CP2K-UK

Supporting Advances in Atomistic Simulation Capability

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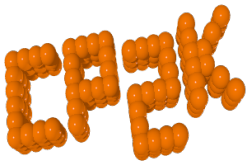

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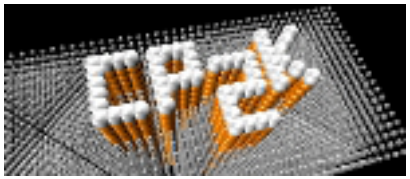
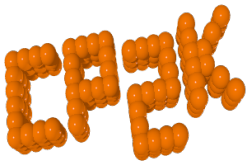
CP2K Overview

"CP2K is a program to perform atomistic and molecular simulations of solid state, liquid, molecular, and biological systems. It provides a general framework for different methods such as e.g., density functional theory (DFT) using a mixed Gaussian and plane waves approach (GPW) and classical pair and many-body potentials."



From www.cp2k.org (and original home page from 2004!)



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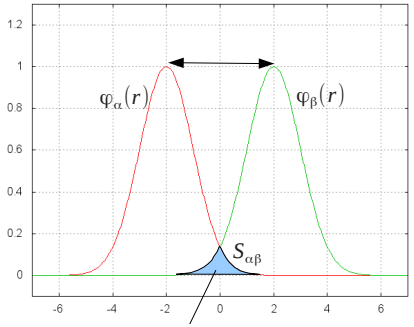
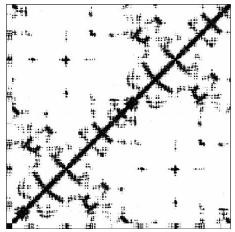
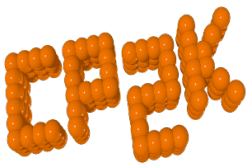
CP2K Overview

- QUICKSTEP DFT: Gaussian and Plane Waves Method (VandeVondele *et al*, Comp. Phys. Comm., 2005)
  - Advantages of atom-centred basis (primary)
    - Density, Overlap, KS matrices are sparse
  - Advantages of plane-wave basis (auxiliary)
    - Efficient computation of Hartree potential
  - Efficient mapping between basis sets
    - -> Construction of the KS Matrix is ~O(n)





- Orbital Transformation Method (VandeVondele & Hutter, J. Chem. Phys., 2003)
  - Replacement for traditional diagonalisation/density mixing(non-metallic systems only)
    - Cubic scaling but ~10% cost



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CP2K Overview

- Many Hamiltonians:
  - Classical
  - DFT (GPW, GAPW + vDW)
  - LS-DFT
  - TD-DFT (LR and RT)
  - Hybrid Hartree-Fock
  - post-HF (MP2, RPA, G0W0)
  - Combinations (QM/MM, mixed)
- Simulation tools:
  - MD (various ensembles)
  - Monte Carlo, Global Optimisation
  - Minimisation (GEO/CELL_OPT)
  - Properties (Spectra, excitations …)
- Open Source
  - GPL, www.cp2k.org
  - 1m loc, ~2 commits per day
  - ~20 core developers

