CP2K-UK 4TH ANNUAL USER MEETING

Welcome & Project Update

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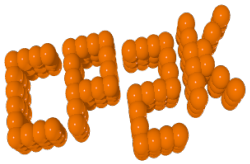
@ibethune @CP2Kproject



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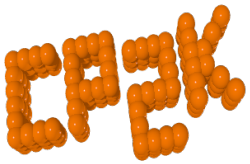
Introduction

- Welcome!
- 40+ attendees from 20+ institutions
- Experienced and novice users
  - Network, learn from others' experience
- Highlight opportunities for training & support
- Update on latest developments

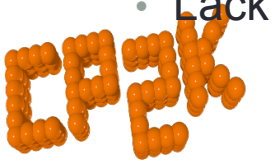


Background: CP2K-UK

- CP2K is a powerful tool
  - DFT, Classical, Hybrid-DFT, TDDFT, LS-DFT, MP2/RPA/G0W0, QM/MM
  - MD, MC, Relaxation, 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 (4Q17)
    - EPSRC: Materials Chemistry Consortium, UKCP
    - NERC: Mineral Physics

- 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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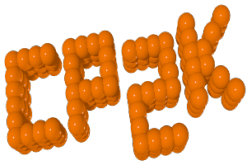
Support for UK CP2K Users

- CP2K-UK: EPSRC Software for the Future
  - £500,000, 2013-2018
  - EPCC, 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
  - 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:
      - www.cp2k.org/events:2016_summer_school:index
  - All CP2K events at www.cp2k.org/news
    - Archived info at www.cp2k.org/docs#workshops
  - Also notification by email

Science & Technology Facilities Council

archer

PRACE

Queen's University Belfast

CP2K

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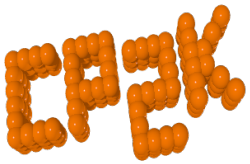
The University of Edinburgh

Support for Users

- 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)
    - Merging in user contributions
  - 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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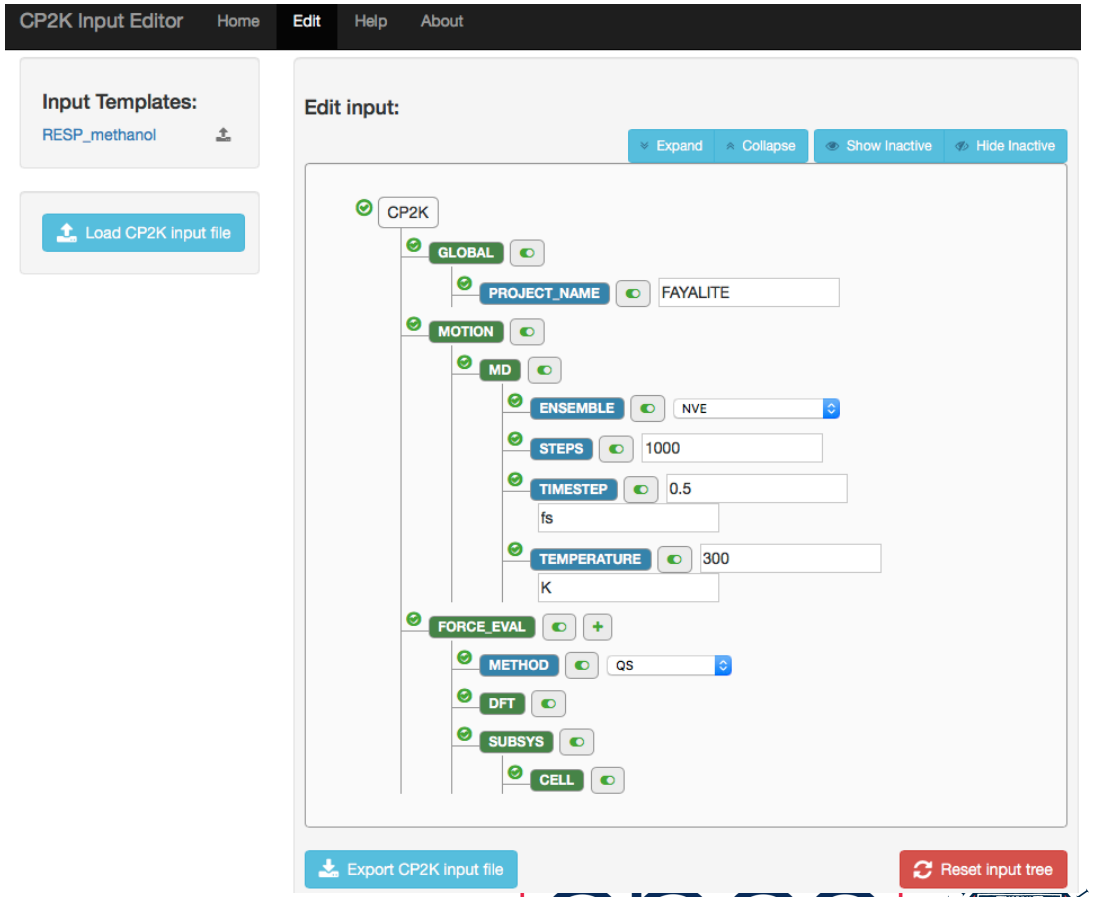
Support for Users

- 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

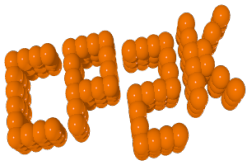
http://cp2k-www.epcc.ed.ac.uk/cp2k-input-editor



Support for Developers

- Development projects
  - 3 year PDRA developer post at KCL (2013-2016)
    - 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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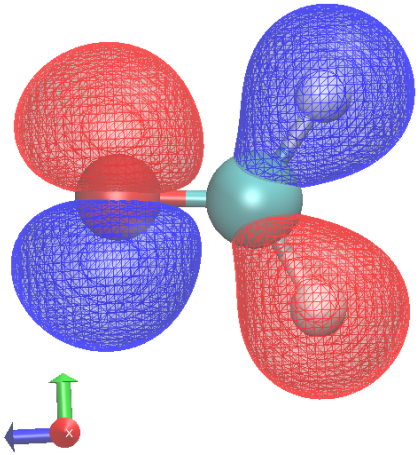
Support for Developers



