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CP2K-UK: EPSRC Investment with International Impact

Impact of international research software collaboration

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Background: CP2K-UK

- CP2K is a powerful tool
  - DFT, Classical, Hybrid-DFT, TDDFT, LS-DFT, MP2/RPA/G0W0, QM/MM
  - MD, MC, Geometry Optimisation, NEB, Free Energy Tools
  - Suitable for simulations in range of EPSRC target areas

- CP2K is popular (and growing)
  - 2nd most heavily used code on ARCHER (£0.5m per year)
  - Growing users of CP2K on national service:
    - 42 (2Q14) -> 72 (1Q15) -> 116 (1Q16) -> 132 (1Q17) -> 173 (1Q18)
    - EPSRC: Materials Chemistry Consortium, UKCP
    - NERC: Mineral Physics

New release!
CP2K 5.1 (Oct 2017)

- CP2K can be hard to use
  - 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 (+ STFC), 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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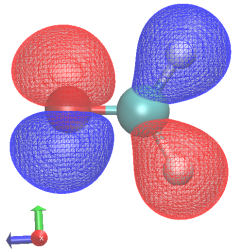
CP2K-UK Project Highlights

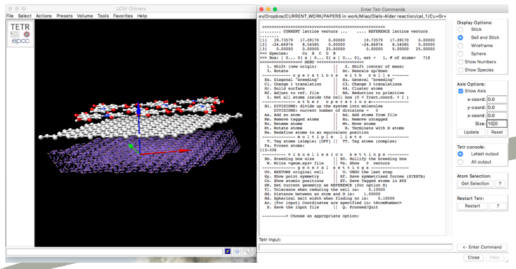


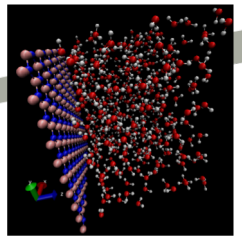
User Support

- Annual User Meetings
  - 270 people (12% international)
- 2 CP2K UK Summer Schools
  - 90+ people (47% international)
- Training Days / group visits / workshops
- CP2K Installation + debugging
- Code review + patches
- Letters of support
- CP2K Toolchain installer

Development

- CP2K Input Editor
  - http://cp2k-www.epcc.ed.ac.uk/cp2k-input-editor
- Plugins for USCF Chimera
  - https://www.cp2k.org/tools:tetr
- New algorithms (3 additional FTE
  - TDDFT with Hybrid Functionals
- Performance optimization
  - 3.6x speedup for GAPW
  - Memory-efficient Load balancing





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CP2K International Community

★ Developers

- STFC Hartree Centre
- EPCC
- University of Lincoln
- University of Zurich
- Paul Scherrer Institute
- IBM Research Zurich
- Aalto University

★ Contributors

- University College London
- University of Bonn
- University of Pisa
- University of Rijeka

★ Collaborators

- Heriot-Watt University
- Trinity College Dublin
- University of Hull
- King's College London
- University College London
- CNRS/ Chimie ParisTech
- TU Dresden
- Lomonsov Moscow State University
- TU Vienna

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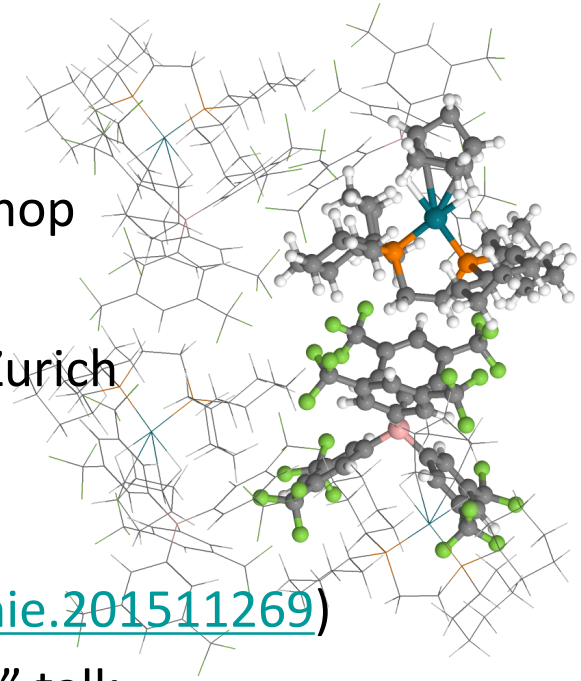
Case study: Solid-state catalysis