CP2K

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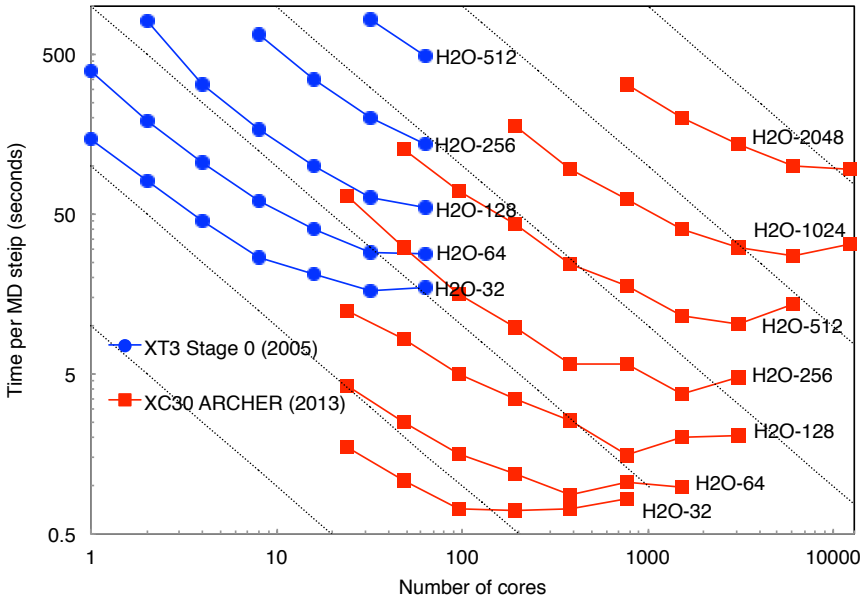
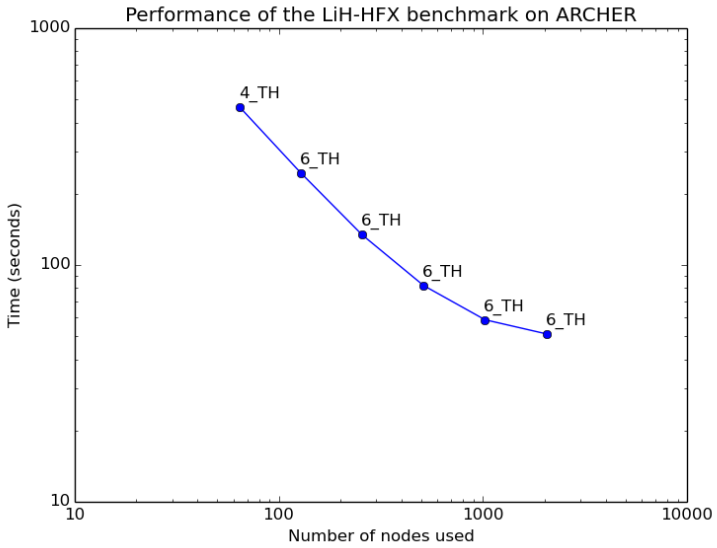
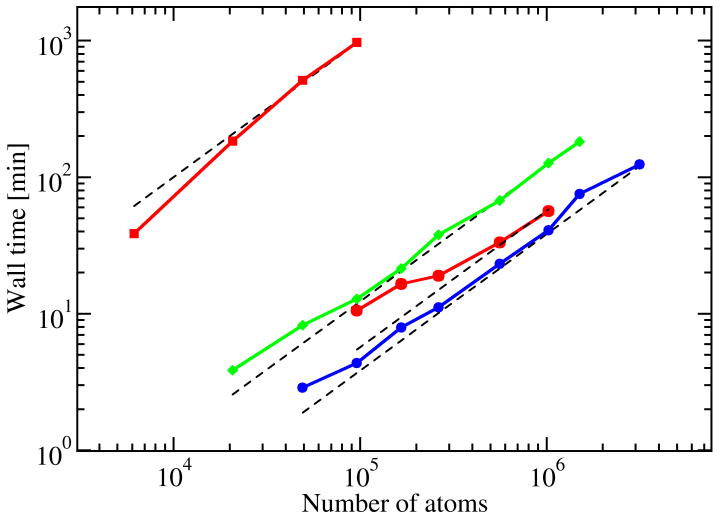
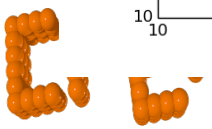
CP2K Overview

- Efficient algorithms and scalable implementations:
  - Fast *ab initio* MD with local XC
  - 10,000s+ cores for single and double-hybrid DFT
    - MPI+OpenMP helps here
  - LS-DFT for millions of atoms