- 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

CP2K

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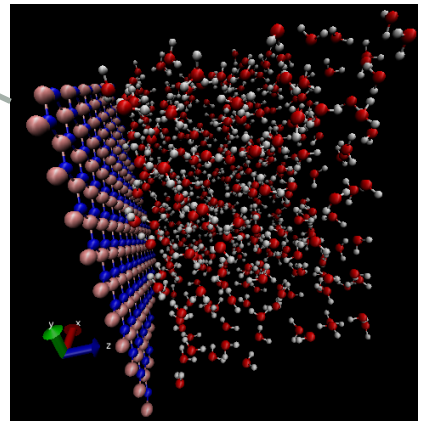
Support for Developers

- 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



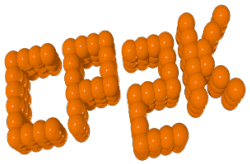
Nodes of ARCHER	45	48	64	96
Original Code	1427	1176	1371	1278
Modified Algorithm	1312	1057	1241	1168
Improvement	8.8%	11.3%	10.5%	9.4%

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

- CP2K-UK project exists to support and grow the CP2K user community - how can you get involved?
  - Let us know what support you need
    - Via discussion session & feedback forms, or ad hoc
    - Provide support visits to individuals & groups
  - Contribute to the CP2K website / wiki
  - Join the CP2K discussion forum
    - http://groups.google.com/group/cp2k
  - Present at next year's user meeting



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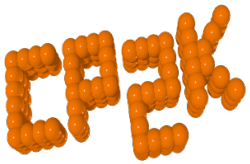
Community Involvement

- 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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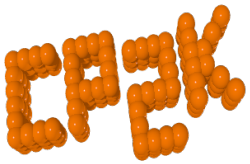
Summary

- CP2K-UK exists to support your research using CP2K!
- Aim to improve confidence and competence in the user community
- User engagement and feedback is key
- Opportunity to get bespoke support for new development projects within your group
  - Support requests to i.bethune@epcc.ed.ac.uk



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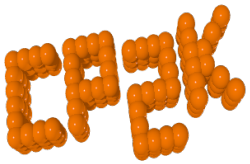
Acknowledgements

- EPSRC (EP/K038583/1)

EPSRC
Engineering and Physical Sciences Research Council

- Joost VandeVondele & Jürg Hutter
- Lev Kantorovich, Ben Slater & Matt Watkins
- Jochen Blumberger, Patricia Hunt, Jorge Kohanoff, Angelos Michaelides, Philip Moriarty, Carole Morrison, Alex Shluger & Michiel Sprik



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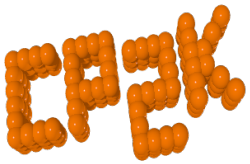
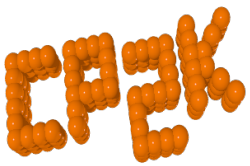
Any questions?





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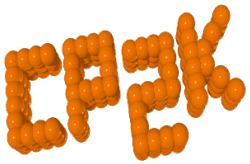
Lightning talks

- 3 minute summaries of research using CP2K:
  - Razak El-Maslmane, University of York
  - Dibyajyoti Ghosh, University of Bath
  - Nico Holmberg, Aalto University
  - Zheng Jiang, University of Southampton
  - Sanliang Ling, University College London
  - Fiona Reid, EPCC
  - Guido Falk von Rudorff, University College London



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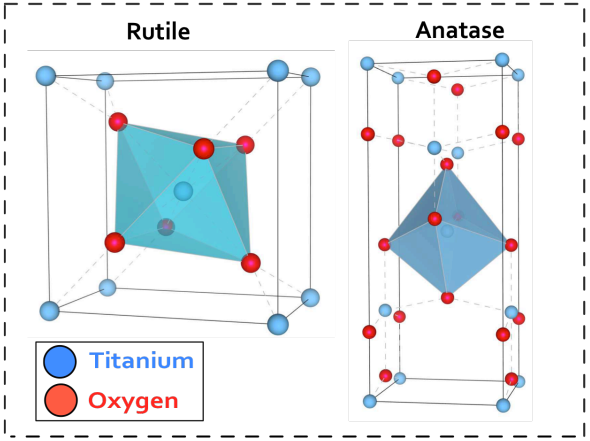
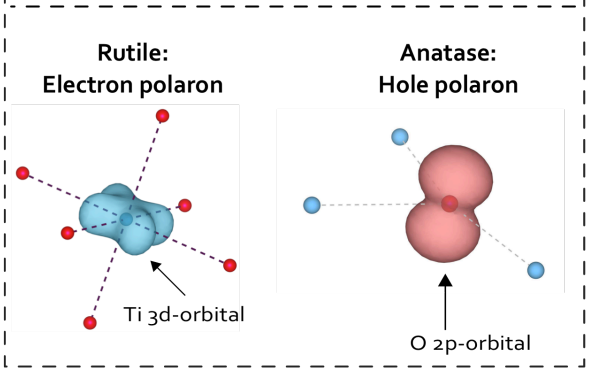
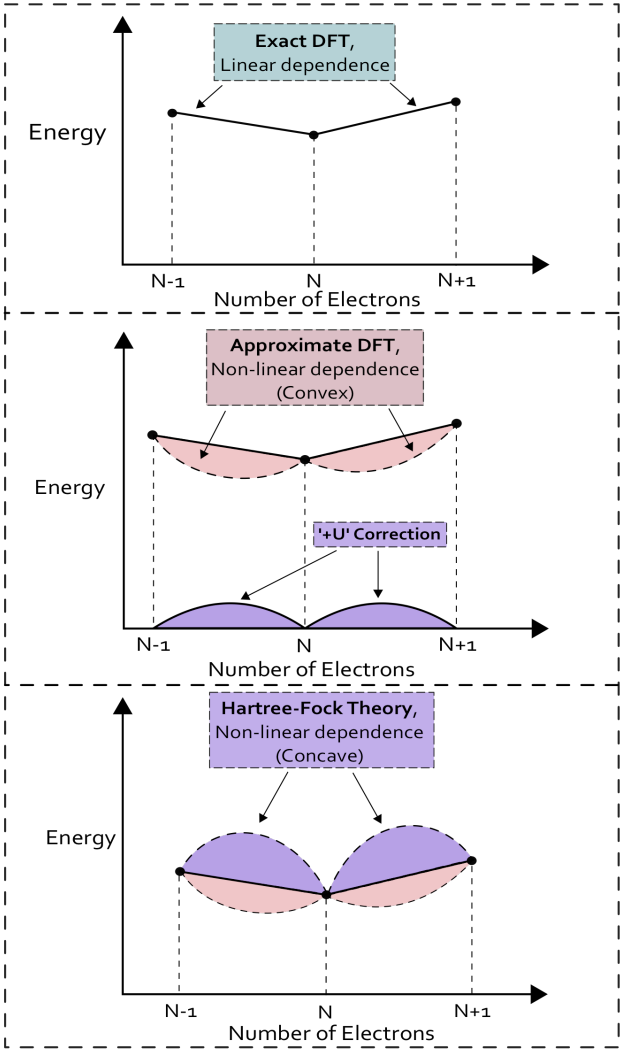
Charge Trapping in Bulk TiO_2
Rutile and Anatase

