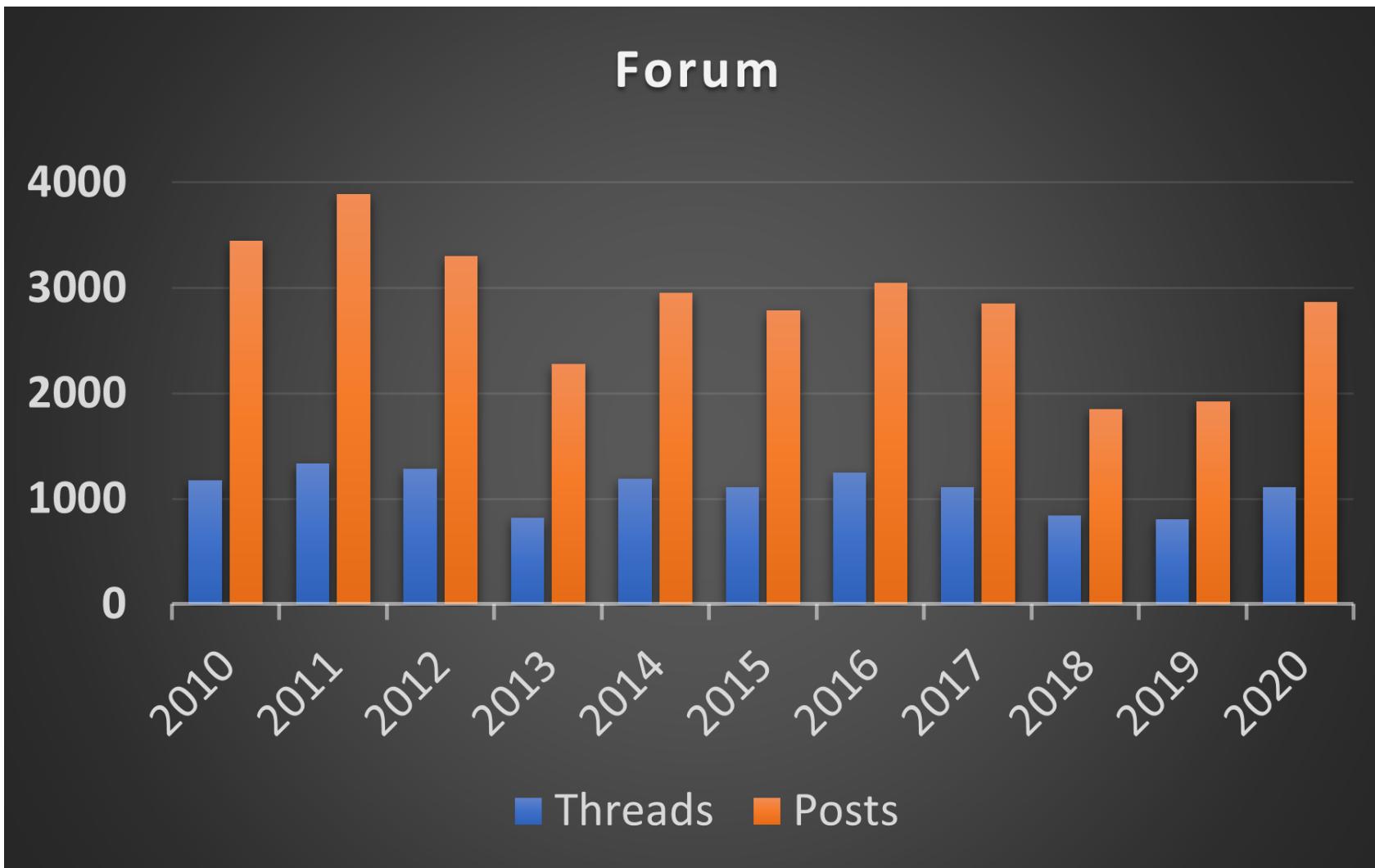
# QUANTUM ESPRESSO: the impact

1,800+ active users



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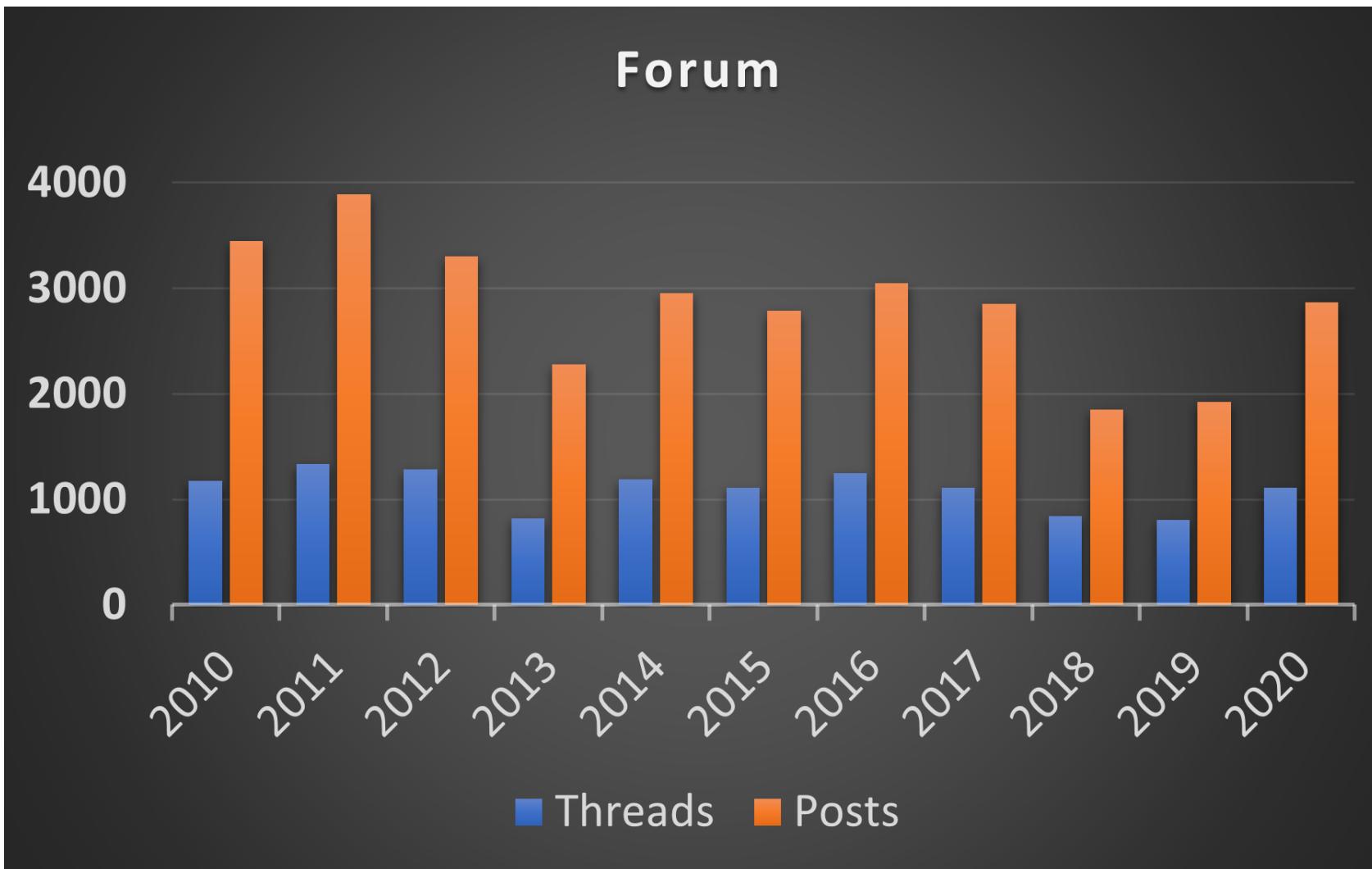


2,000+ citations/year



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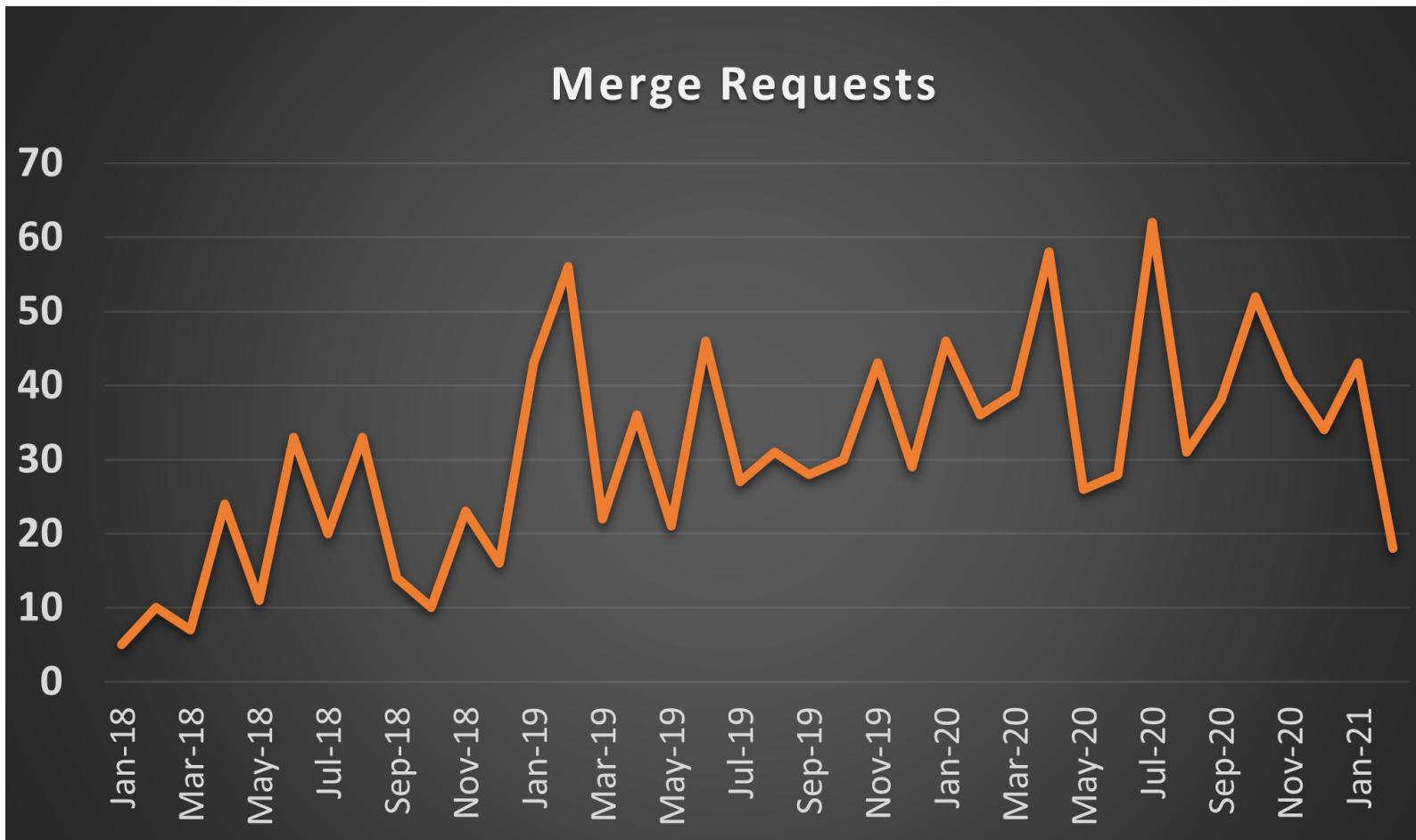
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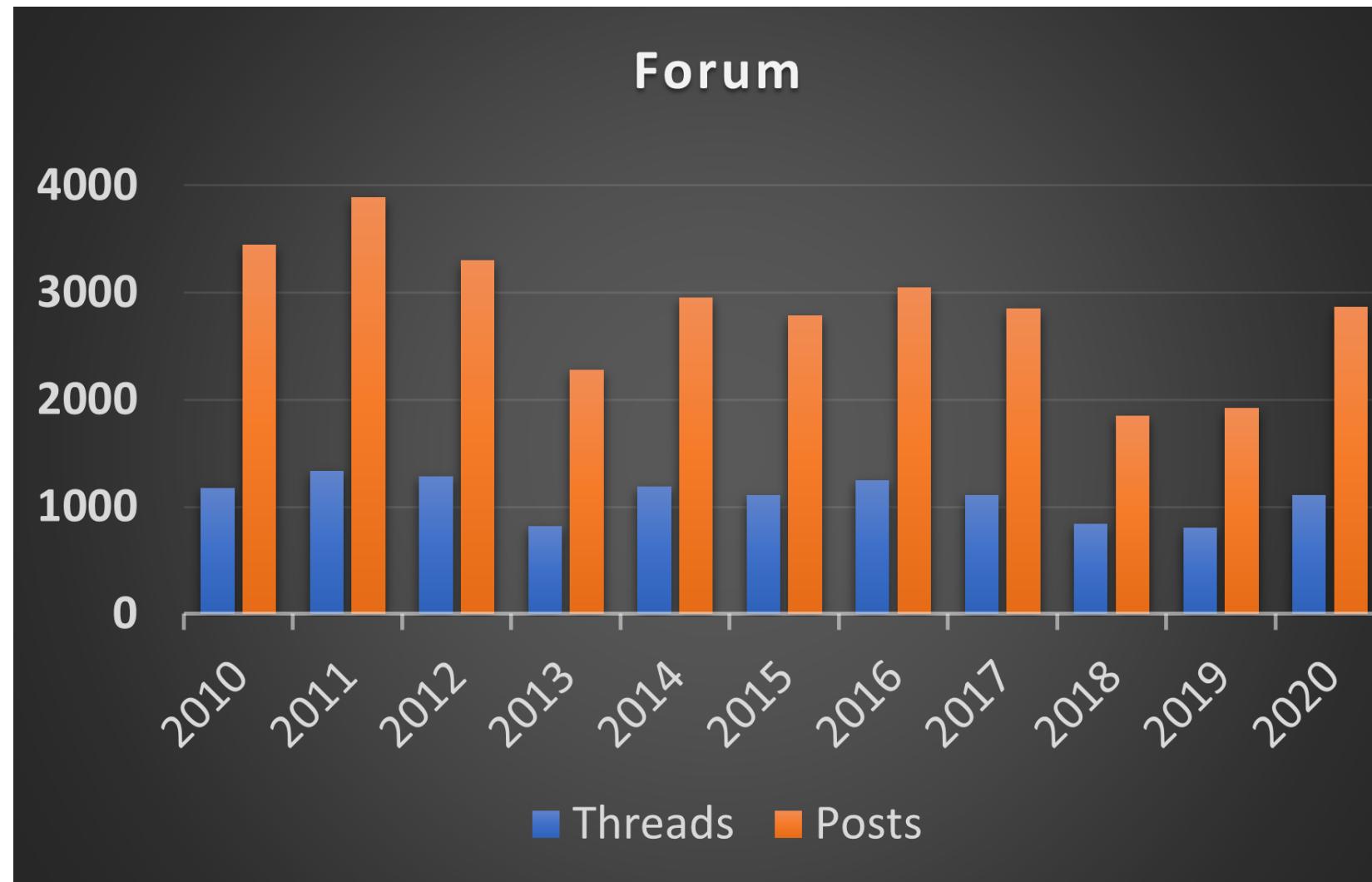