CP2K Applications

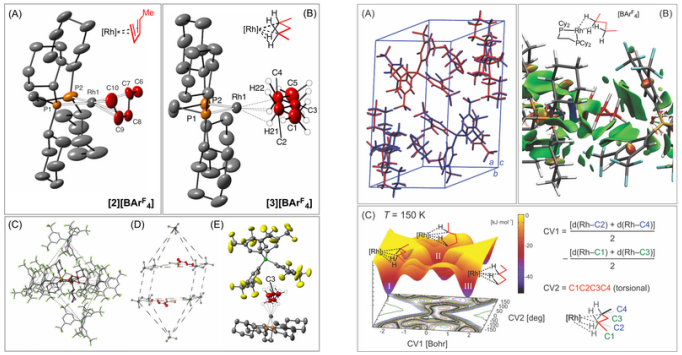
www.cp2k.org/science

Alkane Complexes

International Edition: DOI: 10.1002/anie.201511269
German Edition: DOI: 10.1002/ange.201511269

A Rhodium–Pentane Sigma-Alkane Complex: Characterization in the Solid State by Experimental and Computational Techniques

F. Mark Chadwick[+], Nicholas H. Rees, Andrew S. Weller, Tobias Krämer[+], Marcella Iannuzzi, and Stuart A. Macgregor**



Large variation of vacancy formation energies in the surface of crystalline ice

M. Watkins[1,2,3], D. Pan[4], E. G. Wang[5], A. Michaelides[1,2,3], J. VandeVondele[6] and B. Slater[1,3]*

[1]Department of Chemistry, Christopher Ingold Building, 20 Gordon Street, University College London, London WC1H 0AJ, UK, [2]London Centre for Nanotechnology, University College London, London WC1H 0AJ, UK, [3]TYC@UCL, University College London, London WC1H 0AJ, UK, [4]Institute of Physics, Chinese Academy of Sciences, PO Box 603, Beijing 100190, China, [5]School of Physics, Peking University, Beijing 100871, China, [6]Institute of Physical Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland. *e-mail: b.slater@ucl.ac.uk.

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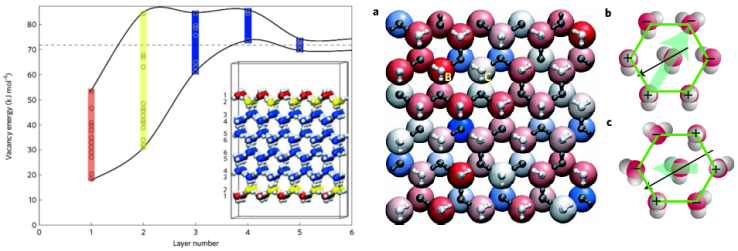


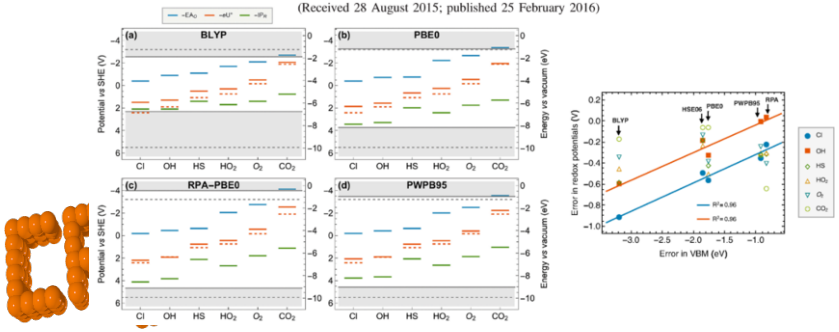
PRL 116, 086402 (2016) PHYSICAL REVIEW LETTERS week ending 26 FEBRUARY 2016

Calculation of Electrochemical Energy Levels in Water Using the Random Phase Approximation and a Double Hybrid Functional

Jun Cheng[*]
Collaborative Innovation Center of Chemistry for Energy Materials, State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, People's Republic of China and Department of Chemistry, University of Aberdeen, Aberdeen AB24 3UE, United Kingdom

Joost VandeVondele[†]
Department of Materials, ETH Zurich, Wolfgang-Pauli-Strasse 27, CH-8093 Zurich, Switzerland

(Received 28 August 2015; published 25 February 2016)