Me: **Razak Elmaslmane**
Supervisor: **Keith McKenna**
University of York







DFT+U (VASP)

Rutile (N+1 Electrons)	Anatase (N-1 Electrons)
Conduction Band	Conduction Band
0.5 eV	1.6 eV
2.1 eV	2.3 eV
Valence Band	Valence Band
$U\{Ti_{3d}\}=2.80$	$U\{Ti_{3d}\}=2.30$
$U\{O_{2p}\}=4.70$	$U\{O_{2p}\}=3.85$

Hybrid DFT (CP2K)

Rutile (N+1 Electrons)	Anatase (N-1 Electrons)
Conduction Band	Conduction Band
0.5 eV	1.4 eV
2.9 eV	3.1 eV
Valence Band	Valence Band
a = 0.125	a = 0.125

Finite size effects not (yet) considered for hybrid DFT results

Bulk TiO_2 Modifications

DFT+U → Non-linearity changes dramatically

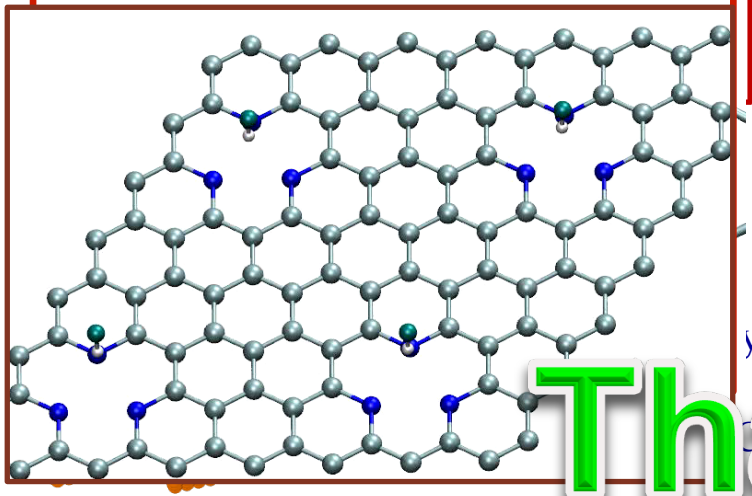
Hybrid DFT → Non-linearity changes very little

BOMD, CP2K and Me

Trapping Gaseous Pollutants on Defective Graphene Sheet

Selective trapping

Increased trapping capacity



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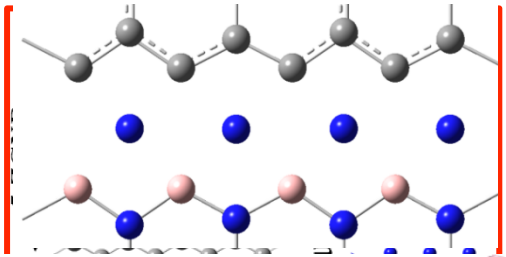
Dibyajyoti Ghosh

Line Defects at the Heterojunction of Hybrid Boron Nitride/Graphene Nanoribbons



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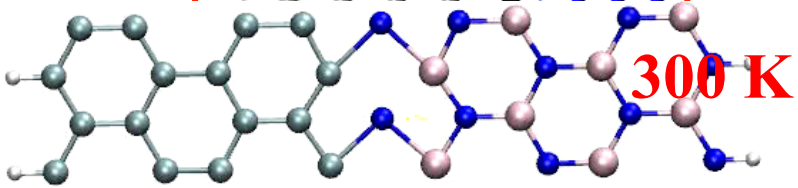

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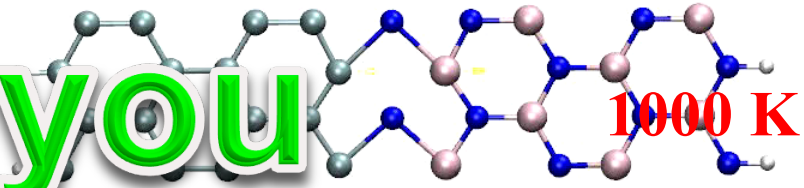
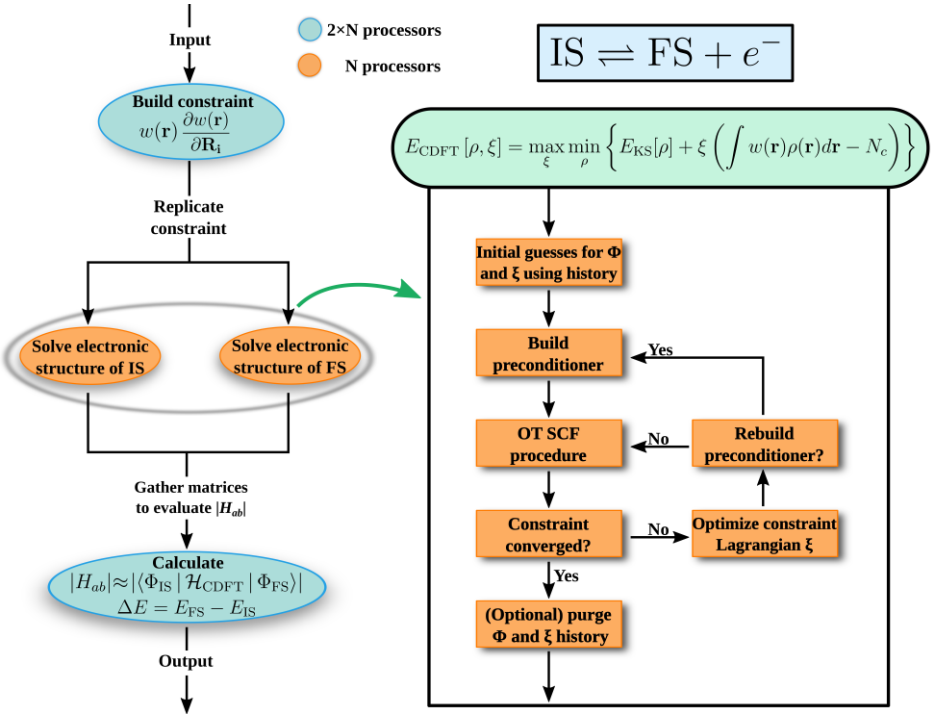


