Performing solid-state Density Functional Theory calculations on LUMI-C

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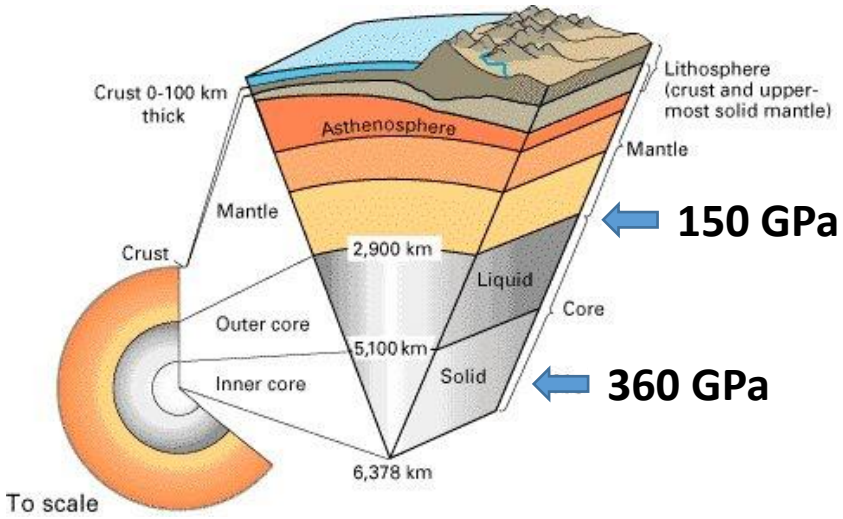
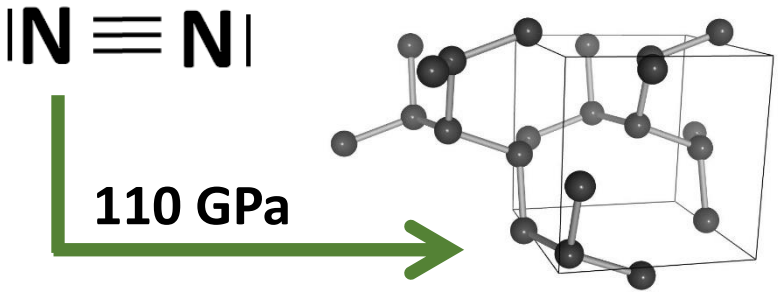
Solid state chemistry and physics

Properties of matter at high pressure above 10 000 atm (1 GPa) up to 1 000 000 atm (100 GPa)