50+ active developers, ≈50 merges/month on git



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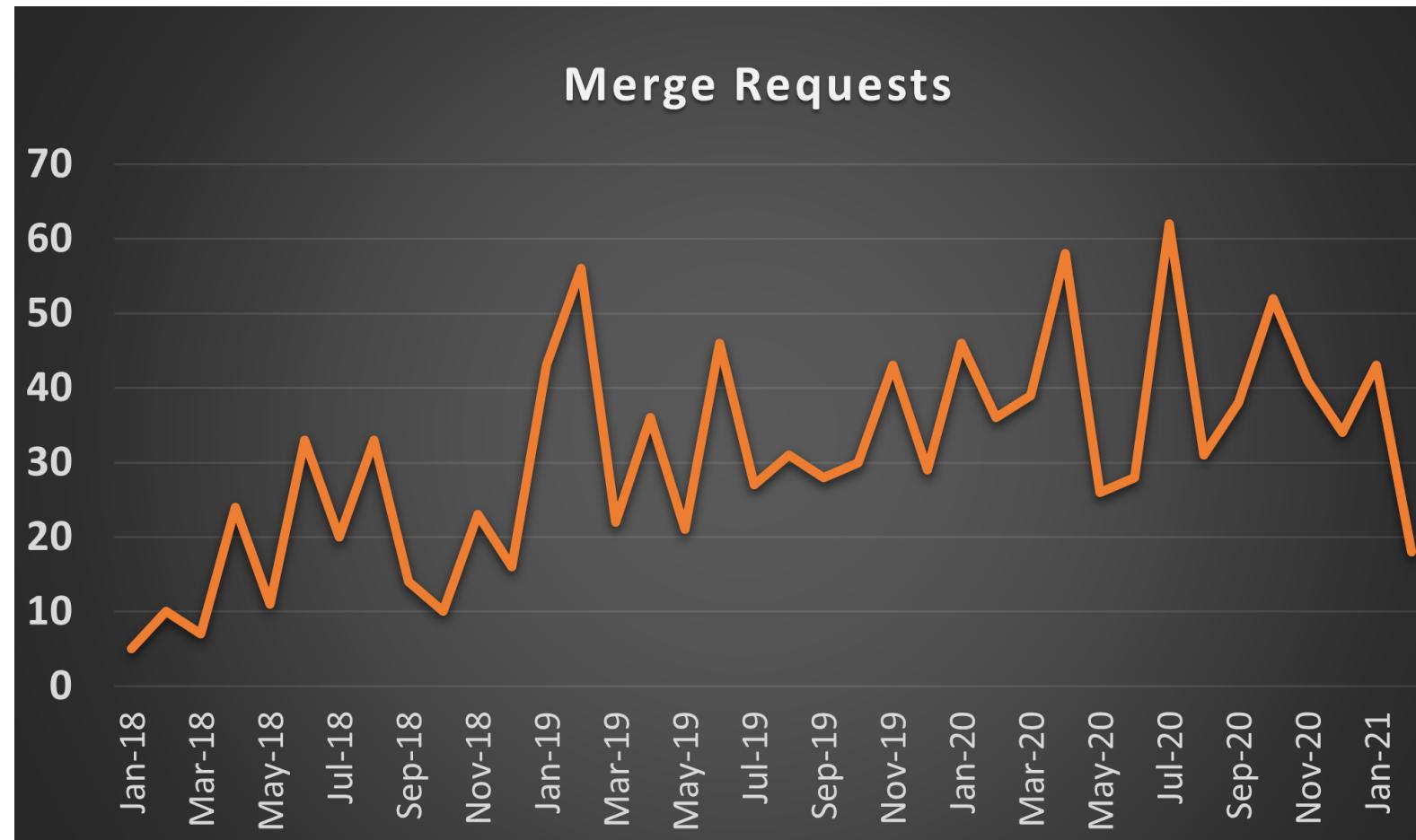
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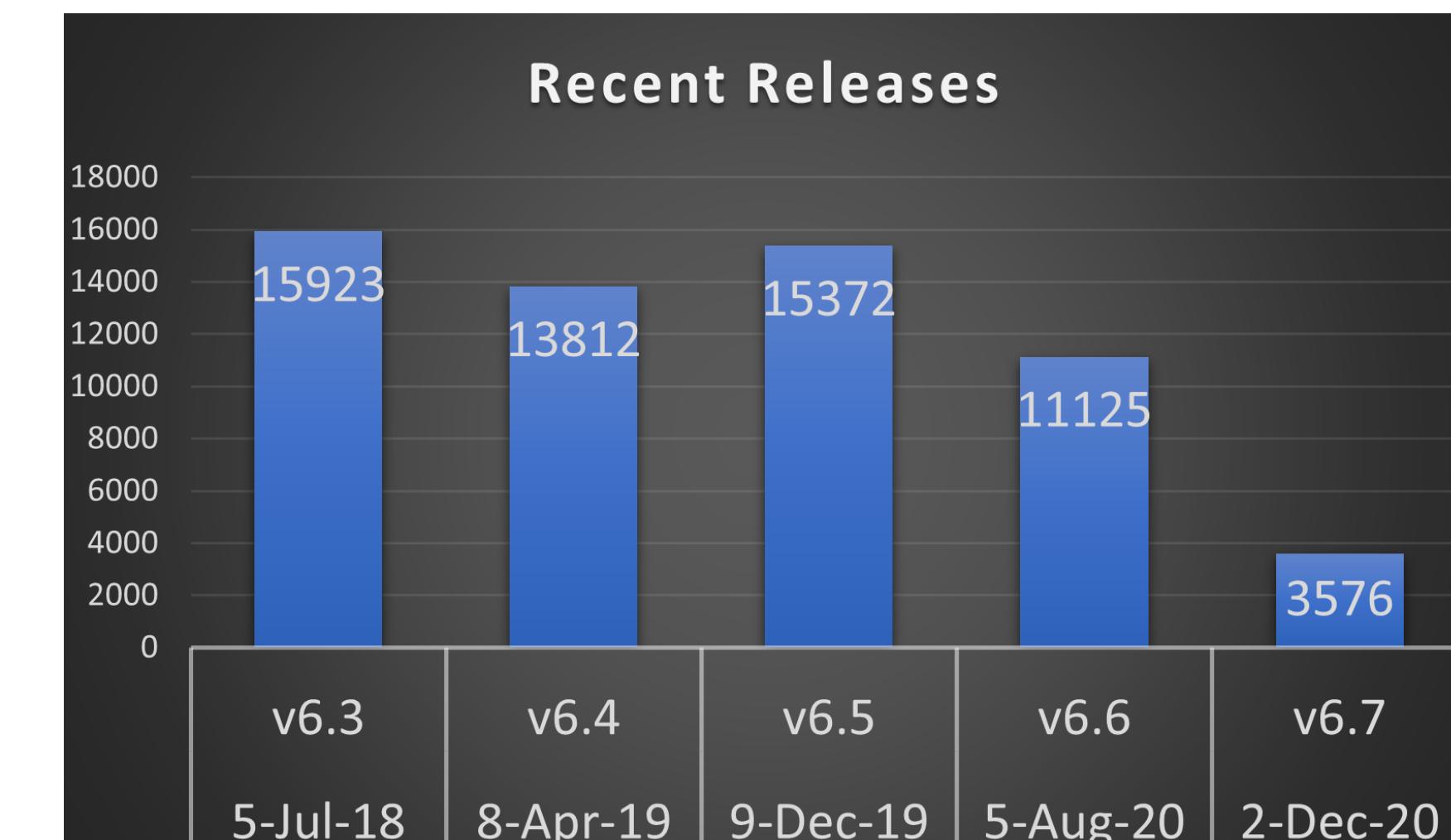
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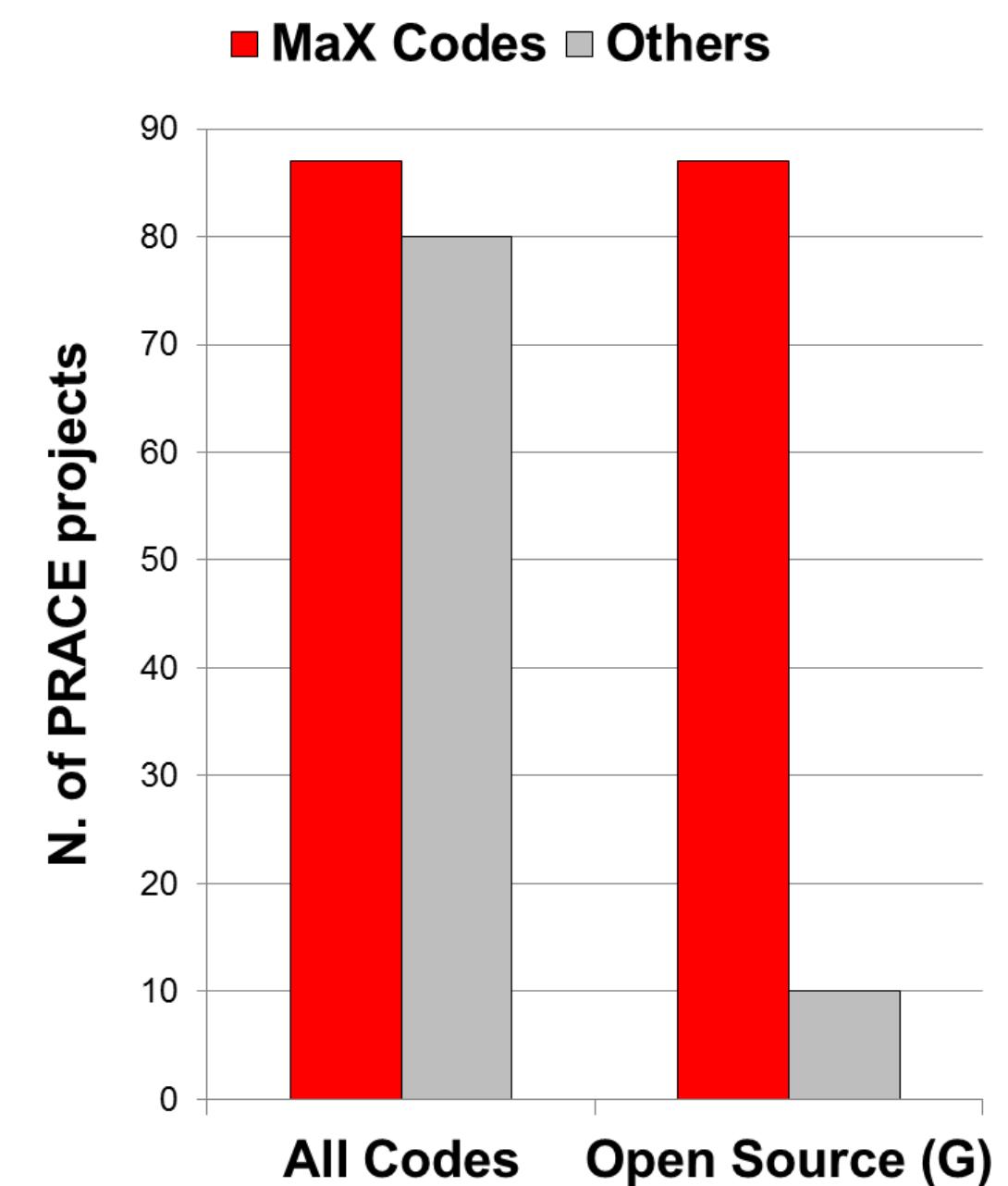
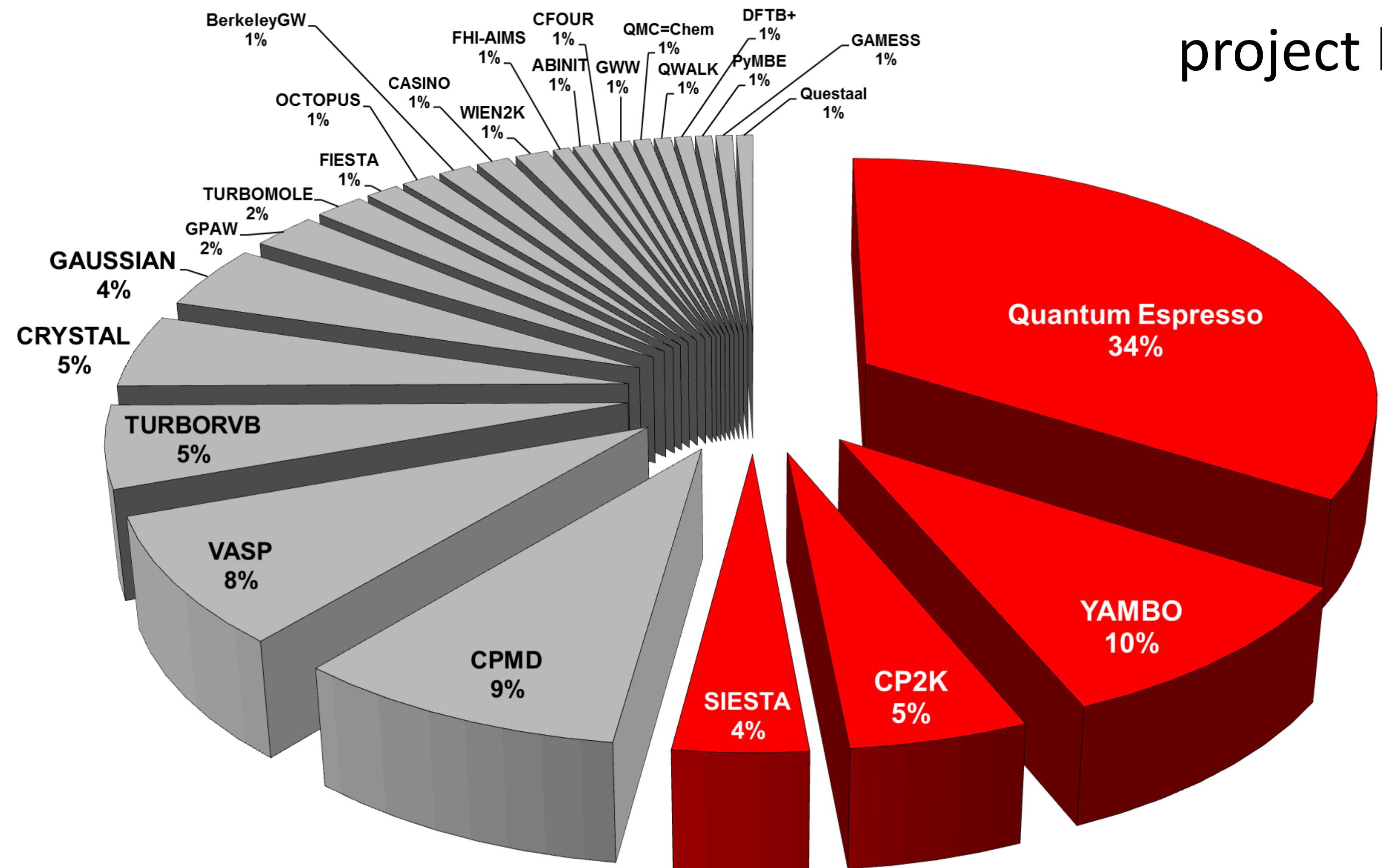
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10-15,000 downloads/release