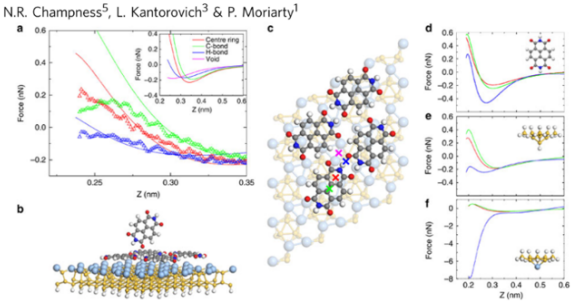
nature COMMUNICATIONS

ARTICLE

Received 6 Dec 2013 | Accepted 22 Apr 2014 | Published 30 May 2014 DOI: 10.1038/ncomms4931 OPEN

Mapping the force field of a hydrogen-bonded assembly

A.M. Sweetman[1,*], S.P. Jarvis[1,*], Hongqian Sang[2,3,*], I. Lekkas[1], P. Rahe[4], Yu Wang[2], Jianbo Wang[2], N.R. Champness[5], L. Kantorovich[3] & P. Moriarty[1]



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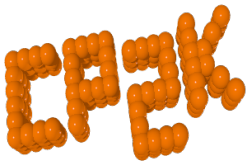
CP2K Usage

- Growing popularity in UK community
  - 2nd most heavily used code on ARCHER
  - Growing users of CP2K on national service:
    - 42 (2Q14) -> 72 (1Q15) -> 116 (1Q16) -> 132 (4Q17)
    - EPSRC: Materials Chemistry Consortium, UKCP
    - NERC: Mineral Physics

- but…
  - Large feature set leads to complexity
  - Few default settings -> hard to set up systems from scratch
  - Lack of documentation



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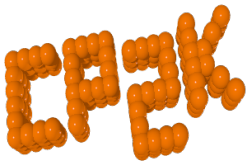
Support for UK CP2K Users

- CP2K-UK: EPSRC Software for the Future
  - £500,000, 2013-2018
  - EPCC, UCL (+ Lincoln), KCL
    - + 7 supporting groups

EPSRC
Pioneering research and skills

- Aims
  - Grow and develop existing CP2K community in UK
  - Lower barriers to *usage* and *development* of CP2K
  - Long-term sustainability of CP2K
  - Extend ability of CP2K to tackle challenging systems



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Support for Users

- Training Events
  - Annual User Group Meetings
    - Mon 9th January 2017 in Edinburgh
  - 14 days CP2K training during 2016
    - Collaborations with ARCHER, PRACE, MCC, UKCP & STFC
    - Visits to research groups (QUB)
  - CP2K Summer School
    - 23rd – 26th Aug 2016 @ King's College London
    - Majority from UK people
    - Slides and exercises still available:
      - https://www.cp2k.org/events:2016_summer_school:index
  - All CP2K events at www.cp2k.org/events
  - Also notification by email