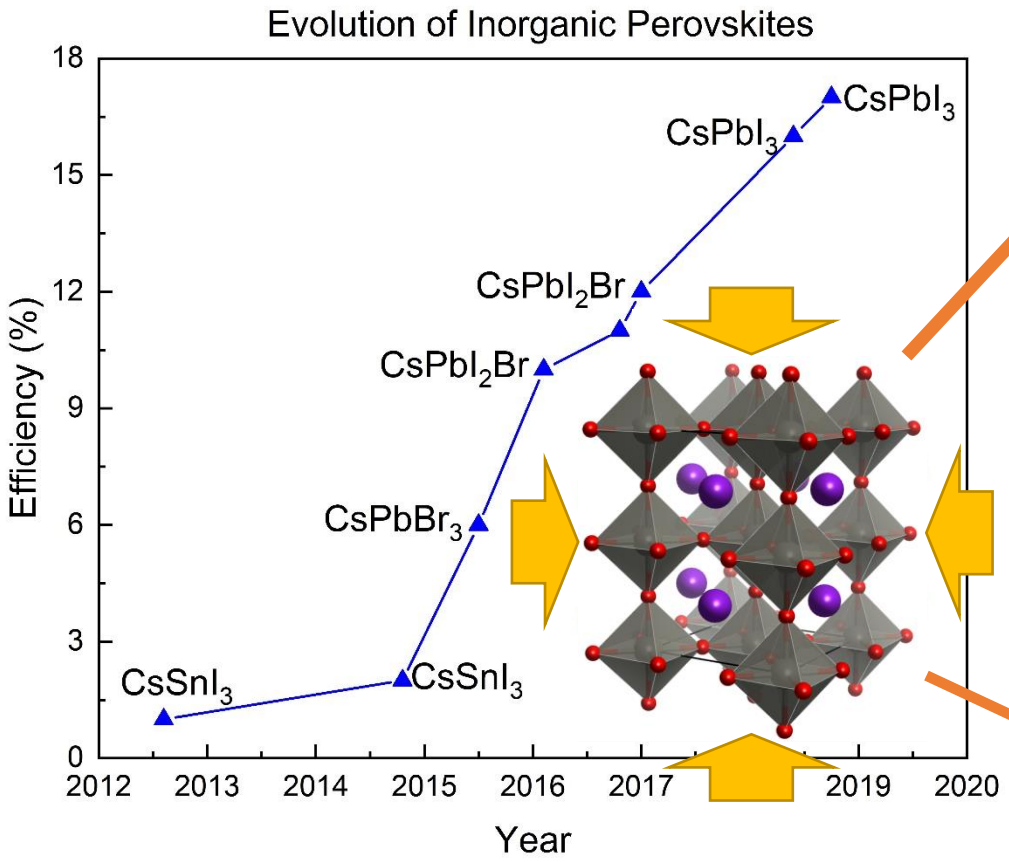
Recreating extreme environments

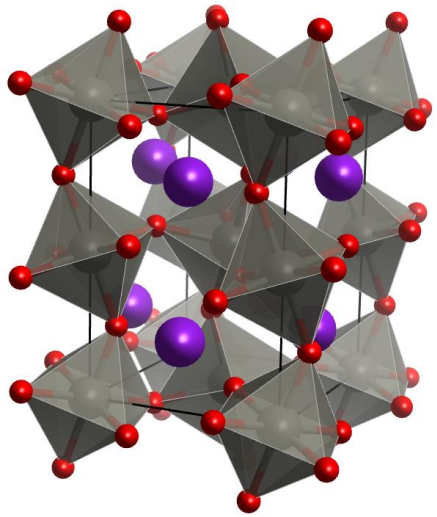


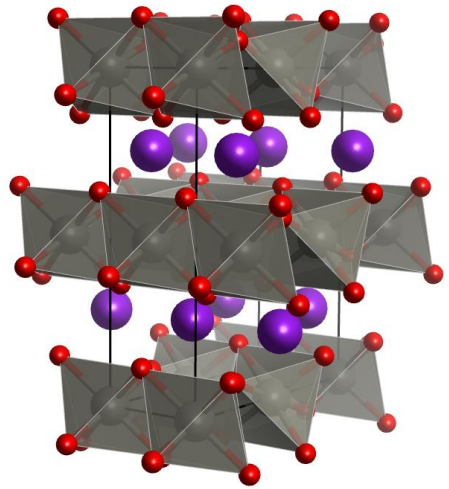
Novel chemistry



Pressure as a tuning parameter