# QUANTUM ESPRESSO: the impact



QUANTUM ESPRESSO on the marketplace

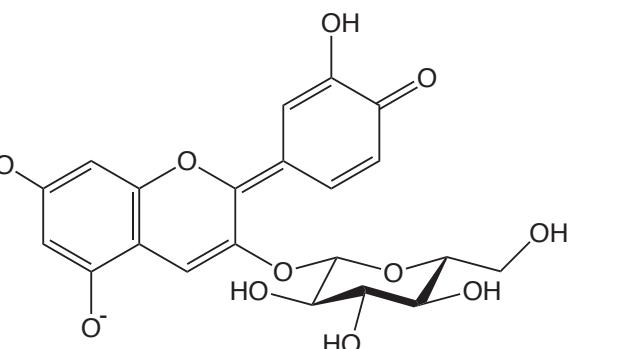
custom-built solutions



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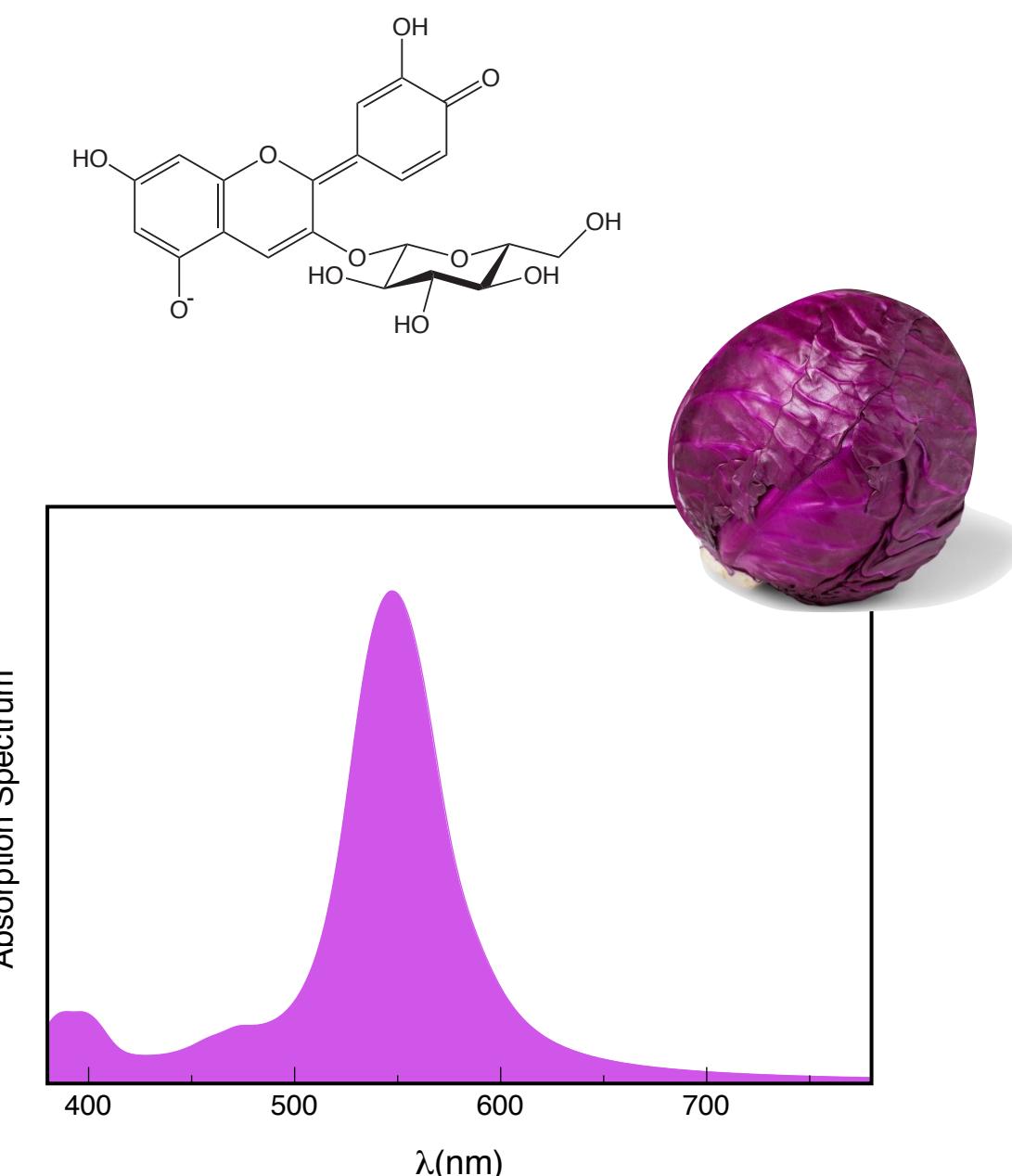
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MARS



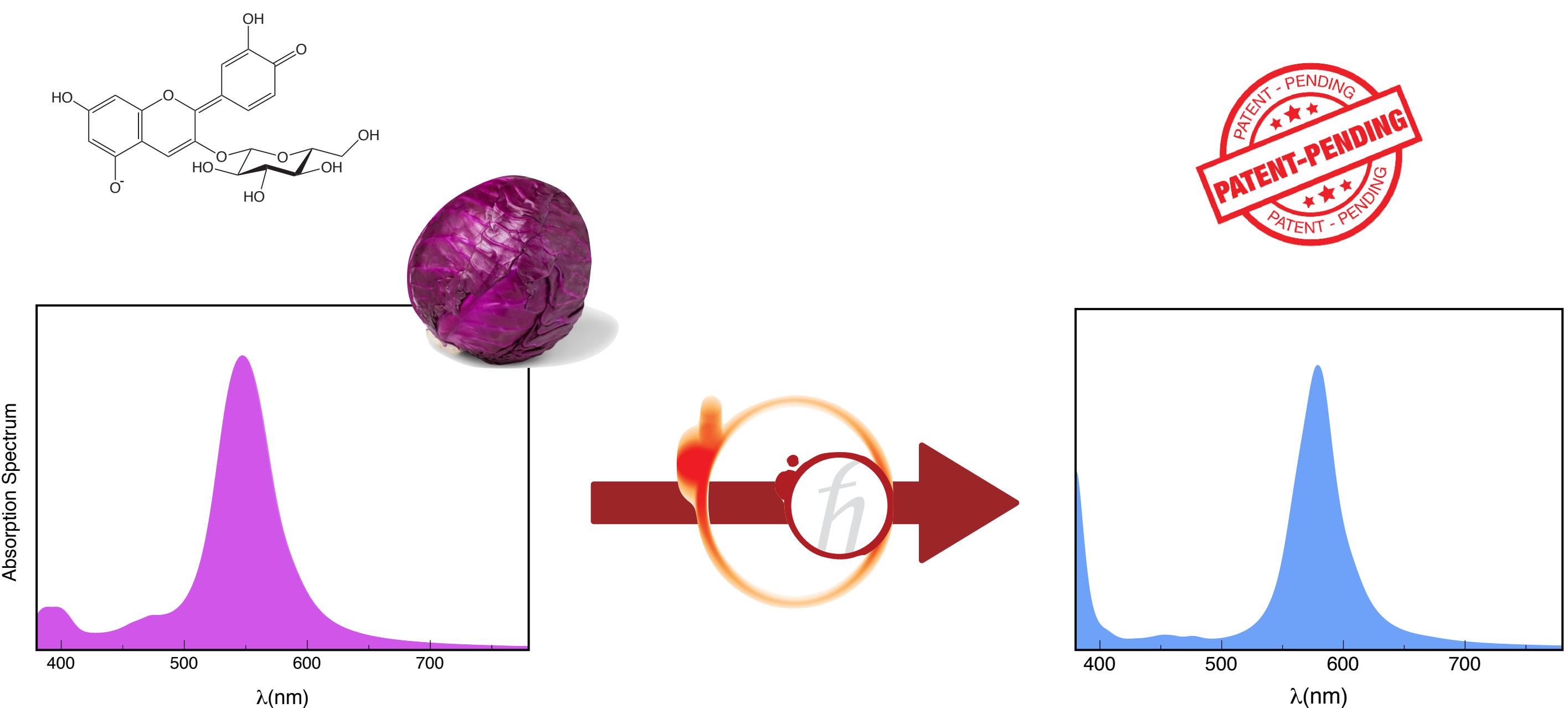
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## custom-built solutions



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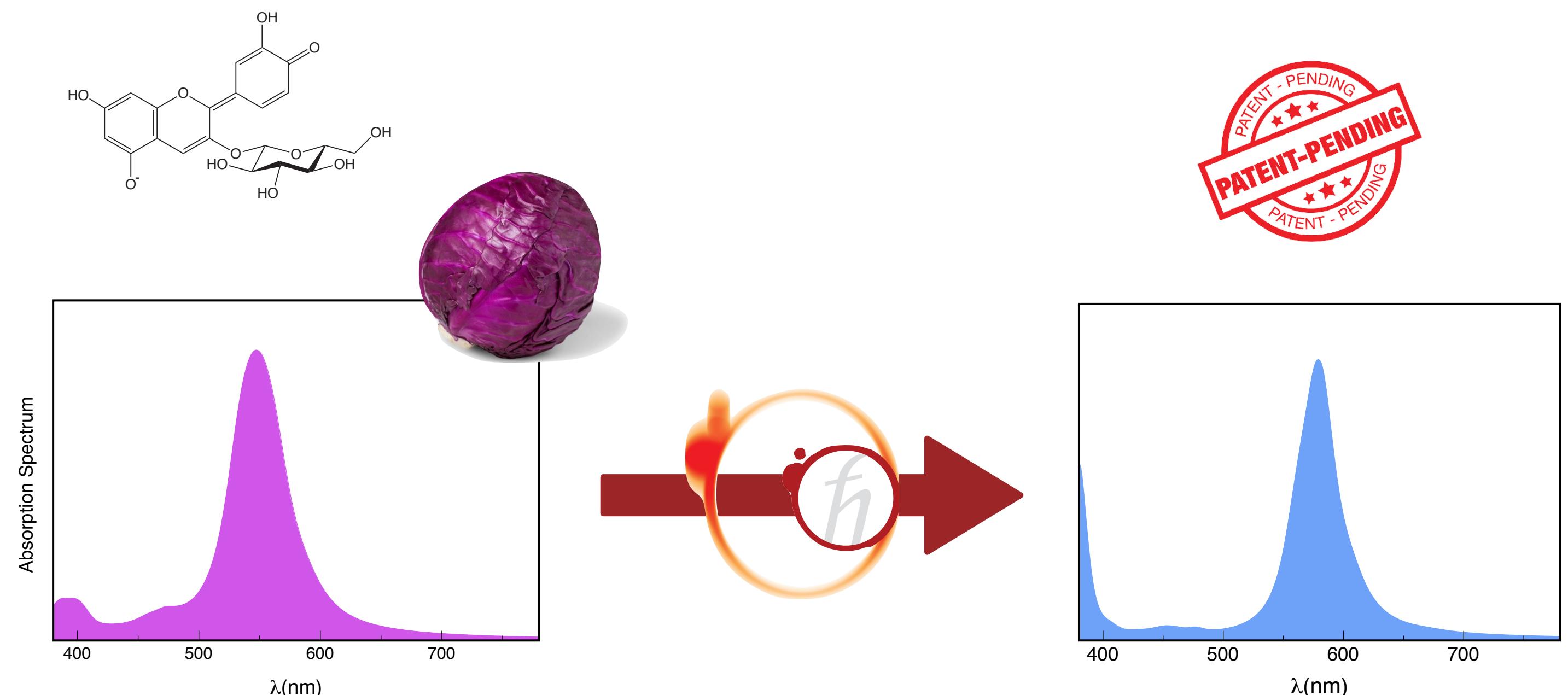
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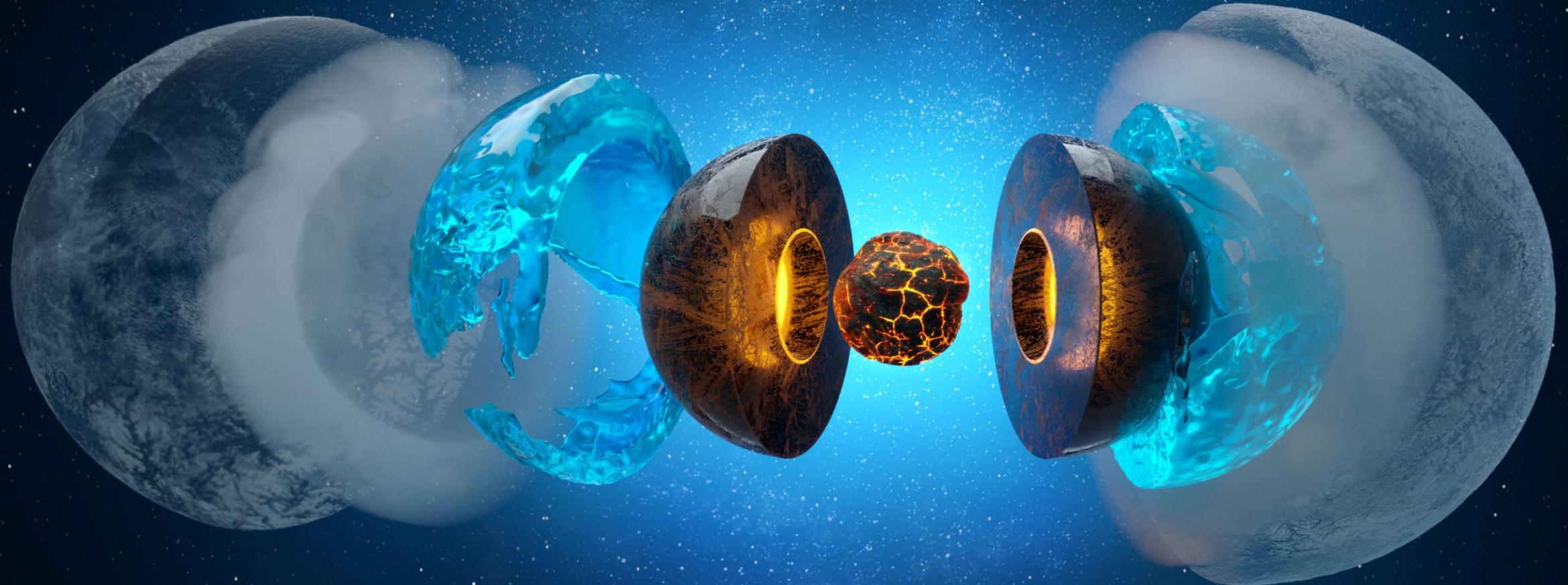
turn-key solutions

