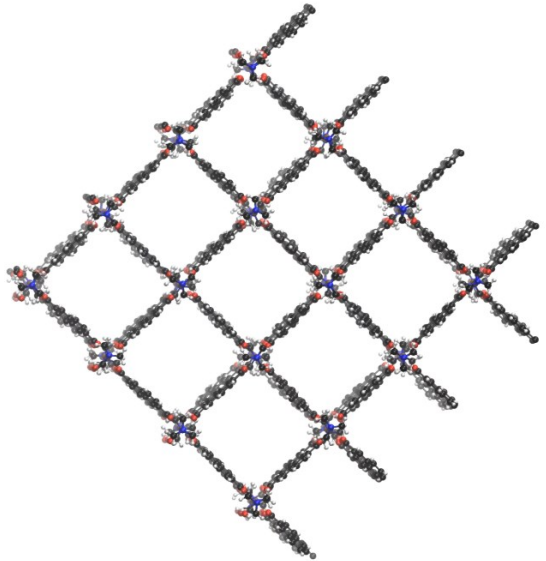
UNIVERSITÄT
LEIPZIG



Chemistry Meets HPC

What we use all these machines for

Leipzig, 19.10.2022

Dr. Patrick Melix

A COMPUTATIONAL CHEMIST'S DREAM WORLD

DREAM WORLD

Hardware:

- 10GHz CPUs, float64 optimized, 1000 per Node
- 10TB of memory, direct connection to each core
- Fast, reliable, global filesystem
- No runtime limits
- No queuing time
- Linearly scaling software on any number of nodes and cores

DREAM WORLD

- No script time limits on headnodes, but please kill all these left-over processes from other people (*not mine obviously*)!
- Lots of example job scripts
- Software installed and updated quickly upon request
- Easy way to use Jupyter notebooks on headnodes
- Up to date hot fix list for common issues until cluster is updated
- Separate CPU, GPU and mixed resources
- Maintain CPU only resources
- Web Interface for usage and project tracking

ACKNOWLEDGEMENTS

- Prof. Thomas Heine
- Prof. Francesco Paesani
- Prof. Randall Q. Snurr
- Prof. Ralf Tonner-Zech
- Prof. Omar K. Farha
- Prof. Joseph T. Hupp
- Prof. Timur Islamoglu
- Prof. Petko Petkov
- Dr. Andrew Rosen
- Dr. Megan C. Wasson
- Dr. Debabrata Sengupta
- Fabian Pieck
- Hendrik Weiske
- Qining Wang

Unterstützt von / Supported by

Alexander von Humboldt Stiftung/Foundation

zenodo

NERSC

NOMAD NOVEL MATERIALS DISCOVERY

ZIH Zentrum für Informationsdienste und Hochleistungsrechnen

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Northwestern

DFG FOR2433

U.S. DEPARTMENT OF ENERGY | Office of Science

TECHNISCHE UNIVERSITÄT DRESDEN

UC San Diego

INSTITUTE FOR SUSTAINABILITY AND ENERGY

UNIVERSITÄT
LEIPZIG

THANK YOU FOR YOUR KIND ATTENTION!