Thank you

Efficient constrained DFT implementation for condensed phase electron transfer MD simulations[1]

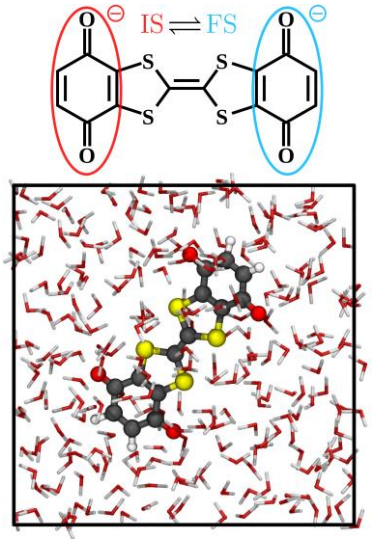
Nico Holmberg, Aalto University, nico.holmberg@aalto.fi

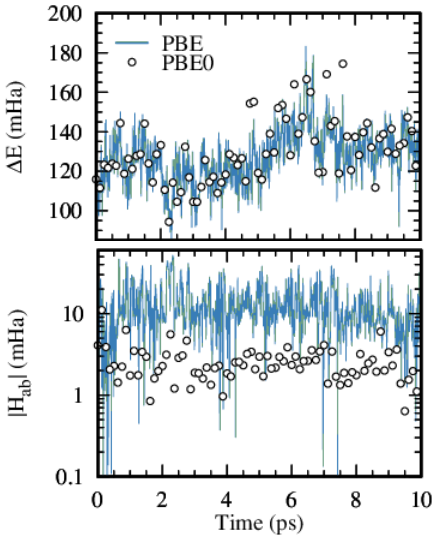


Code not yet in trunk, but available at
https://github.com/nholmber/cp2k-cdft-dev

Electron transfer (ET) parameters directly from two-state MD simulations with explicit solvent

Example: Intramolecular ET in QTTFQ$^-$ (258 water, 12 ps total, 0.5 fs step, 384 MPI cores)



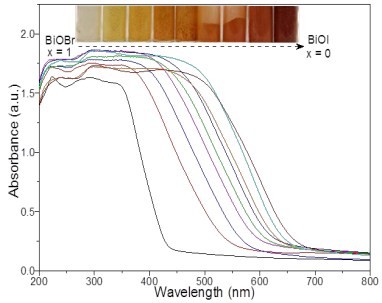


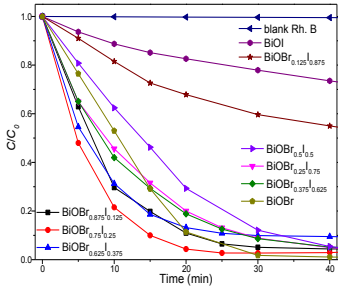
Aalto University
School of Chemical Engineering
CSC
ACADEMY OF FINLAND

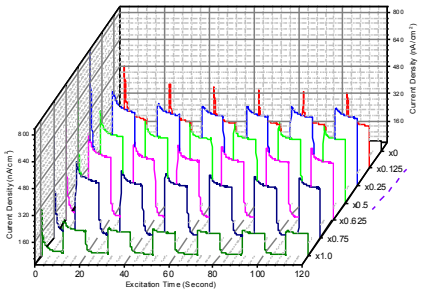
1. Holmberg, N.; Laasonen, K.; *J. Chem. Theory Comput.*, Just Accepted Manuscript, DOI: 10.1021/acs.jctc.6b01085

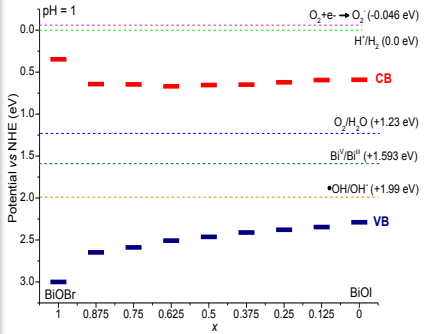
Origin of the Enhanced Photoelectrocatalytic performance of $BiOBr_xI_{1-x}$

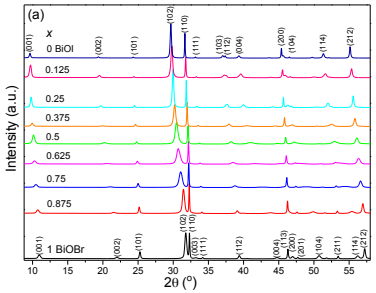
Zheng Jiang, University of Southampton (z.jiang@soton.ac.uk)