A screenshot of the Schrödinger software interface. At the top, there is a navigation bar with links for "ABOUT", "PLATFORM", "PIPELINE", "USER EVENTS", "CAREERS", and "INVESTORS". Below the navigation bar, the word "Quantum ESPRESSO" is prominently displayed in large white letters. A subtitle below it reads "High-performance, open-source QM software for materials simulations". The background of the interface features a dark, abstract visualization of molecular structures and energy bands.



from the supermarket shelf up to the heavens

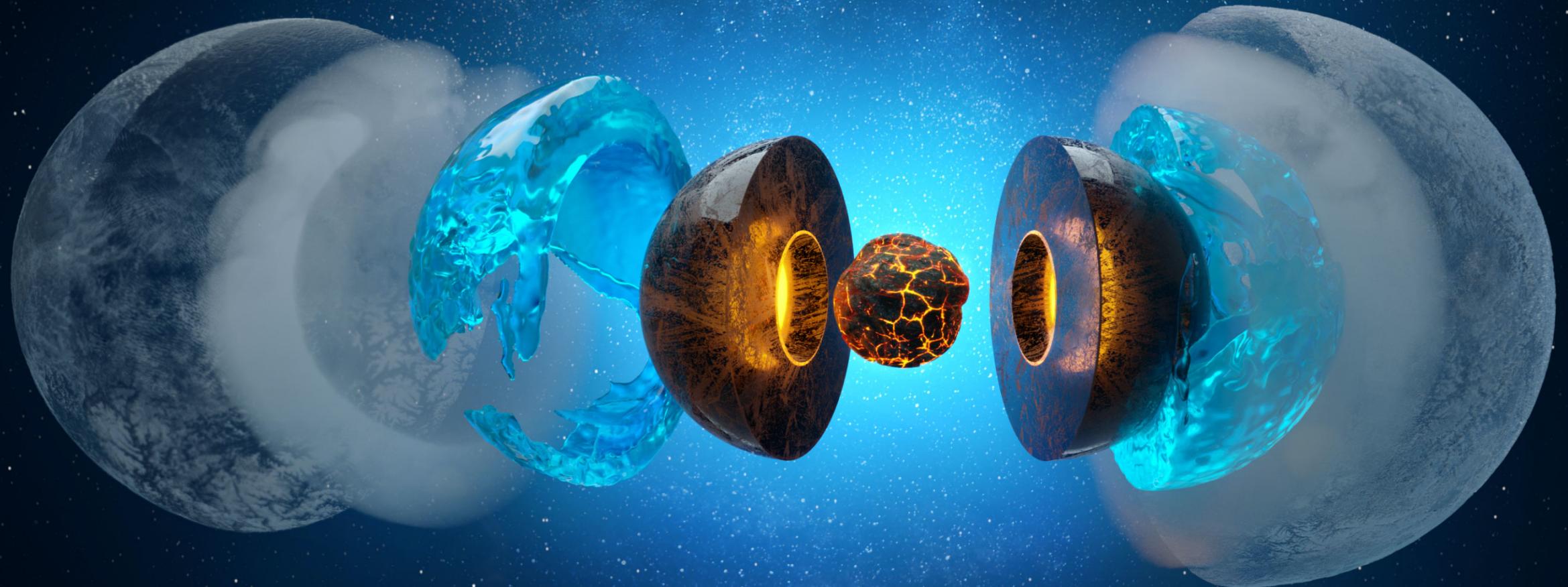
what are the giant icy planets made of?



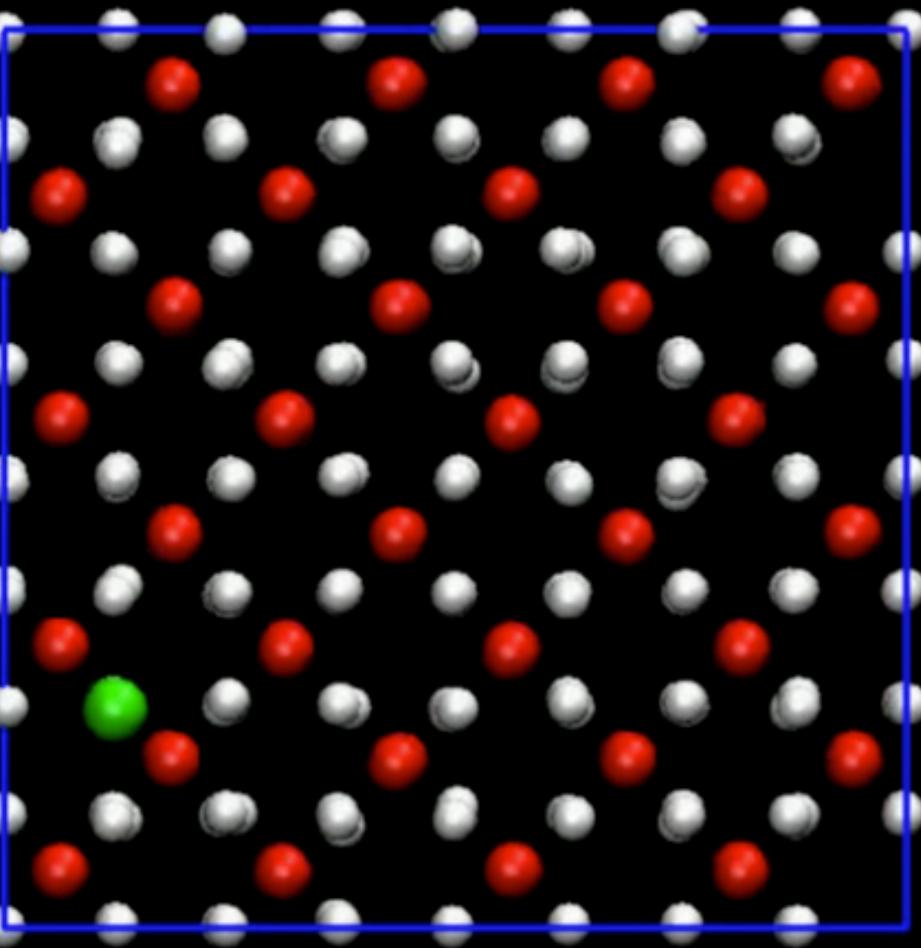
Uranus

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what are the giant icy planets made of?



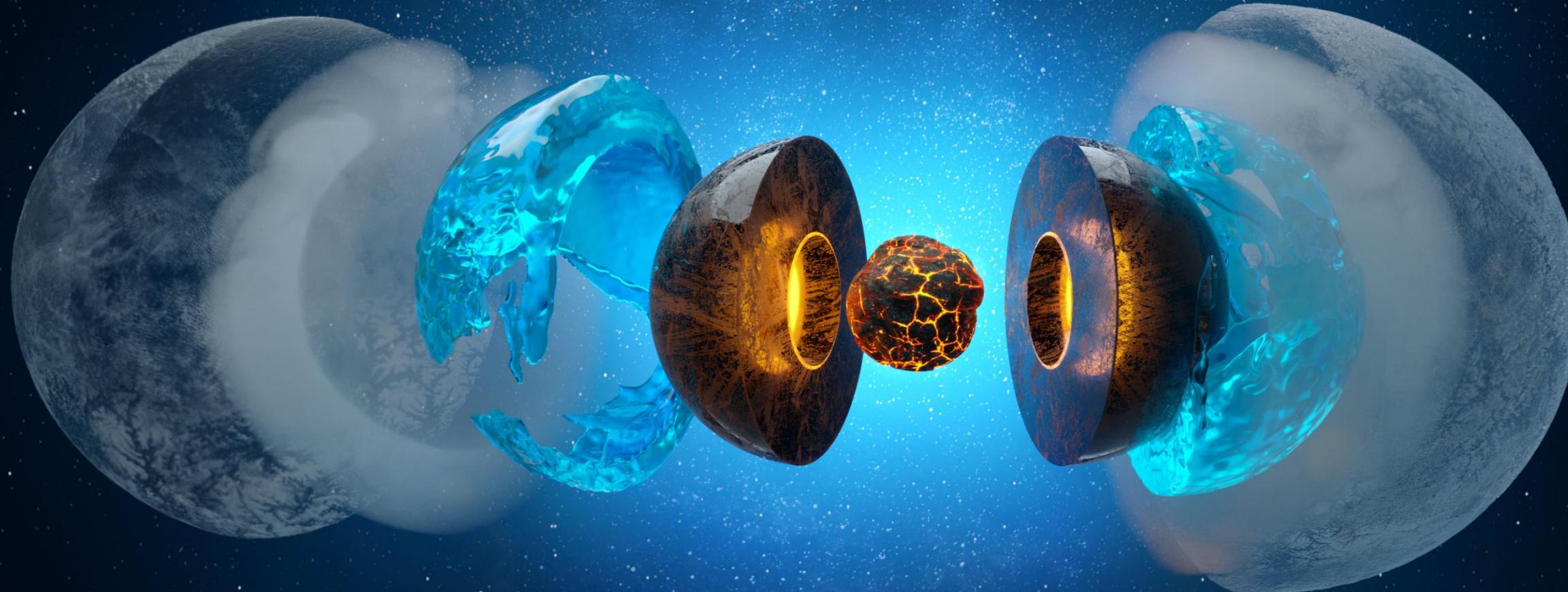
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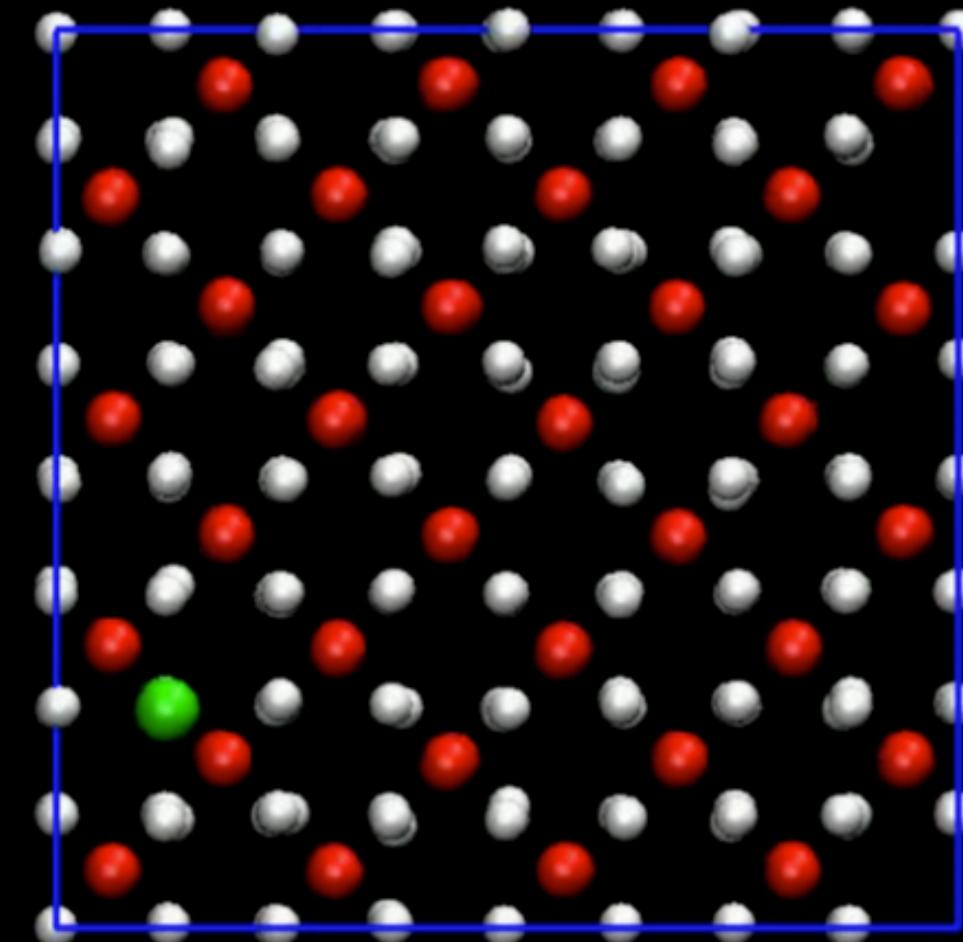
$P=175 \text{ GPa}$   
ice X

