CP2K-UK: EPSRC investment with international impact

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What is CP2K?

CP2K (http://www.cp2k.org) is an powerful and flexible open-source atomistic simulation program, featuring a scalable implementation of Density Functional Theory based on the QUICKSTEP Gaussian and Plane Wave dual basis approach. CP2K is the second-most heavily used code on ARCHER, the UK National HPC Service and has 100s of users in the UK and 1000s worldwide. CP2K has around 20 core developers, mainly in Switzerland and the UK, with many more contributors worldwide.

Collaboration Case Studies

Transistor Modelling: Matt Watkins, University of Lincoln

The EU FP7 Project MORDRED including Alex Shluger (UCL) and Tibor Grasser (Technical University Vienna) achieved the first quantitative models of the mechanisms of transistor gate breakdown fully informed by state-of-the-art atomistic modelling at a quantum mechanical level. The gate dielectric is amorphous and modelling charge trapping in the device that leads to reliability issues requires an accurate energy alignment of channel, gate valence band and conduction band. This required extensive statistical sampling of defect environments and periodic DFT using hybrid density functionals to minimise self-interaction error. The Auxiliary Density Matrix Method implemented in CP2K made sampling 100s of minimisations and NEB calculations per defect type feasible. Atomistic understanding of device degradation in microelectronics devices is an important step forward as devices are becoming ever smaller and nanoscale features begin to dominate their behaviour.

Solid-state catalysis: Tobias Krämer, Heriot-Watt University

In 2015, the CP2K-UK project visited the Macgregor group (Heriot-Watt University) as they needed to be able to model sigma-alkane complexes in a realistic periodic environment, at a scale (750+ atoms) which was unattainable by gas-phase or plane-wave DFT codes. Thanks to an ARCHER RAP grant, and a collaborative visit to Jürg Hutter's group (University of Zurich), they were able to provide atomistic insight into the synthesis process of a Rhodium-Pentane complex as a complement to low-temperature single-crystal X-ray diffraction and solid-state NMR spectroscopy experiments.

CP2K-UK

The CP2K-UK project was funded as part of EPSRC's 2013 "Software for the Future" strategy – with the goal of supporting the developer and user communities of CP2K based in the UK. Over the last 5 years, CP2K-UK has improved the capability of CP2K ('Better Software') and nurtured a growing user community ('Better Research') – leading to improved research outputs and impacts. Some of the project's outcomes:

- A series of annual user group meetings, with 270 participants (12% international)
- A CP2K Summer School in London, 2016, with 59 participants (47% international)
- 3 years FTE of additional funding awarded from ARCHER eCSE to build UK expertise in CP2K development and materials modelling capability
- Supported Dr Clotilde Cucinotta's EPSRC Fellowship, which will develop electronic transport modelling capability in CP2K, with applications in battery technology.
- Enabled code contributions from around the UK and overseas (Finland, France, Germany) to benefit the whole CP2K community.

International Community

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