Contribution ID: **115**

Type: **Workshop**

Exploiting exascale HPC for materials modelling; UK's Excalibur Project

Sunday, 30 November 2025 13:30 (1h 30m)

GULP is one of the leading materials software for modelling materials using the method of interatomic potentials, likewise CASTEP and CP2K are two of the leading electronic structure codes for modelling materials. In this workshop the theory and a practical guide to how these can be employed to exploit HPC will be taught by developers of these codes.

The ChemShell computational chemistry environment will be introduced with a focus on multiscale quantum mechanical/molecular mechanical (QM/MM) modelling of materials systems. The course will cover how to set up QM/MM models for a range of materials chemistry problems and running calculations through interfaces to QM and MM codes including CASTEP and GULP. Recent developments in ChemShell for materials modelling carried out under the PAX-HPC project will be explored.

Presenting Author

Email

Student or Postdoc?

Institute

Registered for the conference?

CHPC User

No

CHPC Research Programme

Workshop Duration

Full day

Primary authors: Prof. WOODLEY, Scott (UCL); Prof. KEAL, Thomas (STFC); Dr PULIGHEDDU, Marcello (STFC); Dr SMITH, Matt (University of York); Dr SOKOL, Alexey (UCL); Dr KV, Rajany (STFC)

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Session Classification: Workshop