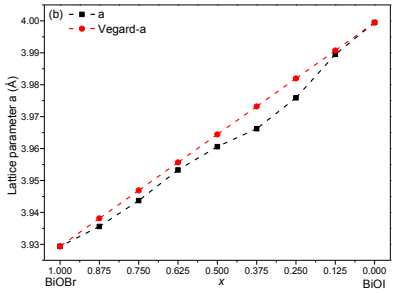


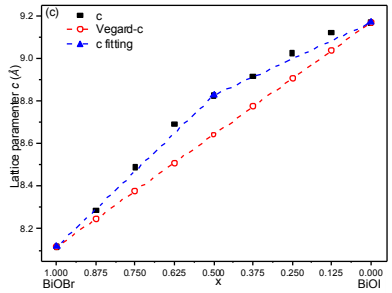


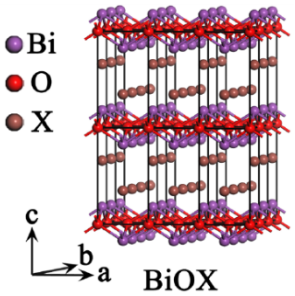


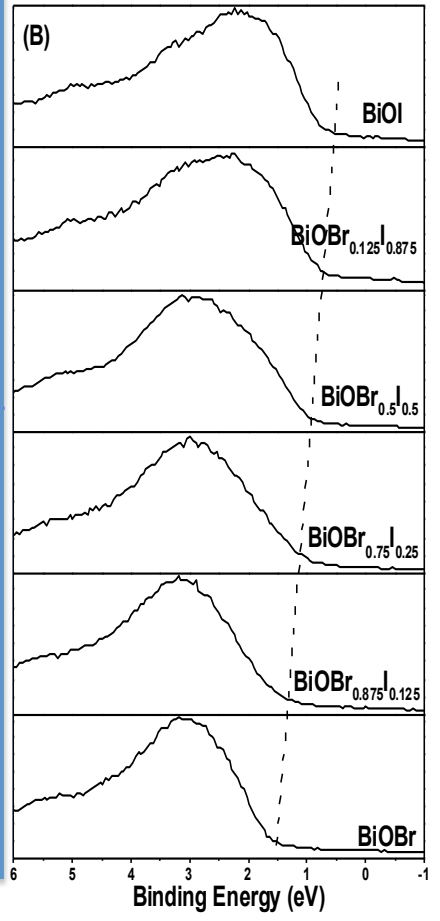


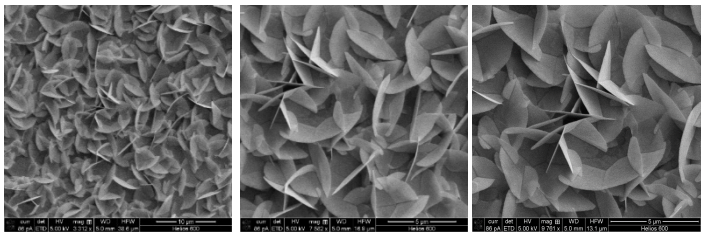


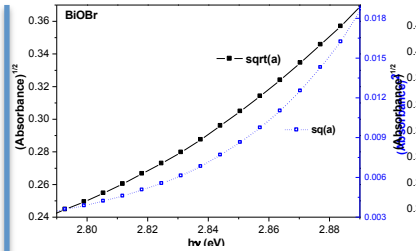


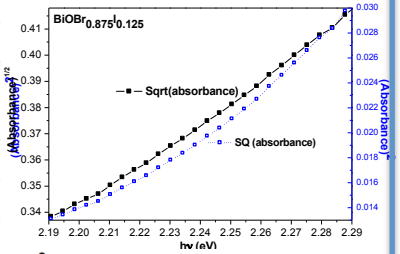


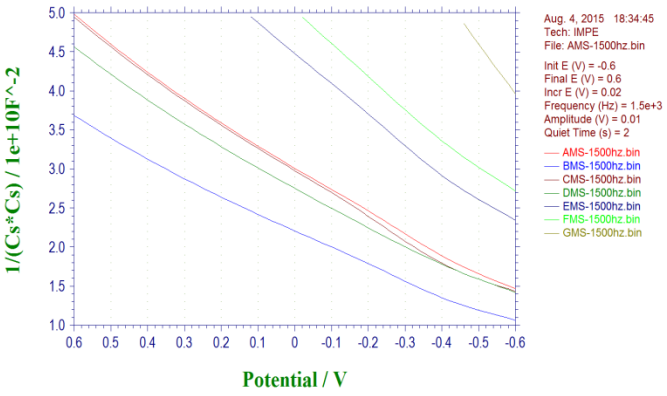