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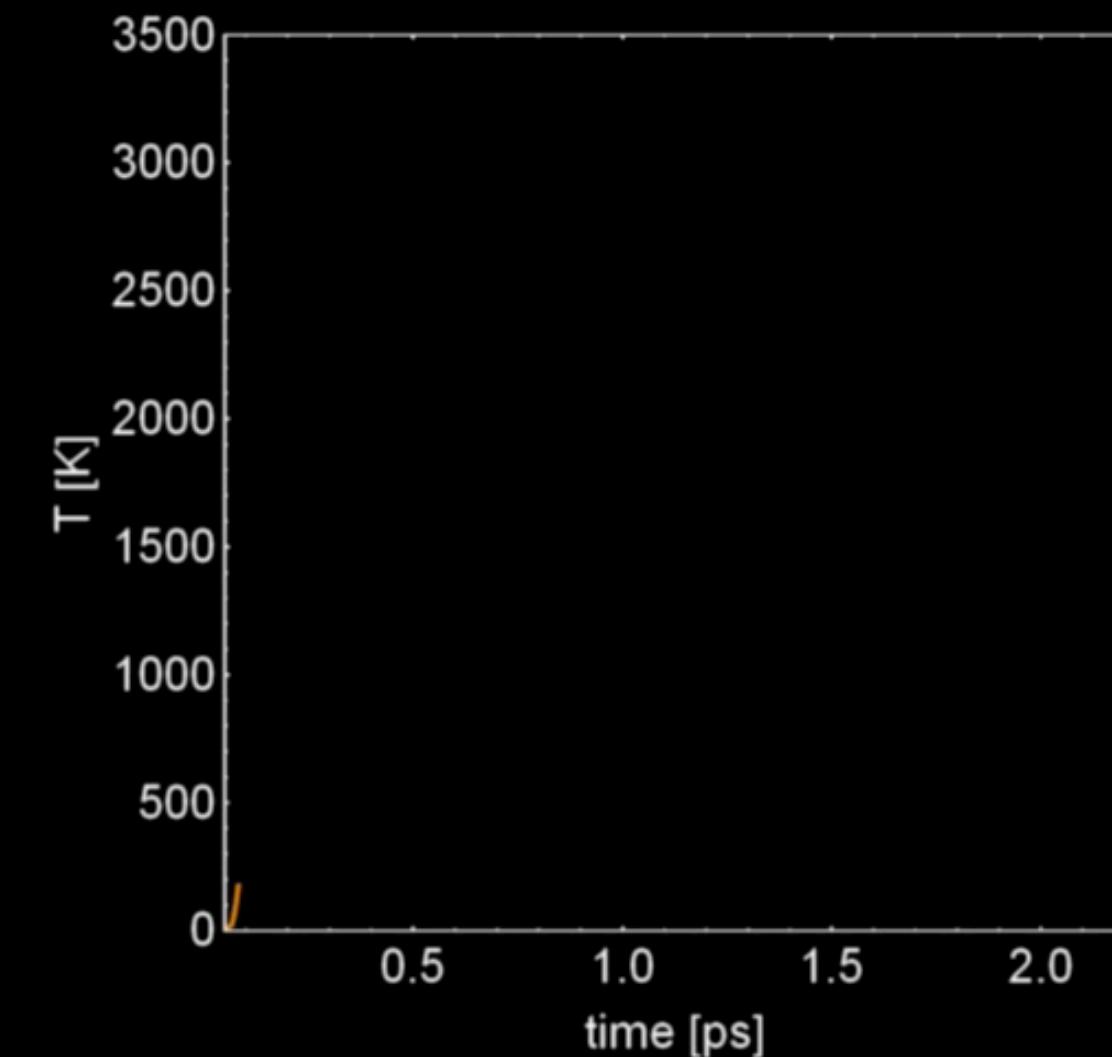
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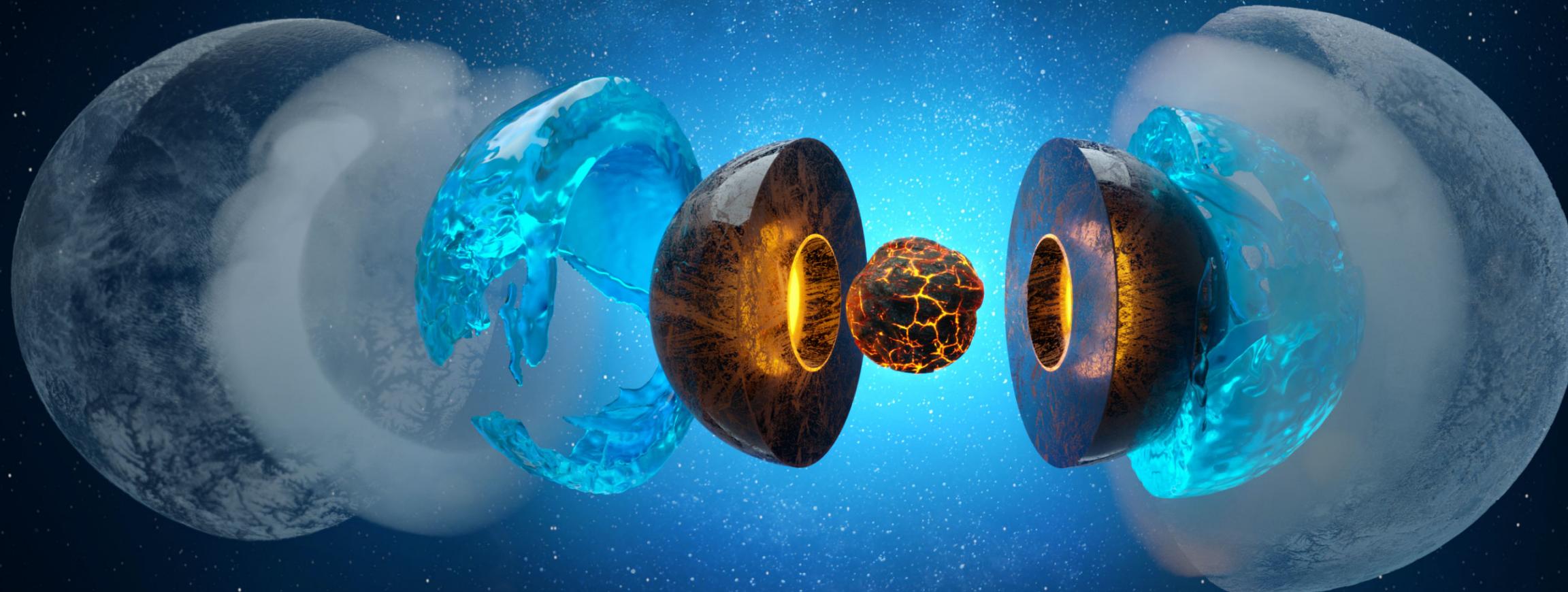


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**nature  
COMMUNICATIONS**

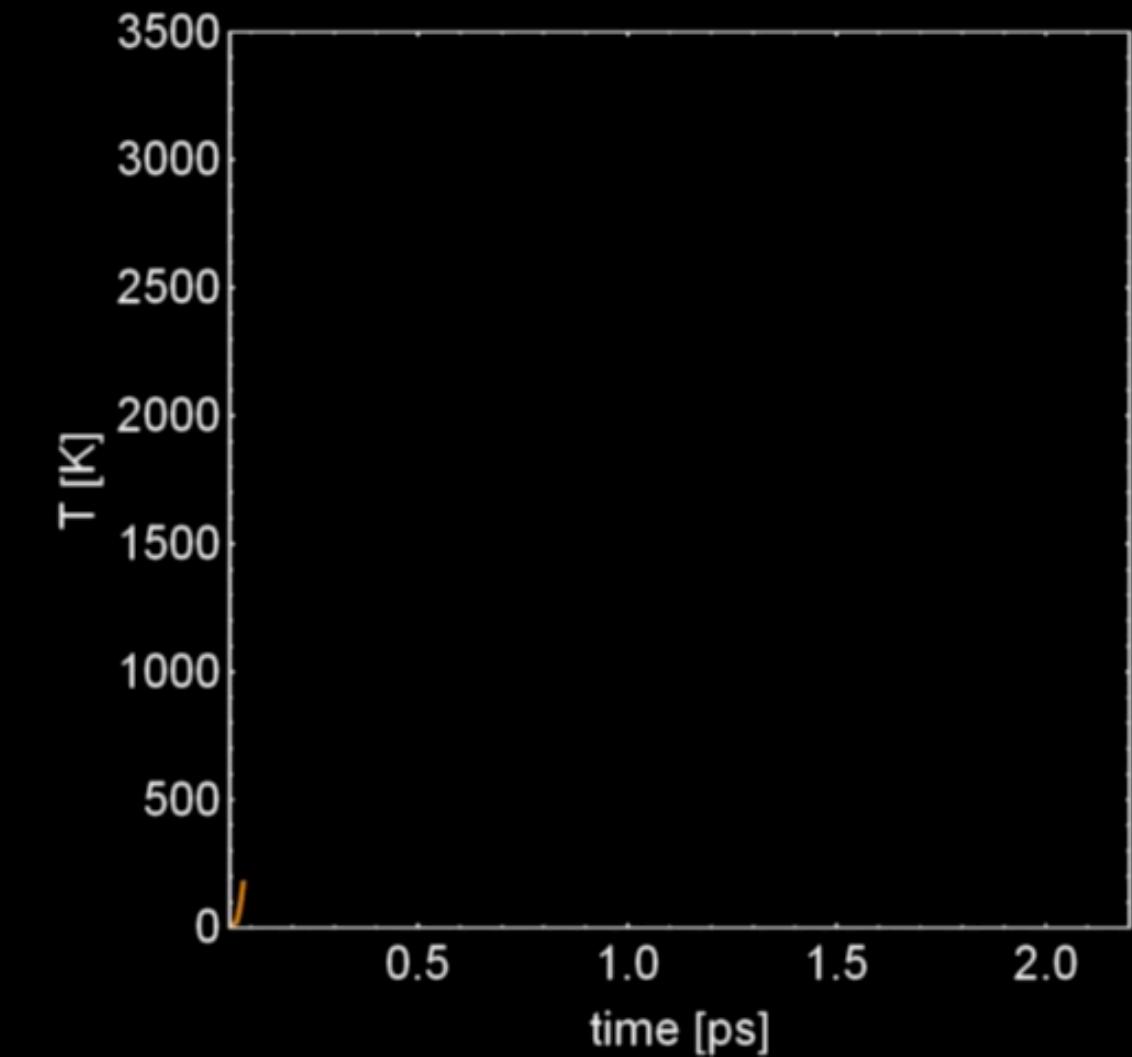
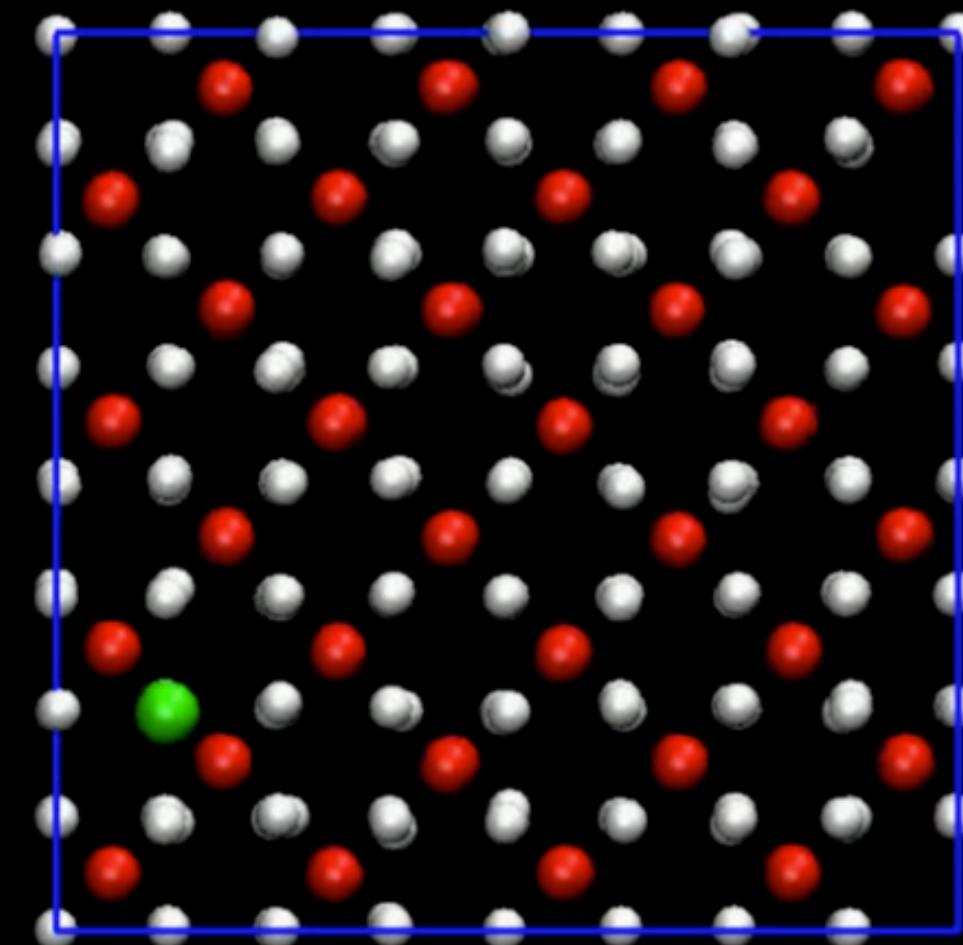
ARTICLE

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

Heat and charge transport in  $\text{H}_2\text{O}$  at ice-giant conditions from ab initio molecular dynamics simulations

Federico Grasselli<sup>1,4</sup>, Lars Stixrude<sup>2</sup> & Stefano Baroni<sup>1,3</sup>