Science & Technology Facilities Council

archer

PRACE

Queen's University Belfast

CP2K

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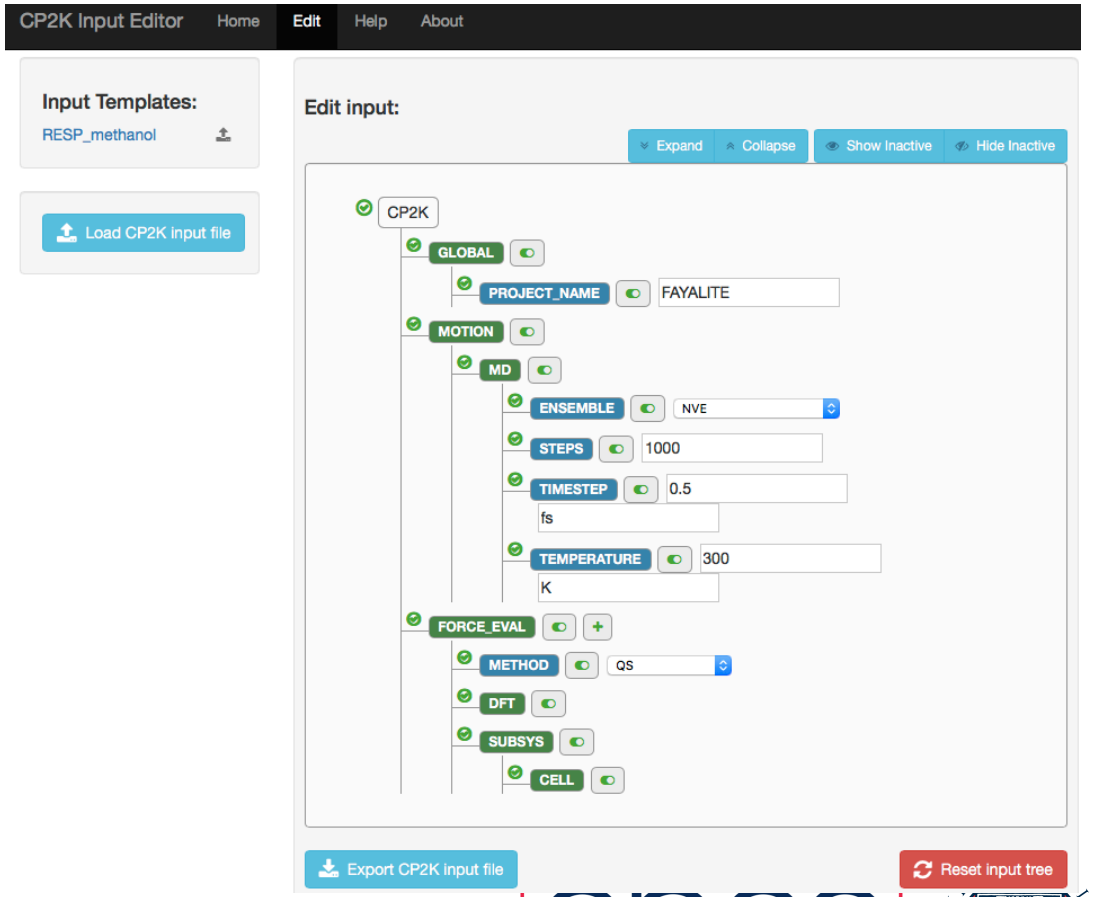
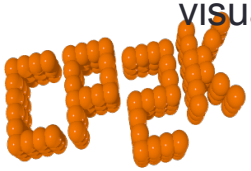
The University of Edinburgh

Support for Users

- Tools & Usability
  - Feedback from tutorials:
    - building an input is hard!
  - CP2K input GUI
  - Validation of input
    - CP2K releases 2.5 – 4.0
  - Keyword Selection
  - Show/hide sections
  - Job templates
  - Tooltip keyword help
  - Import and edit existing input files
  - Currently working on Chimera / tetr integration
    - System set-up and visualisation

http://cp2k-www.epcc.ed.ac.uk/cp2k-input-editor





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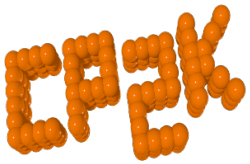
Support for Users

- Ad-hoc bespoke support
  - Help installing CP2K on your cluster
    - Iceberg @ Sheffield, Lancaster HEC, KCL Physics Cluster, QUB …
  - Training days / group visits
  - Debugging
  - Adding functionality (e.g. OPLS torsions)
  - Advice on parallel performance - www.cp2k.org/performance
    - We would like more than just Cray machines!
- Documentation
  - Growing set of ‘HowTo’ guides: https://www.cp2k.org/howto
  - FAQs: https://www.cp2k.org/faq



- Let me know your pain points!