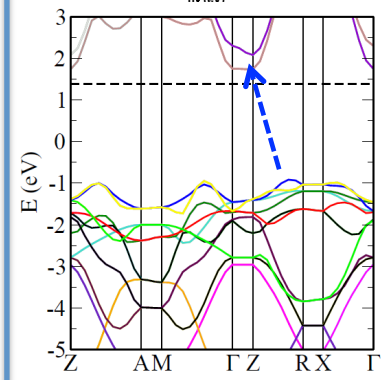


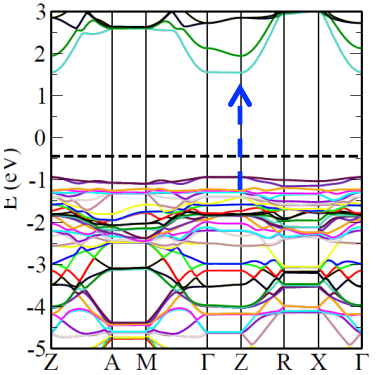








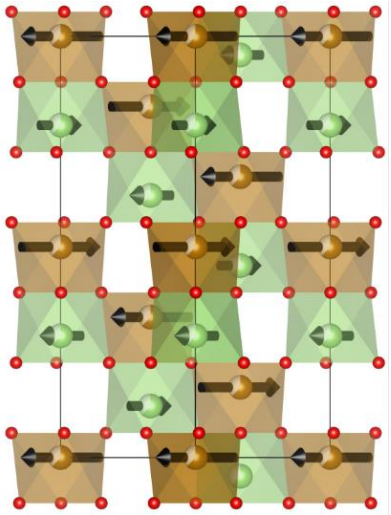




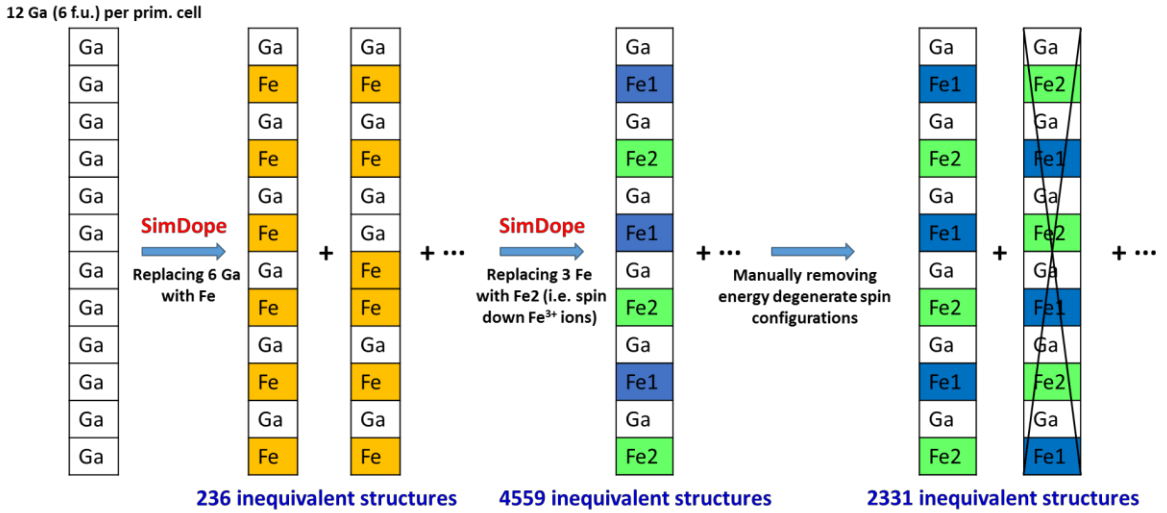
Using HSE06 XC functional, Norm Cons Pot.

Computational Study of Multiferroic Materials Using CP2K

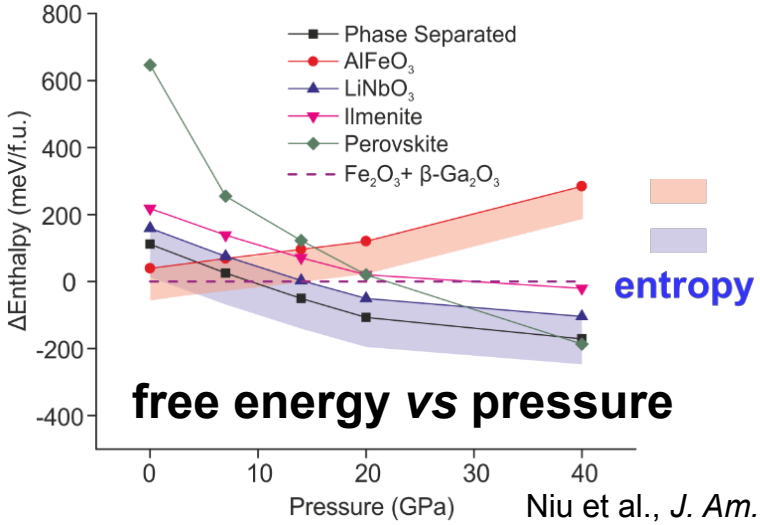
Sanliang Ling, Ben Slater, Furio Cora (UCL Chemistry)