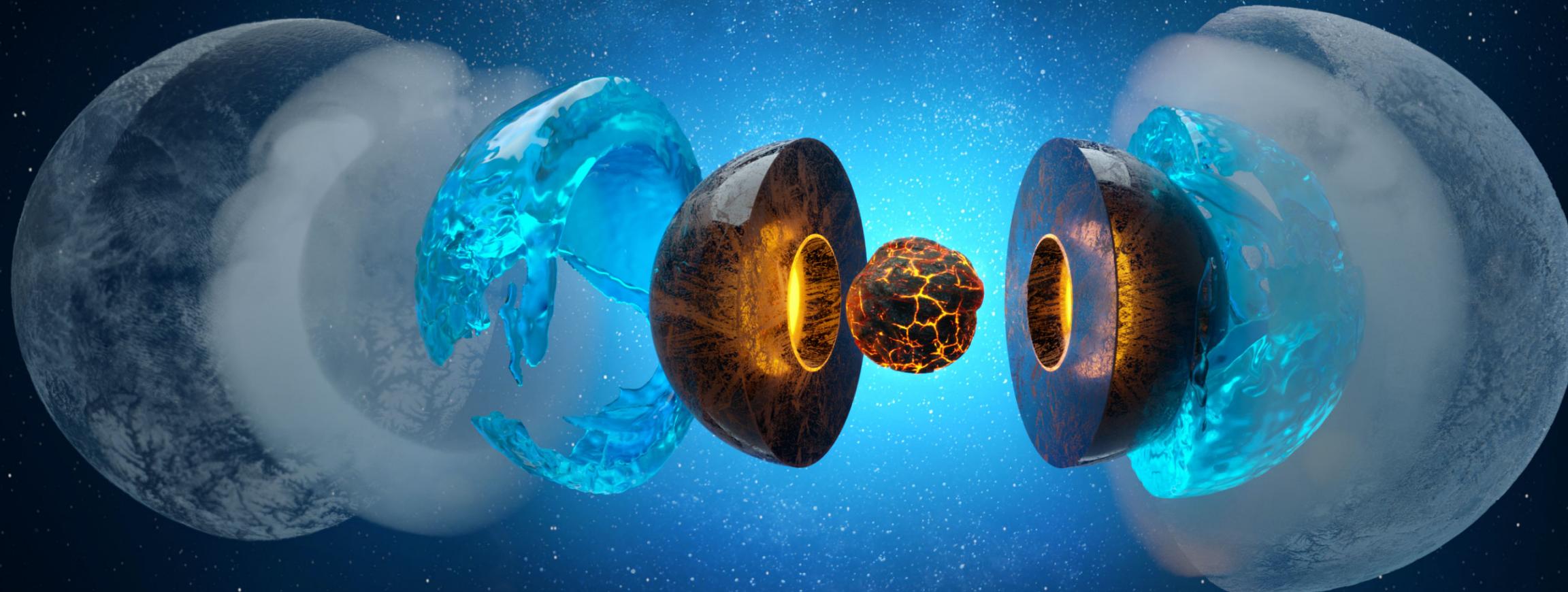
<sup>1</sup>Scuola Normale Superiore, Pisa, Italy; <sup>2</sup>University of Minnesota, Minneapolis, MN, USA; <sup>3</sup>Universität Regensburg, Regensburg, Germany; <sup>4</sup>Universidade de São Paulo, São Paulo, Brazil



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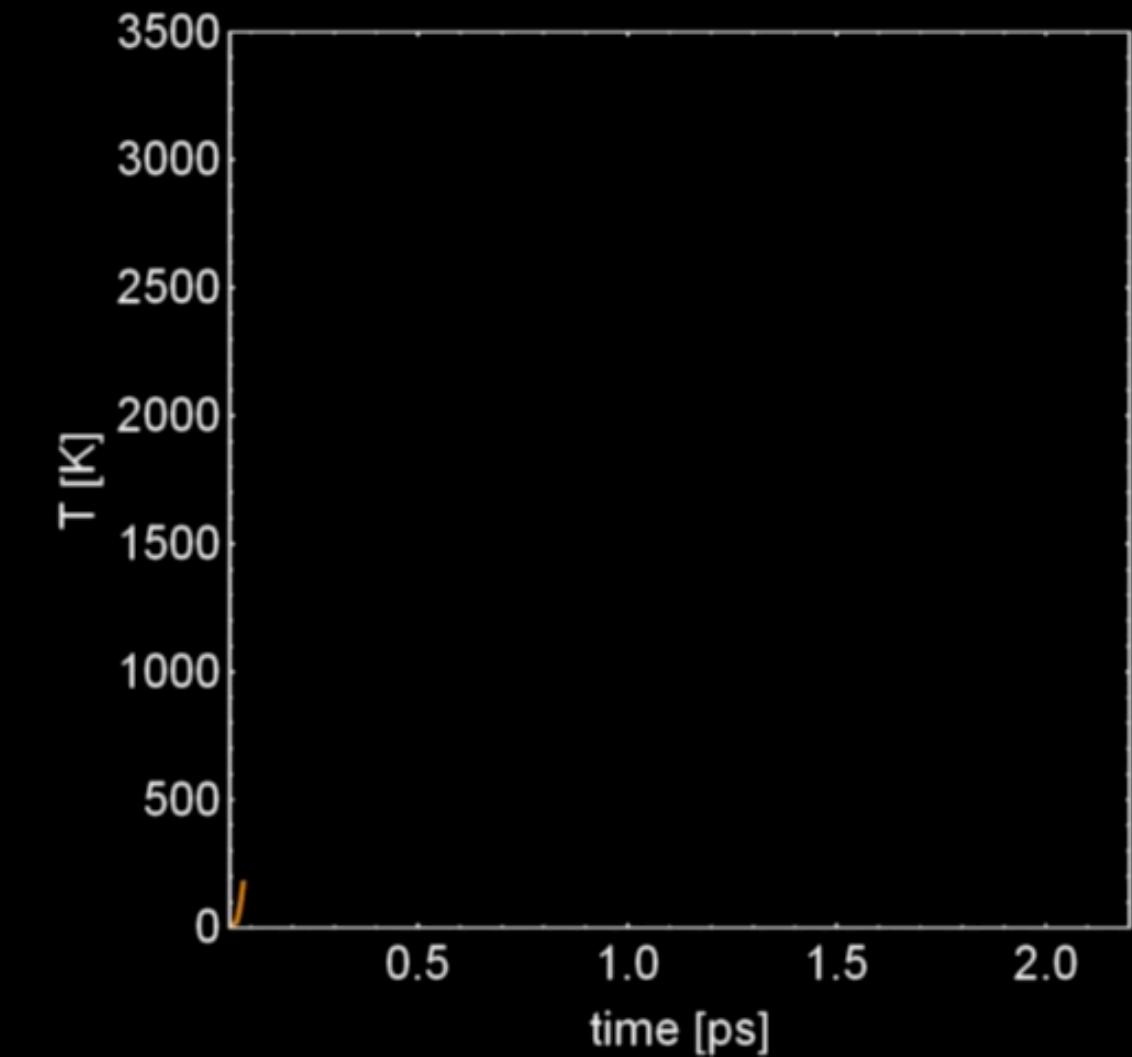
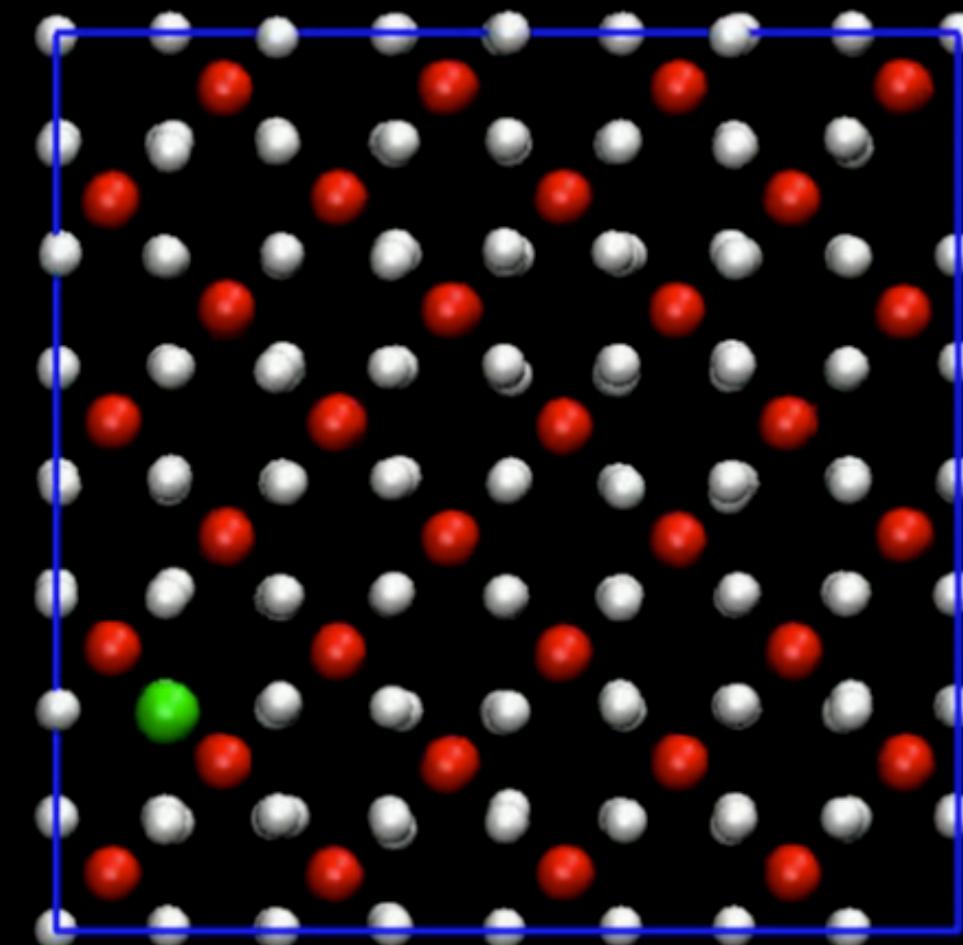
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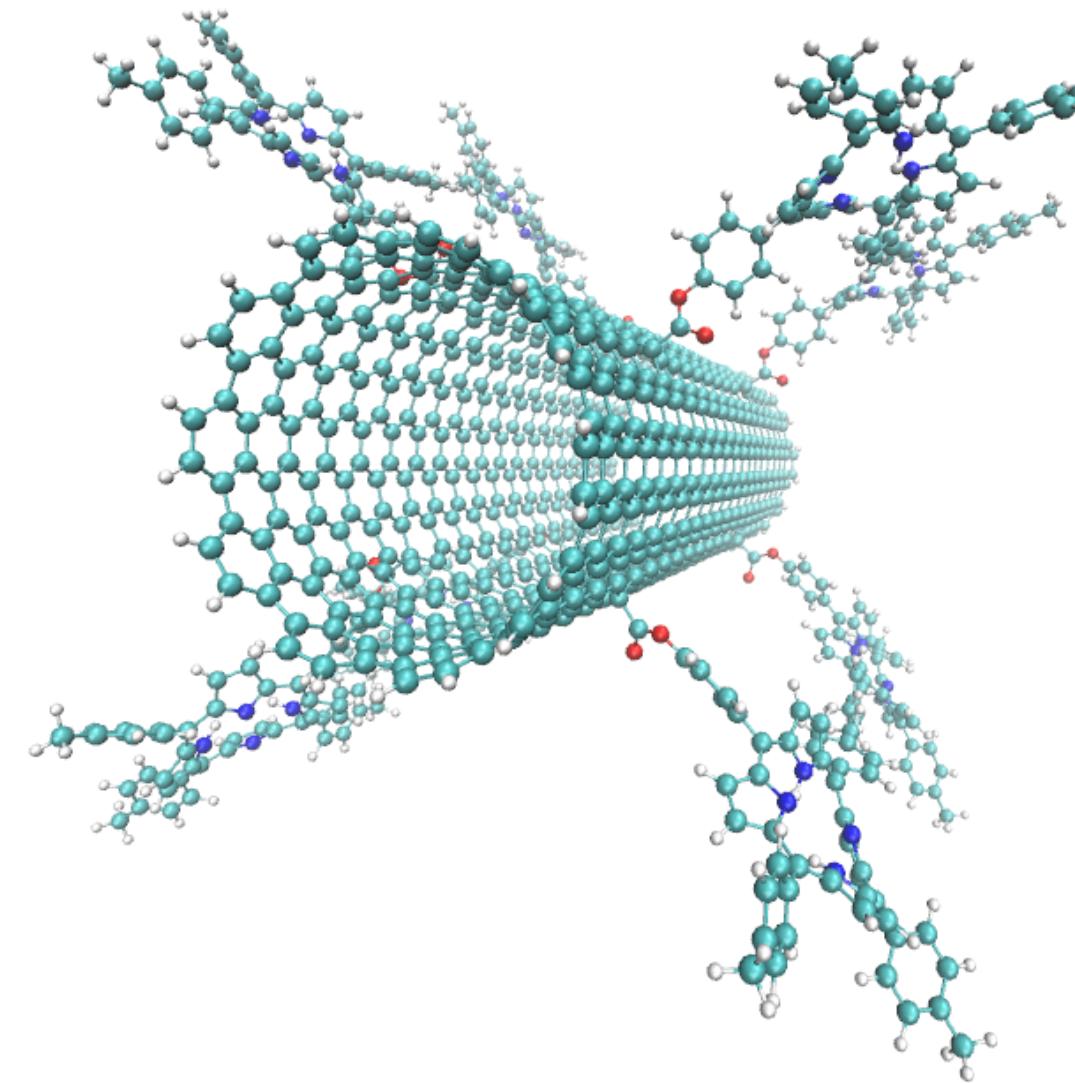
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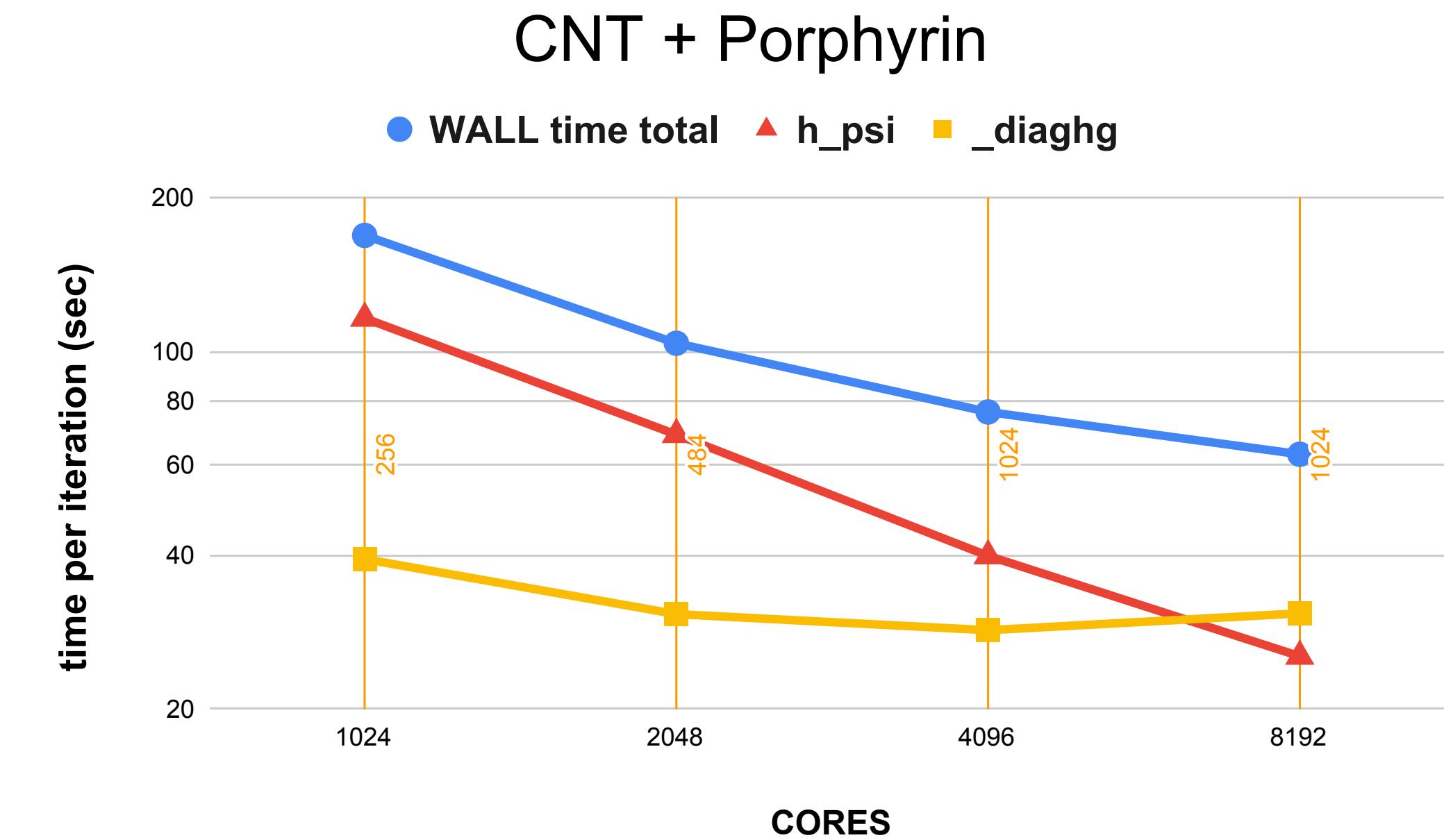
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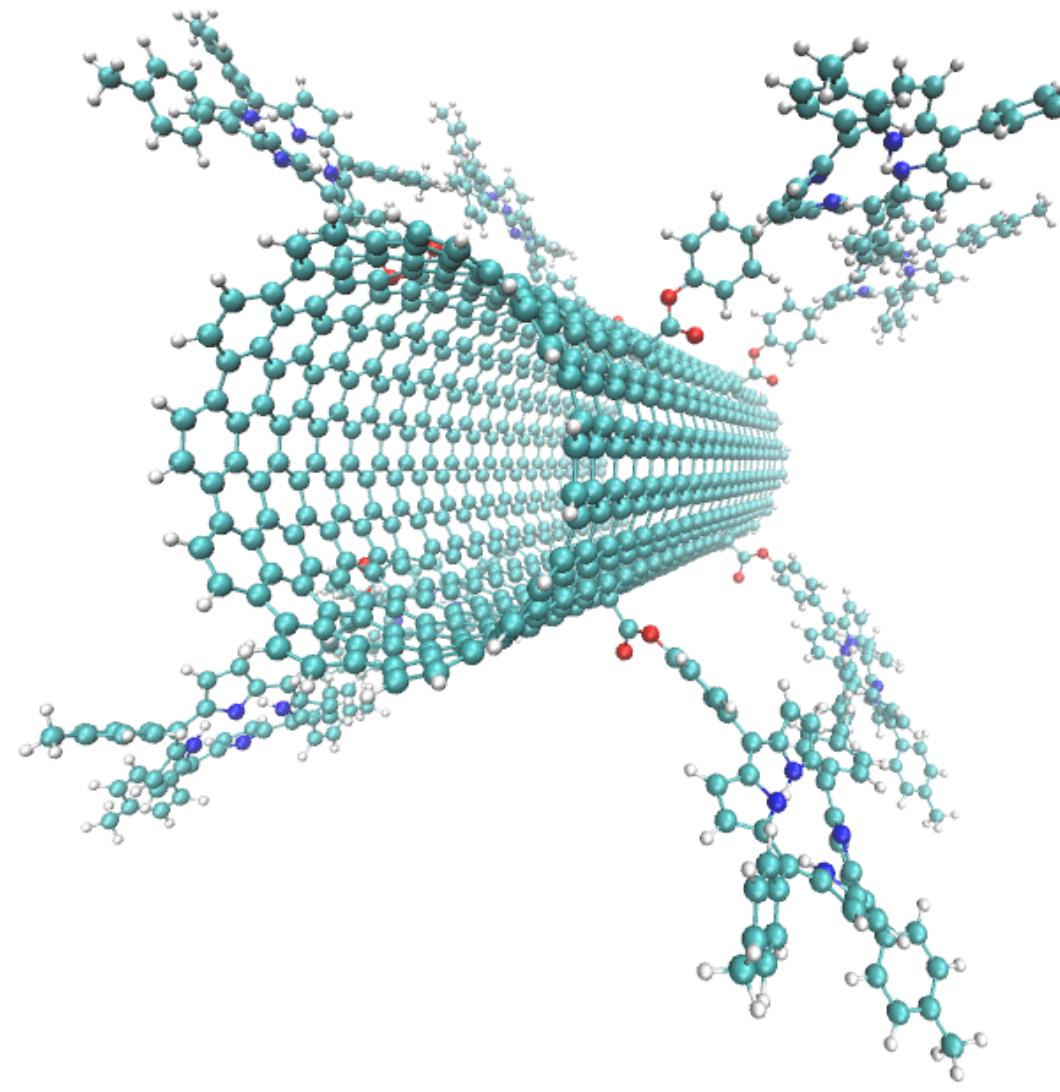