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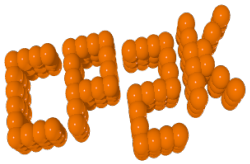
Support for Developers

- Development projects
  - 3 year PDRA developer post at KCL
    - Trailblazer for future (externally funded) projects

  - Langevin Dynamics regions (Kantorovich, 2008, Phys Rev B)
  - BSSE calculations with arbitrary fragments
  - Filter Matrix Diagonalization (Rayson & Briddon, 2009, Phys Rev B)
  - REPEAT charge fitting (Campana *et al*, 2008, JCTC)
  - CP2K Installer
  - Vibrational Initialisation for MD (West & Estreicher, 2006, PRL)



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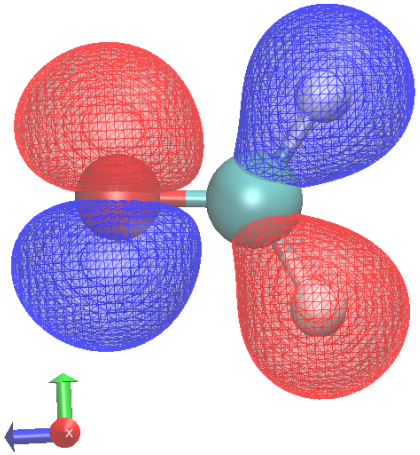
Support for Developers



- External funding
  - Three 12 month funded projects from ARCHER eCSE
  - LR-TDDFT with Hybrid Functionals/ADMM
    - Dec 2015 – Dec 2016 : Sergey Chulkov / Matt Watkins @ Lincoln
    - Maximum Overlap Method
    - MO visualisation output in Molden format
    - See https://www.archer.ac.uk/training/virtual/2016-11-23-CP2K-Improvements/TDDFT.slides.html
  - Electron Transport based on Non-Equilibrium Green's Functions Methods
    - Dec 2016-Dec 2017
    - Sergey / Matt @ Lincoln, Lev Kantorovich @ KCL, Artem Fediai @ TU Dresden

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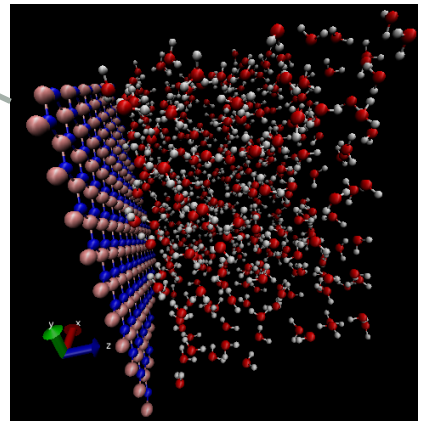
Support for Developers

- CP2K performance improvements
  - Started Dec 2015 - Mark Tucker @ EPCC
  - Large, load imbalanced systems (~10% speedup, GBs memory saving)
  - GAPW (3.6x speedup!)
  - vDW-corrected XC functionals (~5% speedup)
  - K-points
  - See https://www.archer.ac.uk/training/virtual/2016-11-23-CP2K-Improvements/CP2K-virtual-tutorial.pdf



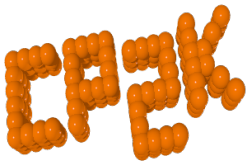
Nodes of ARCHER	45	48	64	96
Original Code	1427	1176	1371	1278
Modified Algorithm	1312	1057	1241	1168
Improvement	8.8%	11.3%	10.5%	9.4%

Table 2: Overall Run Time (seconds).

- Charged cluster of 216 water molecules in 34Å^3 box
- TZV2P MOLOPT basis set
- PBC off
- ~10% speedup

Community Involvement

- Interested in contributing to development?
  - Opportunity to get 6-12 months funding via ARCHER eCSE calls (next 31st Jan & 9th May 2017) for *"Improvements to code which allows new science to be carried out"*
    - Have a 'killer feature' that you *need* in CP2K?
    - Interested in working on a development project? Let me know…
- Acknowledge support from CP2K-UK grant (EP/K038583/1) in publications (and tell me!)
  - More impact = better chance of future funding
  - Cite CP2K reference papers (check your output!)
- Letters of support available to projects who will use/develop CP2K



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Summary

- CP2K is a powerful tool for materials modeling using DFT
  - + a wide range of other Hamiltonians
- Well suited to use on HPC and cluster systems
- Support for users and developers available through EPSRC-funded CP2K-UK project
- Support requests to i.bethune@epcc.ed.ac.uk