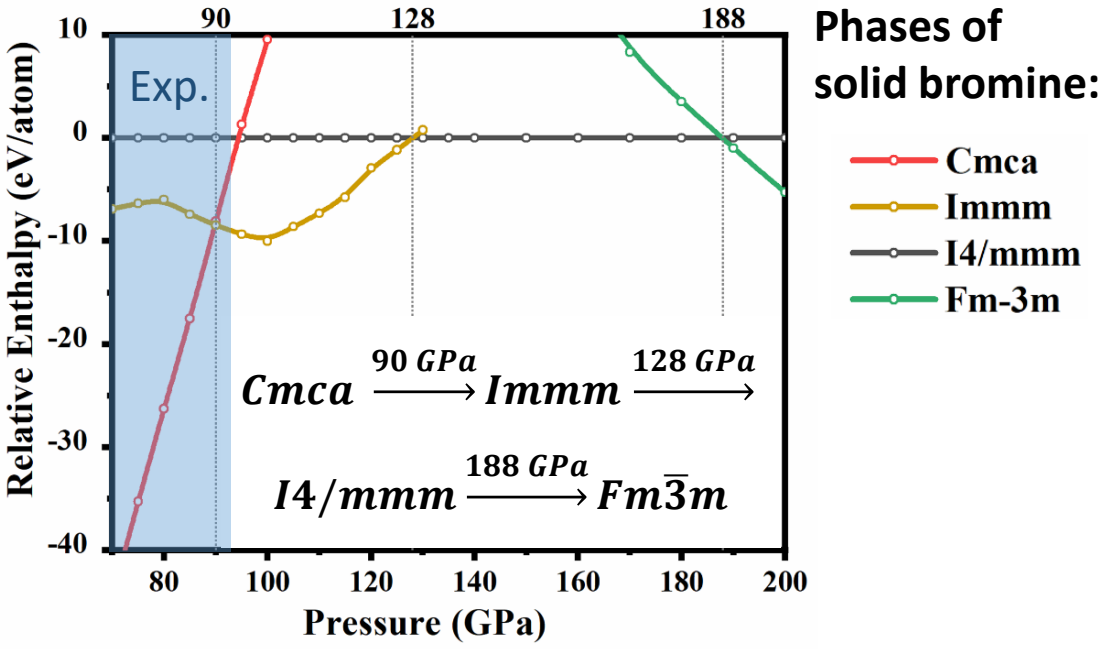




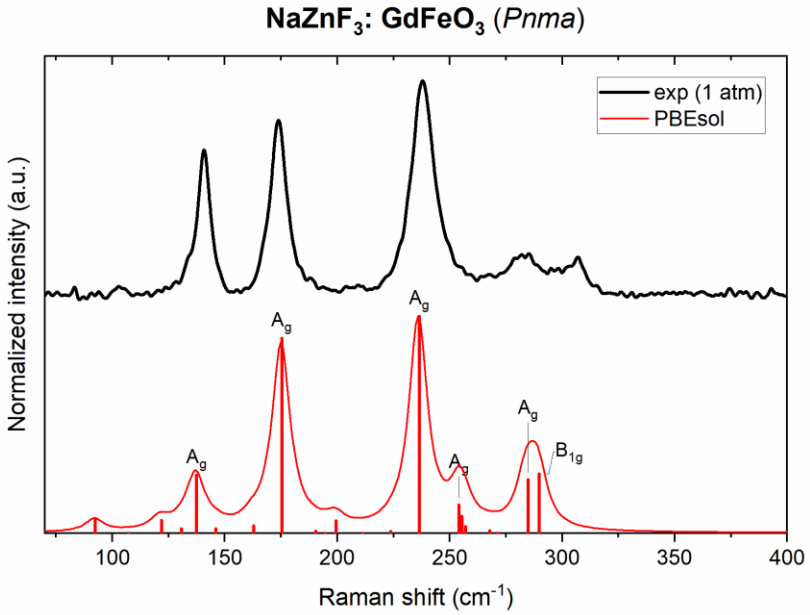


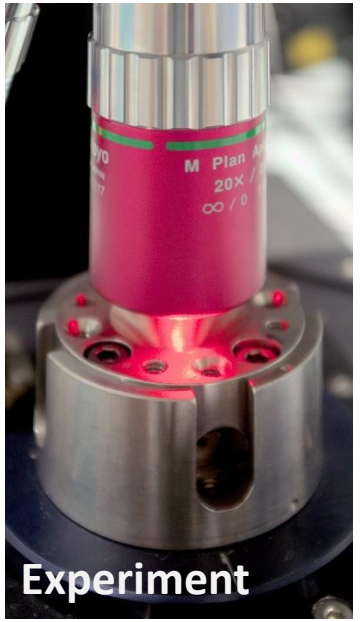
Density functional theory (DFT) modelling in high-pressure studies