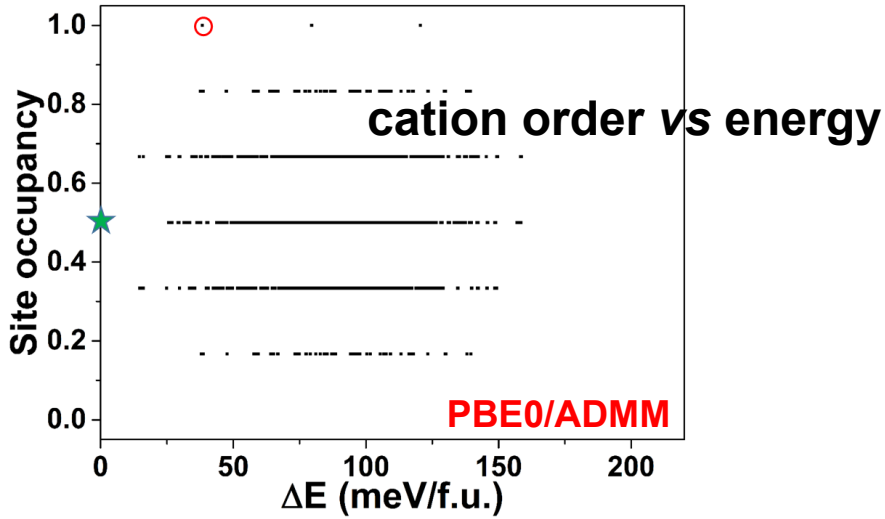


Corundum $ScFeO_3/GaFeO_3$

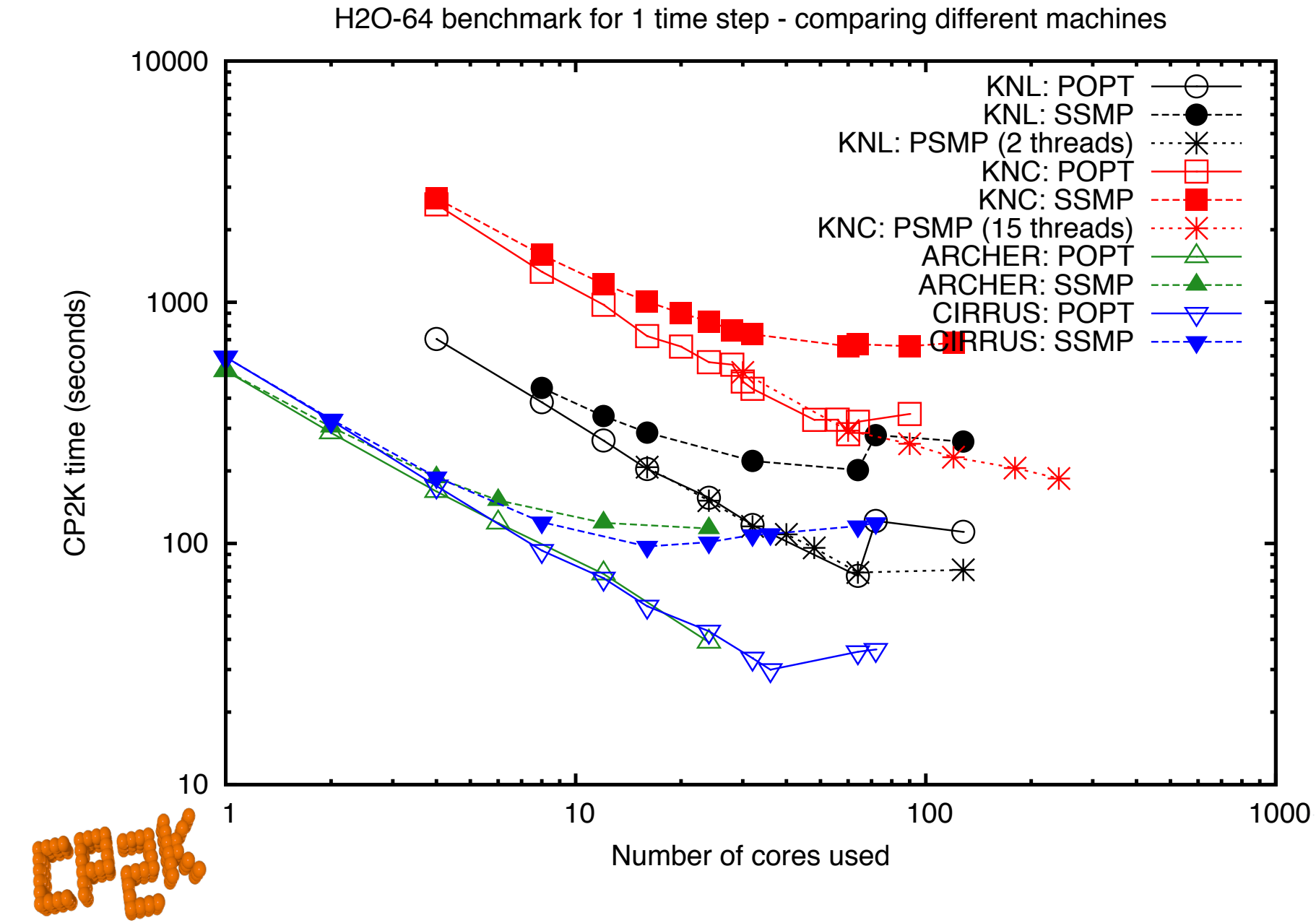


What are the most stable cation and spin distributions?





Niu et al., *J. Am. Chem. Soc.*, 2017, DOI: 10.1021/jacs.6b11128 (in collaboration with Liverpool)


H2O-64 benchmark for 1 time step - comparing different machines
CP2K time (seconds)
Number of cores used
10000
1000
100
10
1
10
100
1000
KNL: POPT
KNL: SSMP
KNL: PSMP (2 threads)
KNC: POPT
KNC: SSMP
KNC: PSMP (15 threads)
ARCHER: POPT
ARCHER: SSMP
CIRRUS: POPT
CIRRUS: SSMP