porphyrin@CNT

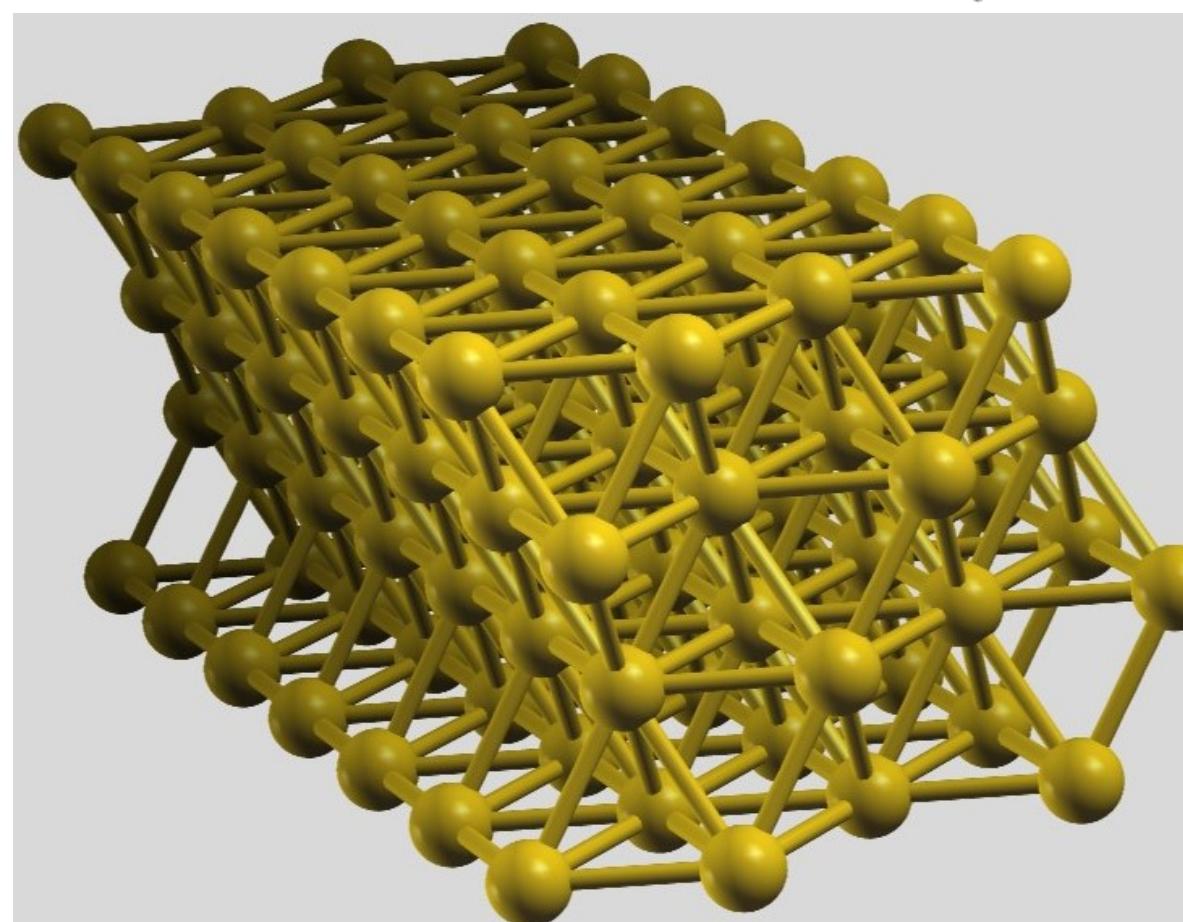
porphyrin@CNT  
1,500+ atoms  
3,200+ electrons  
 $2.4 \times 10^6$  PWs