Predicting high-pressure transformations

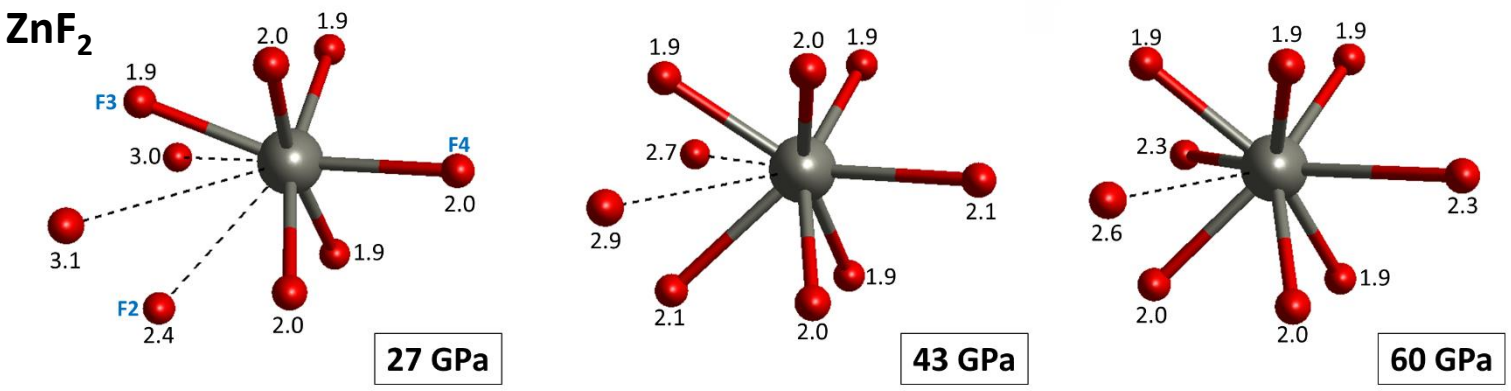


Aiding analysis of experimental data



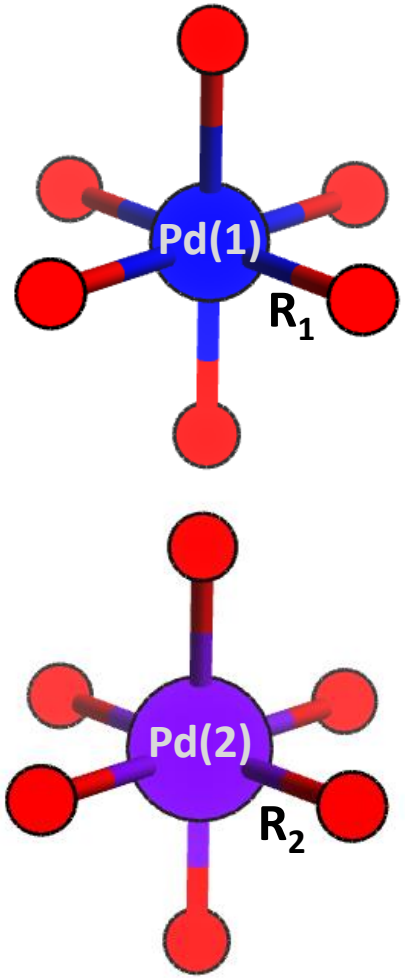


Understanding changes in structure and properties

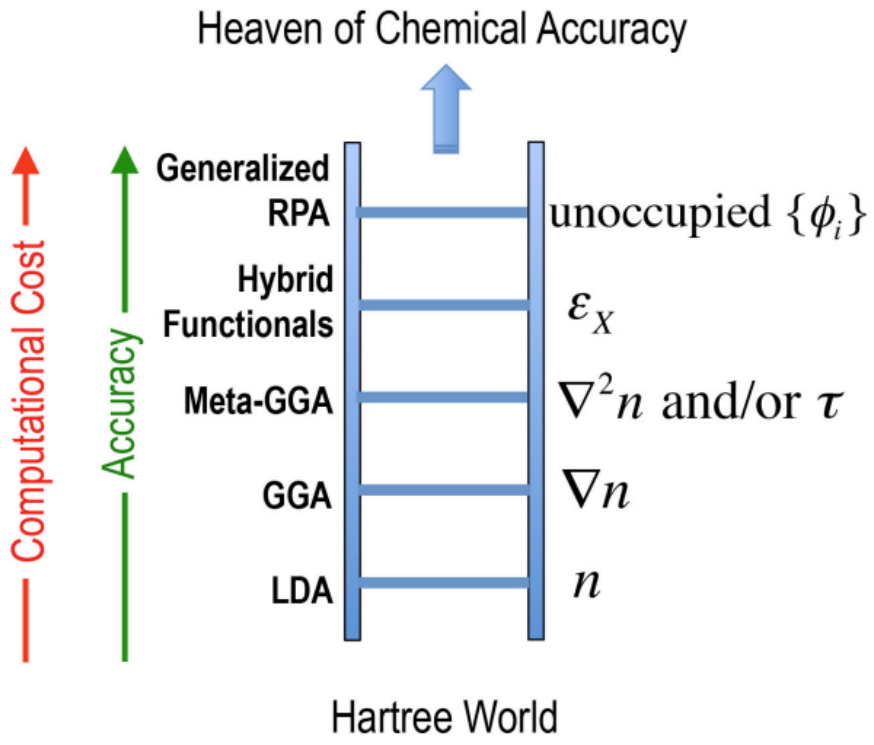


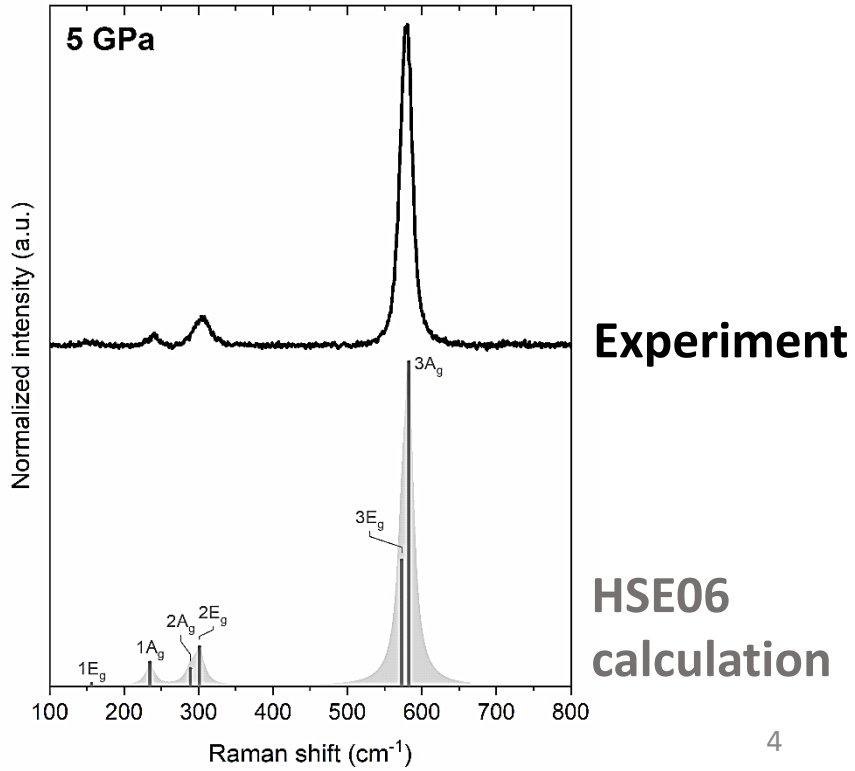
Jacob's ladder of DFT

PdF_3



„Rung"	$\mu_{Pd(1)}$ (μ_B)	$\mu_{Pd(2)}$ (μ_B)	R_2 vs R_1	ω_{3Ag} (cm^{-1})	ω_{3Eg} (cm^{-1})
Experiment	**0.0**	**1.8**	**+14 %**	**564**	**557**
Hybrid functional (HSE06)	0.1	1.6	+13 %	565	551
Meta-GGA (SCAN)	0.2	1.4	+9 %	453	487
GGA (PBE)	0.0	0.0	0 %		





Experiment

HSE06 calculation

Computational cost

Test system: PdF_3 (24 atoms, 186 electrons, 5 k-points)

LUMI-C

1 536 nodes × 128 cpus = 196 608 cpus

Linpack Performance (Rmax) = 6.30 PFlop/s

Rmax per cpu = 32.0 GFlop/s

„Rung”	Time per SCF step (s)
Hybrid functional (HSE06)	479 (x19.4)
Meta-GGA (SCAN)	56.1 (x2.3)
GGA (PBE)	24.7

5 nodes × 128 cpus = 640 cpus

ALTAIR (PCSS)