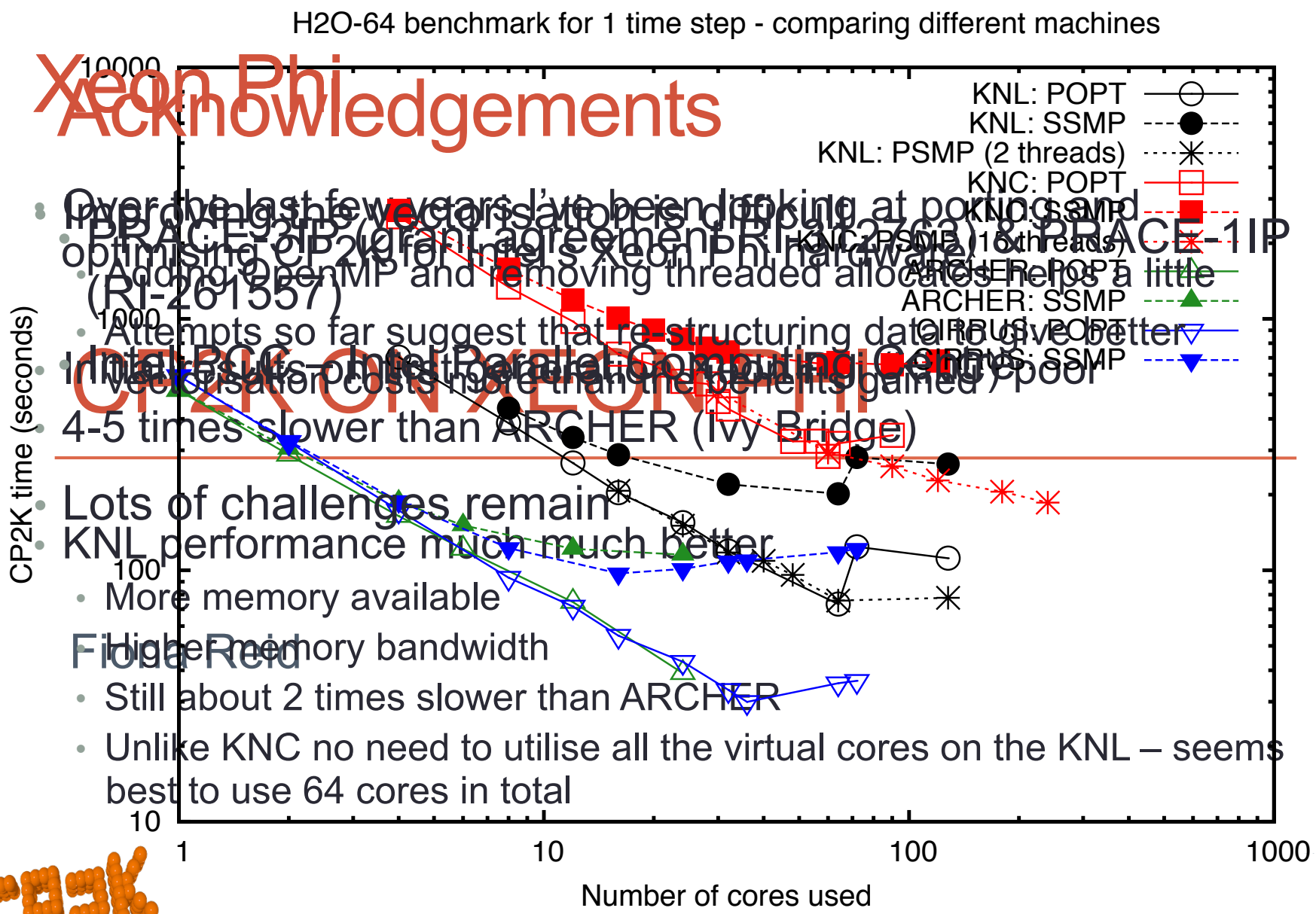
Xeon Phi

Acknowledgements

- Improving the vectorisation is difficult
- PRACE-3IP (grant agreement RI-312763) & PRACE-1IP (RI-261557)
- Initial results – Intel Parallel Computing Centre

CP2K ON XEON PHI

- Over the last few years I've been looking at porting and optimising CP2K for Intel's Xeon Phi hardware
  - Adding OpenMP and removing threaded allocates helps a little
  - Attempts so far suggest that re-structuring data to give better vectorisation costs more than the benefits gained
- 4-5 times slower than ARCHER (Ivy Bridge)
- Lots of challenges remain
- KNL performance much much better
  - More memory available
  - Higher memory bandwidth
  - Still about 2 times slower than ARCHER
  - Unlike KNC no need to utilise all the virtual cores on the KNL – seems best to use 64 cores in total



Fiona Reid

Faster HFX forces in MD runs

$$E_X^{HF} = -\frac{1}{2}\sum_{\lambda\sigma\mu\nu}\left[\sum_i C_{\mu i}C_{\sigma i}\right]\left[\sum_j C_{\nu j}C_{\lambda j}\right]\int d\mathbf{r_1}\int d\mathbf{r_2}\frac{\phi_\mu(\mathbf{r_1})\phi_\nu(\mathbf{r_1})\cdot\phi_\lambda(\mathbf{r_2})\phi_\sigma(\mathbf{r_2})}{|\mathbf{r_2}-\mathbf{r_1}|}$$

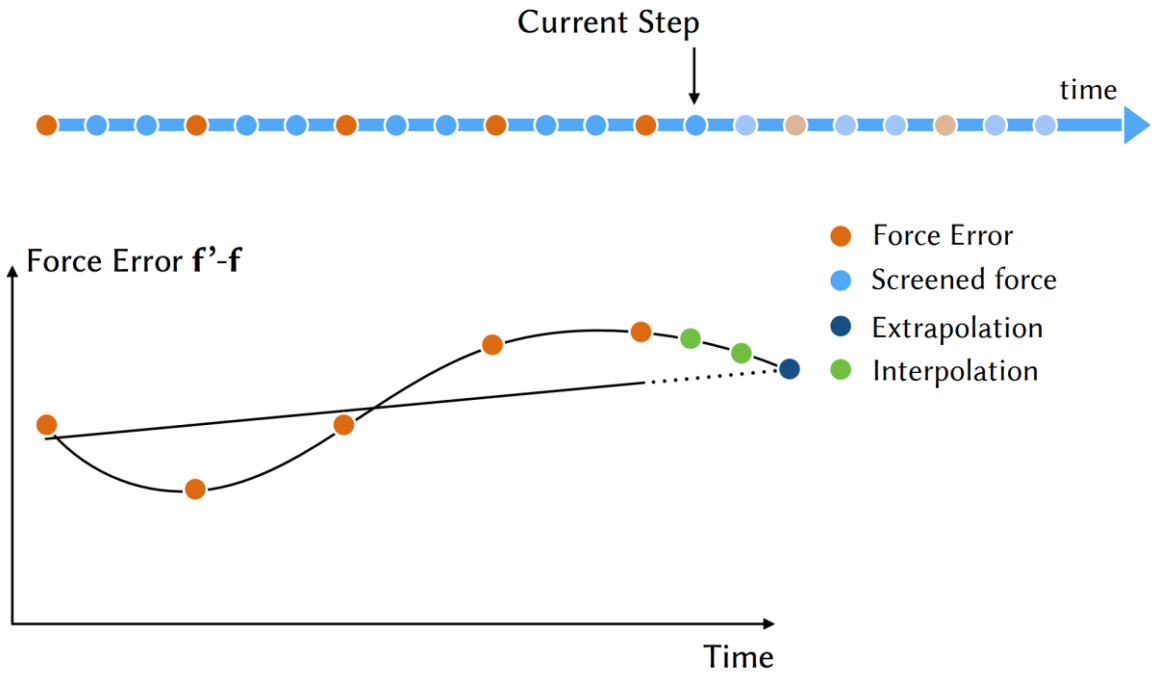
Atomic Orbital Basis

Density Matrix Components

Electron-repulsion integrals (ERI)

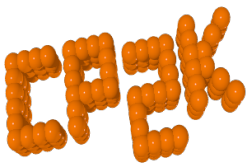
$|\mathbf{F}| > 10^{-3}$: 10^2 per atom

$|\mathbf{F}| < 10^{-9}$: 10^6 per atom



Speed-up:

CoO: 3.0x
FeO: 2.4x



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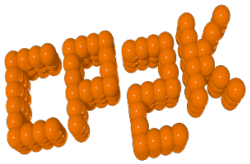
Discussion session

- Suggested topics:
  - CP2K Development projects (Jürg)
  - Getting started with CP2K / Usability (Iain)
  - Hybrid Functional Calculations (Ben & Sanliang)
  - TDDFT (Matt & Sergey)
  - Others?

- What could the CP2K-UK project do in the next year that would give the most help to your research?



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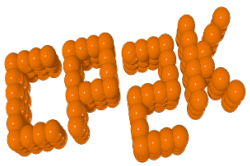

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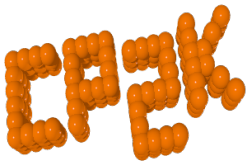
Summary

- Thank *you* very much for coming
- Thanks to all our our speakers
- Please complete feedback forms and return them before you leave
- See you again next year!



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