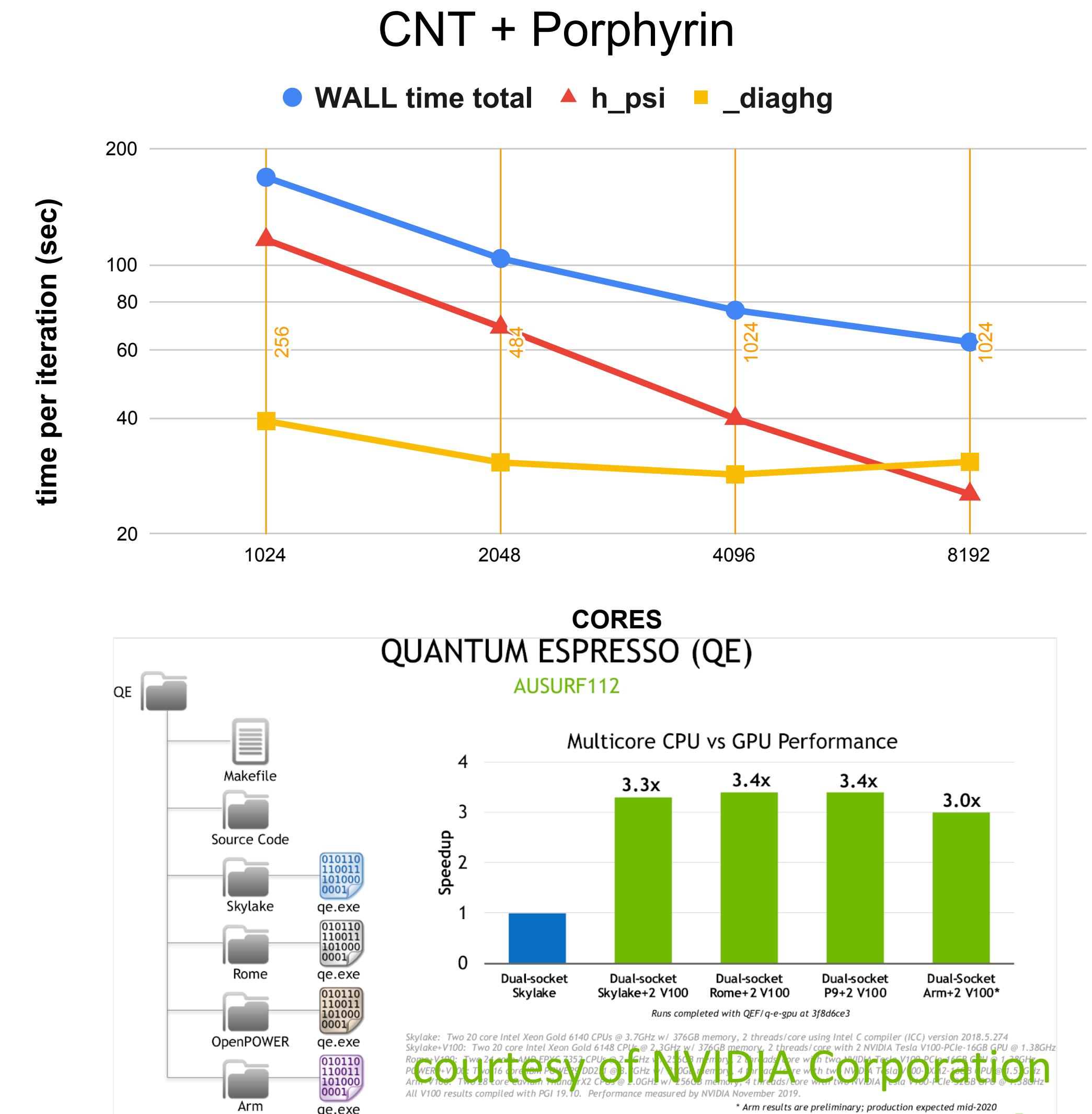
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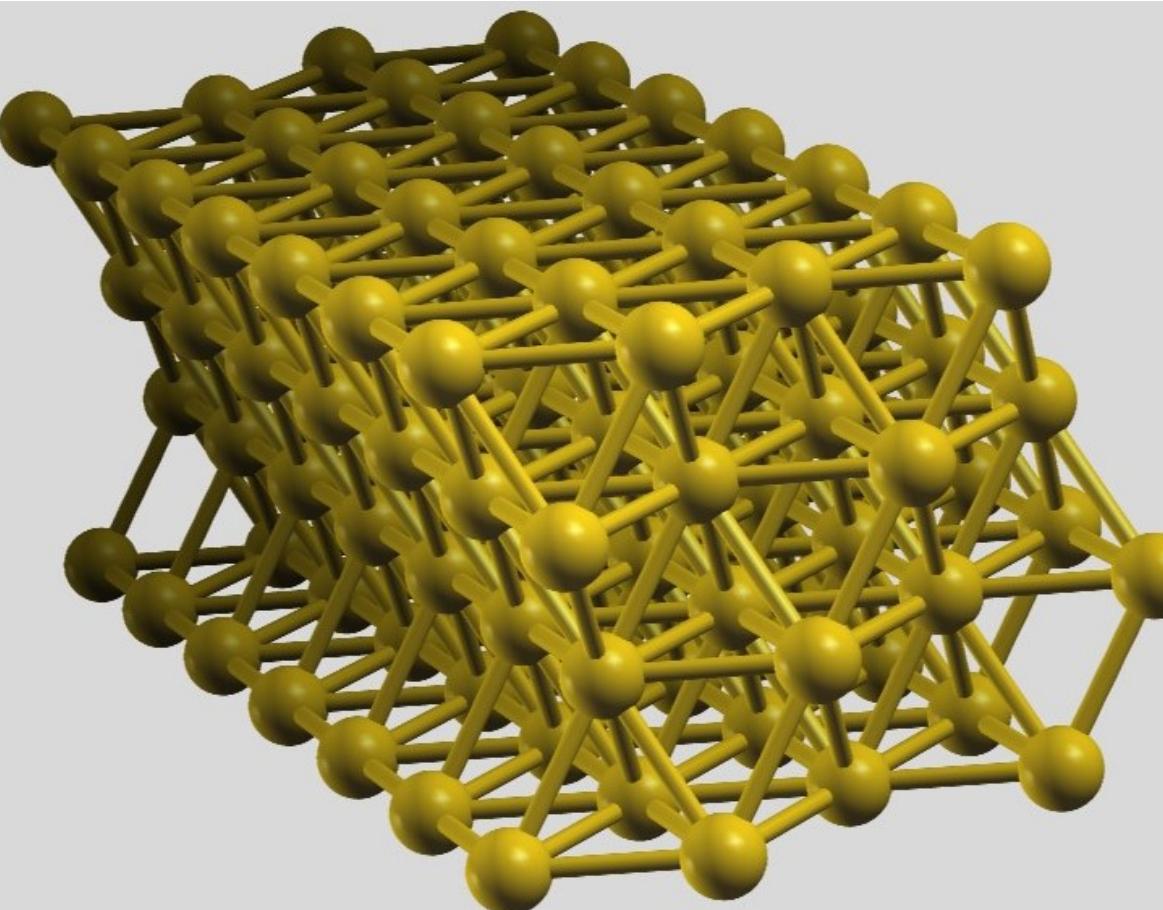
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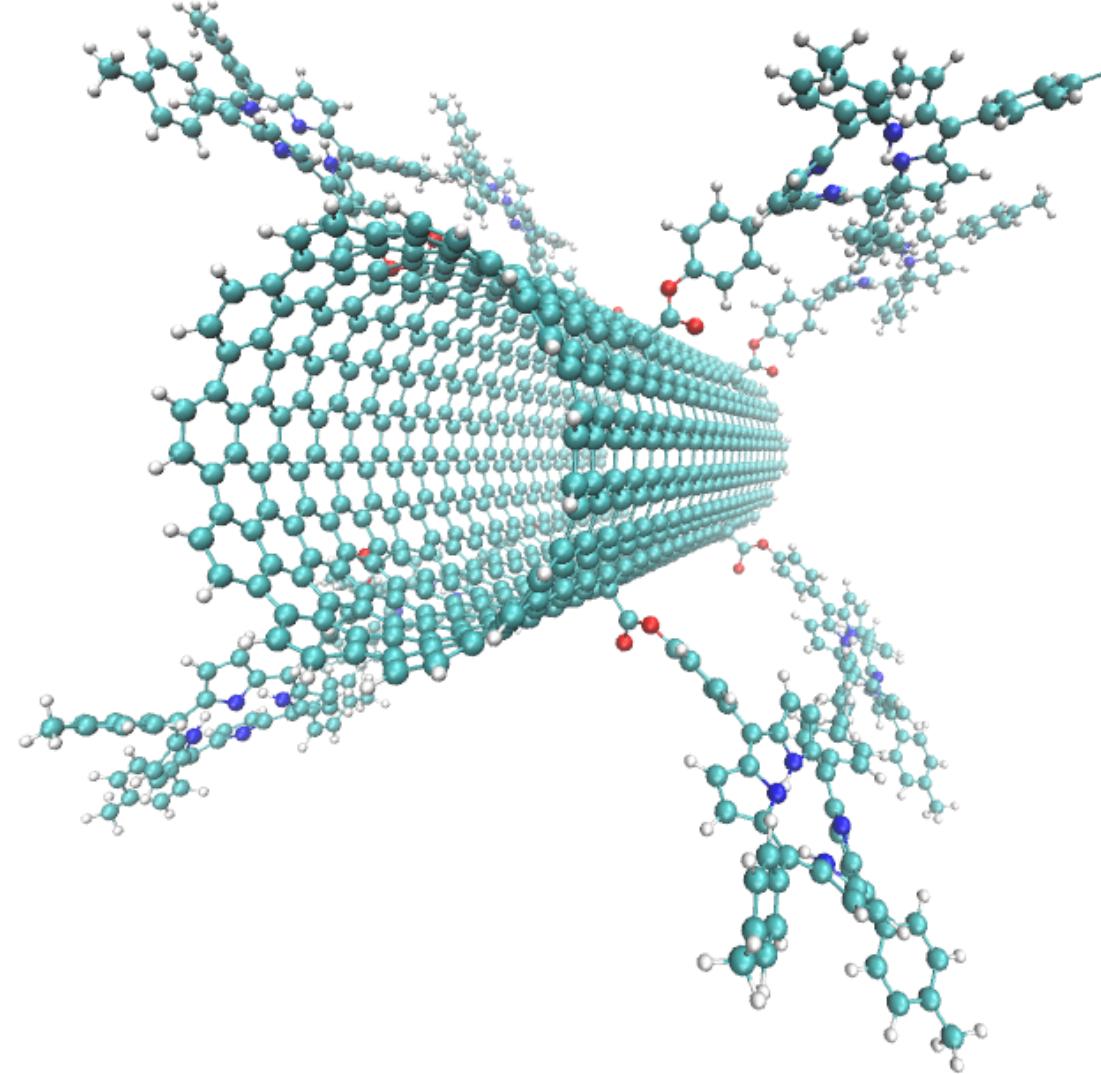
Au<sub>112</sub> surface



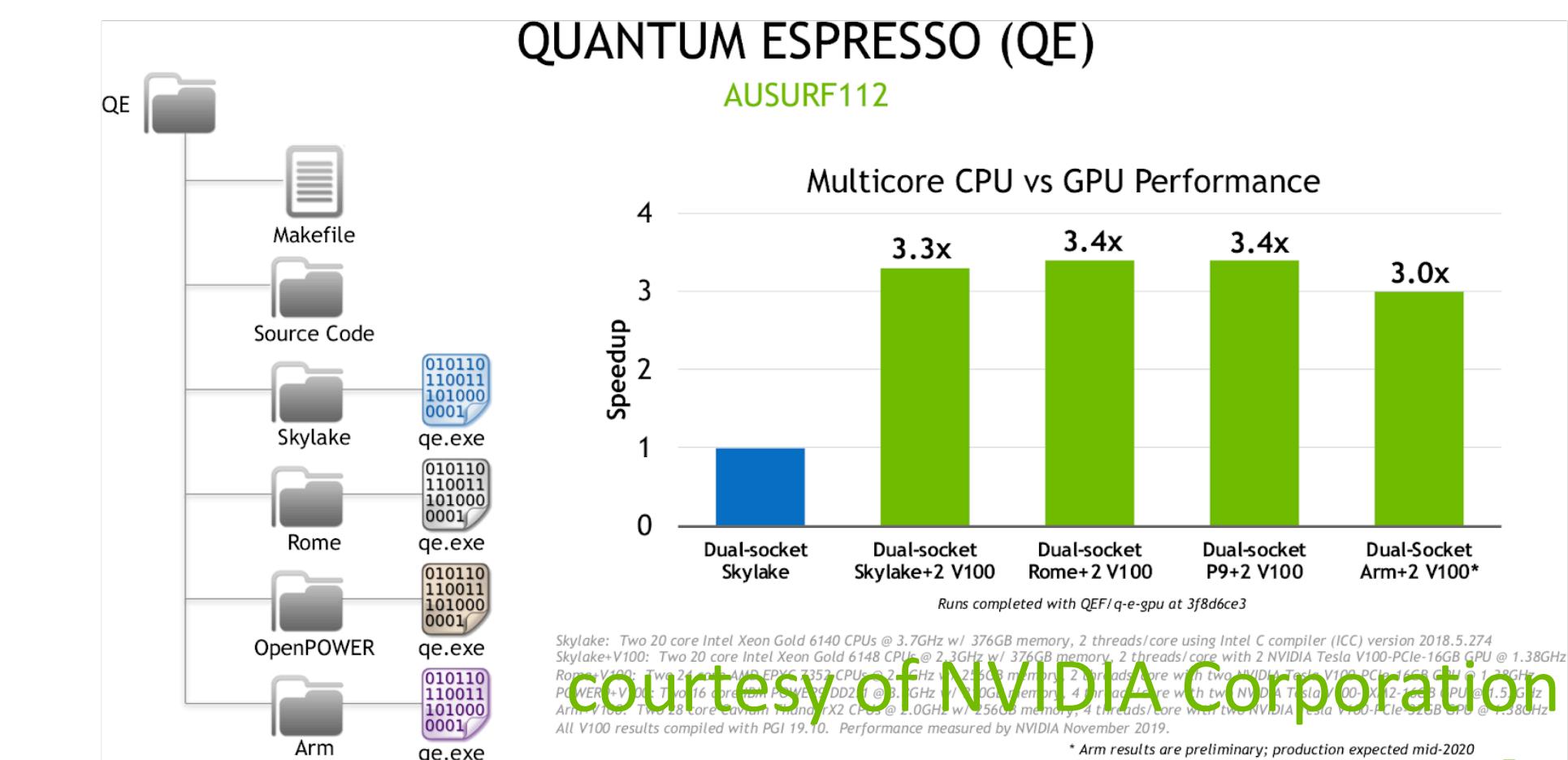
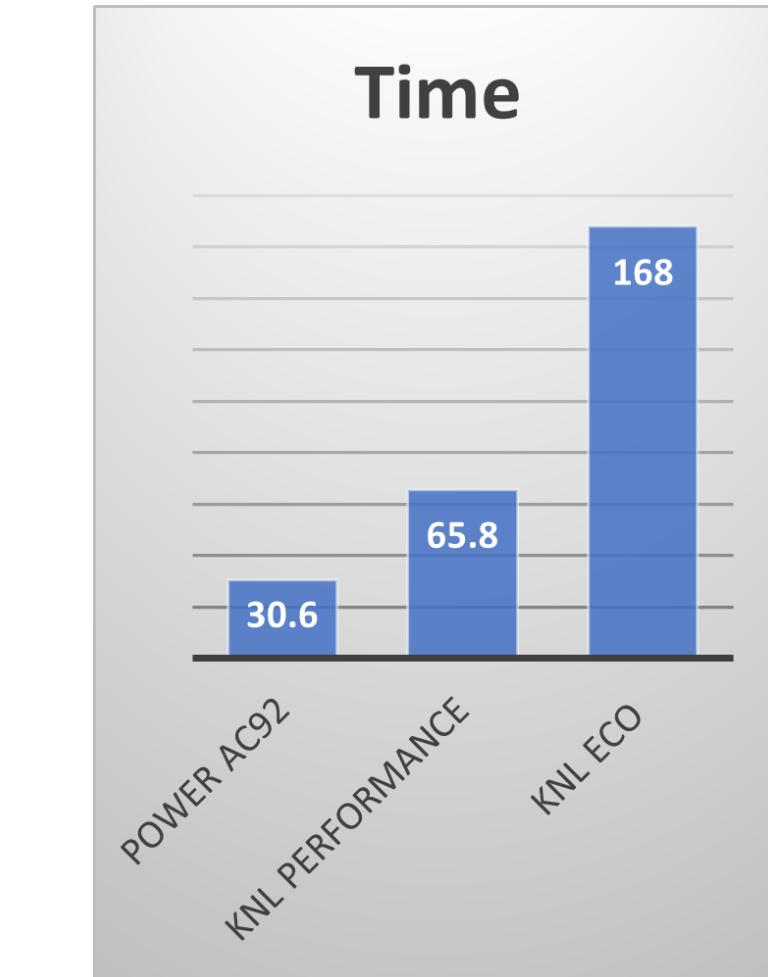
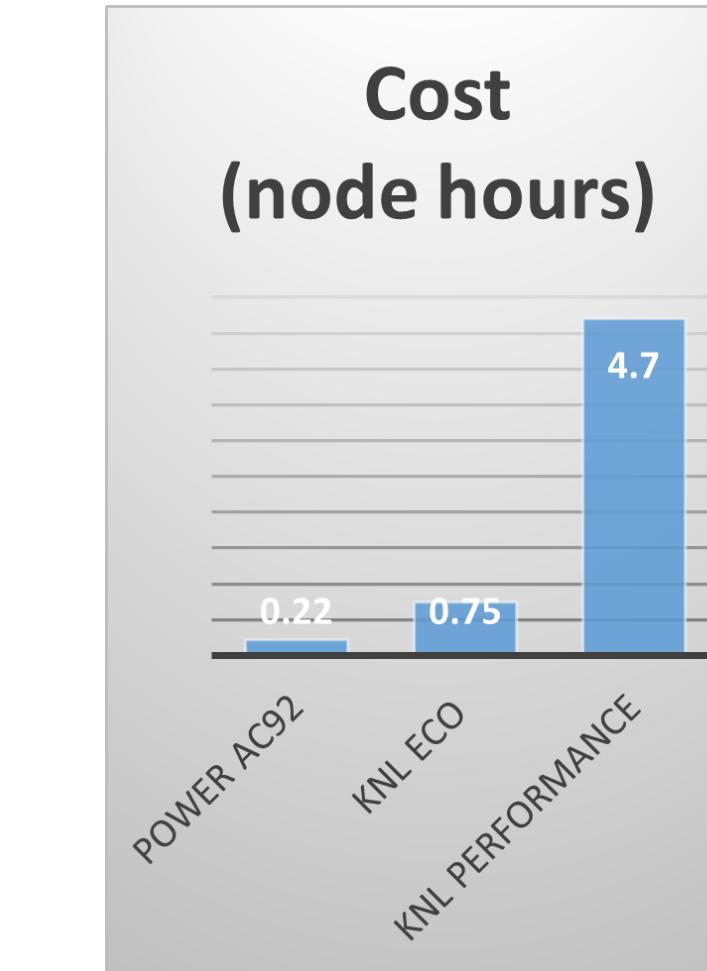
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Au<sub>112</sub> surface



porphyrin@CNT





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