1 320 nodes × 48 cpus = 63 360 cpus

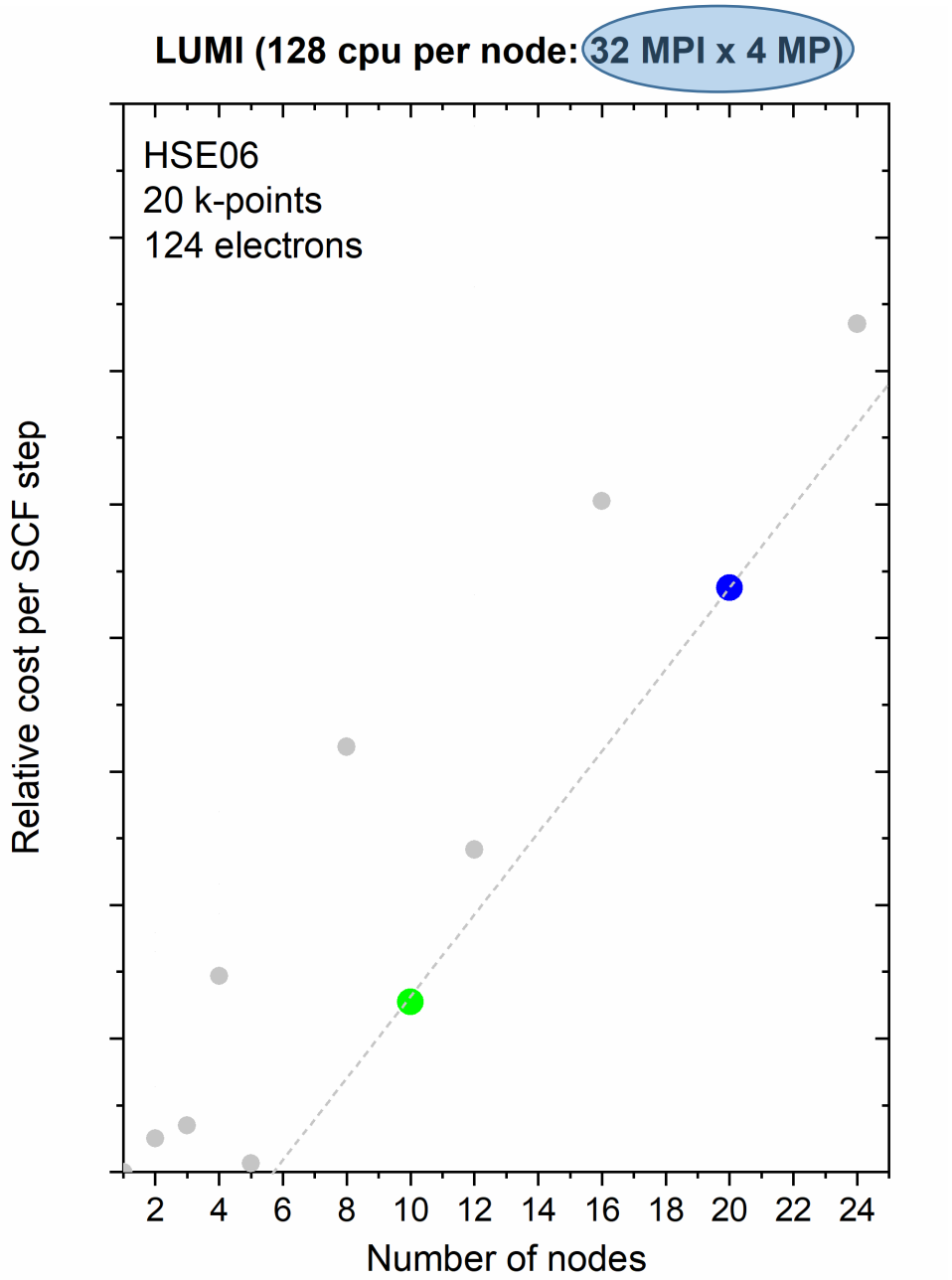
Linpack Performance (Rmax) = 3.53 PFlop/s