- May 2014: CP2K-UK visit to Macgregor group (Heriot-Watt University)
  - Installation, intro to CP2K
- June 2014: ARCHER Instant Access
- Aug 2014: Macgregor group at NSCCS CP2K workshop
- Nov 2014: ARCHER RAP Application
- Feb-Mar 2015: Tobi Krämer visit to, University of Zurich
- Dec 2015: Results!
  - Joint computational / experimental paper in Angewandte Chemie (https://doi.org/10.1002/anie.201511269)
- Feb 2016: TK gives CP2K-UK user meeting "how-to" talk



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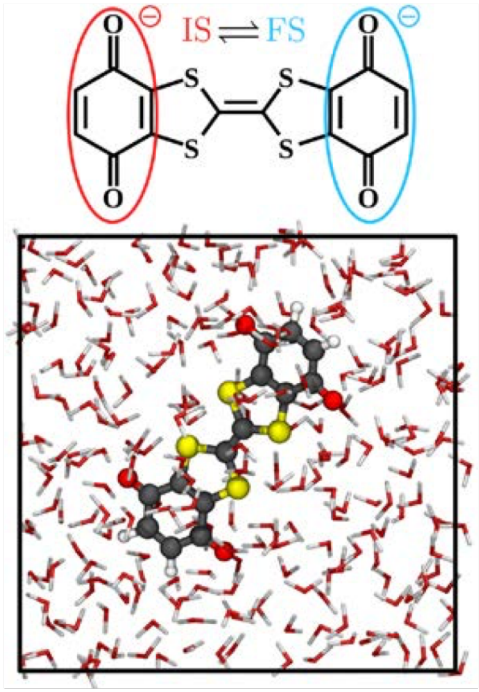
Case study: Constrained DFT

- 2015-2016: Development of Constrained DFT methods at Computational Chemistry group, Aalto University
  - Developed in a fork of CP2K: https://github.com/nholmber/cp2k-cdft-dev
  - Published in JCTC: https://doi.org/10.1021/acs.jctc.6b01085
- Jan 2017: Nico Holmberg lightning talk at CP2K-UK user meeting
- Jan-Feb 2017: Code review, merge CDFT into main CP2K trunk
- Mar 2017: NH given commit permissions to CP2K code
- Jan 2018: NH gives CP2K-UK user meeting “how-to” talk



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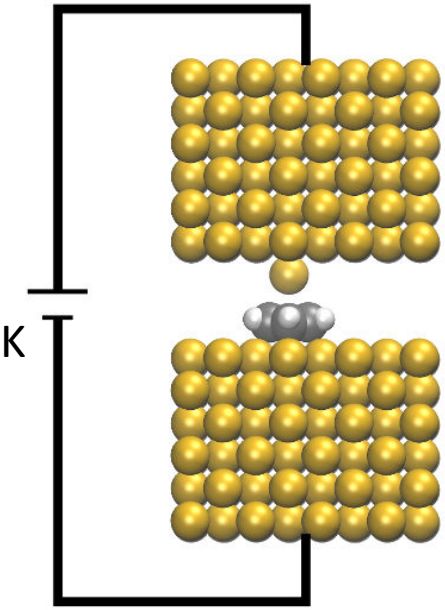
Case study: Transistor Modelling

- 2011-2015: EU FP7 Project MORDRED
  - Collaboration with Alex Shulger (UCL) and Tibor Grasser (TU Vienna)
  - First qualitative ab-initio models of transistor device gate breakdown mechanisms
  - Required efficient hybrid density functionals (ADMM) in CP2K
- 2012: Matt Watkins Co-I of CP2K-UK project
- Apr 2015: MW moves to new Computional Physics Group, University of Lincoln
- Dec 2015: Sergey Chulkov joins from Russia for CP2K developer post
  - Time-dependent DFT with Hybrid Density Functionals
  - Electronic Transport using Non—equilibrium Green's Functions



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- Lev Kantorovich, Ben Slater & Matt Watkins
- Jochen Blumberger, Patricia Hunt, Jorge Kohanoff, Angelos Michaelides, Philip Moriarty, Carole Morrison, Alex Shluger & Michiel Sprik
- Worldwide CP2K community

Interested in learning about how CP2K can impact your work?

Get in touch!

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