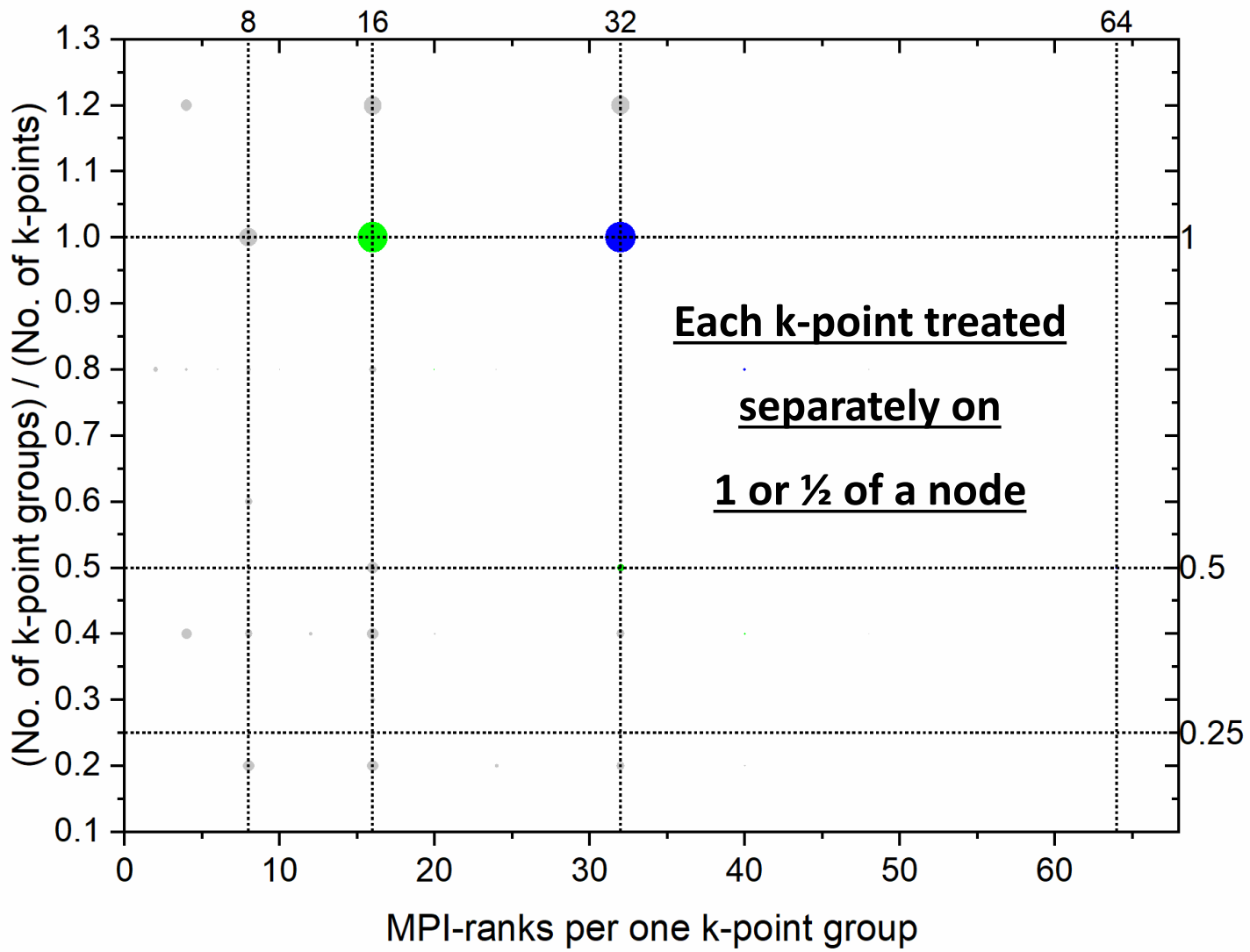
Rmax per cpu = 55.7 GFlop/s

„Rung”	Time per SCF step (s)
Hybrid functional (HSE06)	479 (x32.3)
Meta-GGA (SCAN)	56.0 (x3.1)
GGA (PBE)	17.8

10 nodes × 48 cpus = 480 cpus

Running jobs efficiently on LUMI-C





Outlook

Portable Acceleration of Materials Modeling Software: CASTEP, GPUs, and OpenACC

Matthew Smith and Arjen Tamerus, *University of Cambridge, CB3 0HE, Cambridge, U.K.*

Phil Hasnip, *University of York, YO10 5DD, York, U.K.*

In this article, we present work to port the CASTEP first-principles materials modeling program to accelerators using open accelerator (OpenACC). We discuss the challenges and opportunities presented by graphical processing units (GPU) architectures in particular, and the approach taken in the CASTEP OpenACC port. Whilst the port is still under active development, early performance results show that significant speed-ups may be gained, particularly for materials simulations using so-called "nonlocal functionals," where speed-ups can exceed a factor of ten.

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PL GRID

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