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CP2K-UK 5th Annual User Meeting

Welcome & Project Update

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@ibethune @CP2Kproject

Introduction

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

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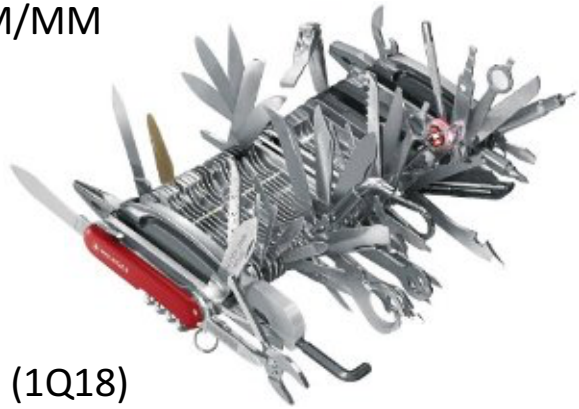
Background: CP2K-UK

- 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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Support for Users

- Training Events
  - Annual User Group Meetings
  - CP2K User Tutorial 2017
    - 3 day workshop at Zurich
    - CP2K-UK travel funding
  - All CP2K events at www.cp2k.org/news
    - Growing archive of lecture, example material: www.cp2k.org/docs#workshops
  - Also notification by email
  - Planning CP2K Summer School 2017

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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, Cambridge …
  - Training days / group visits
  - Debugging
  - Adding functionality
    - Merging in user contributions (OPLS torsions, CDFT…)
  - 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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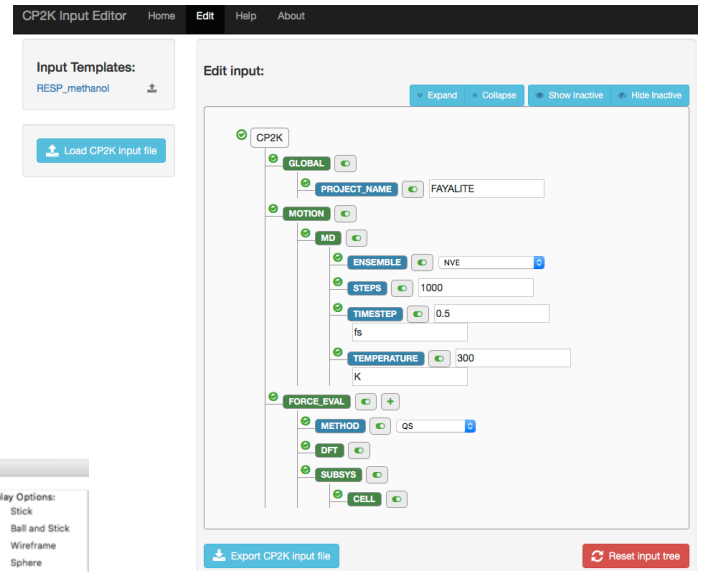
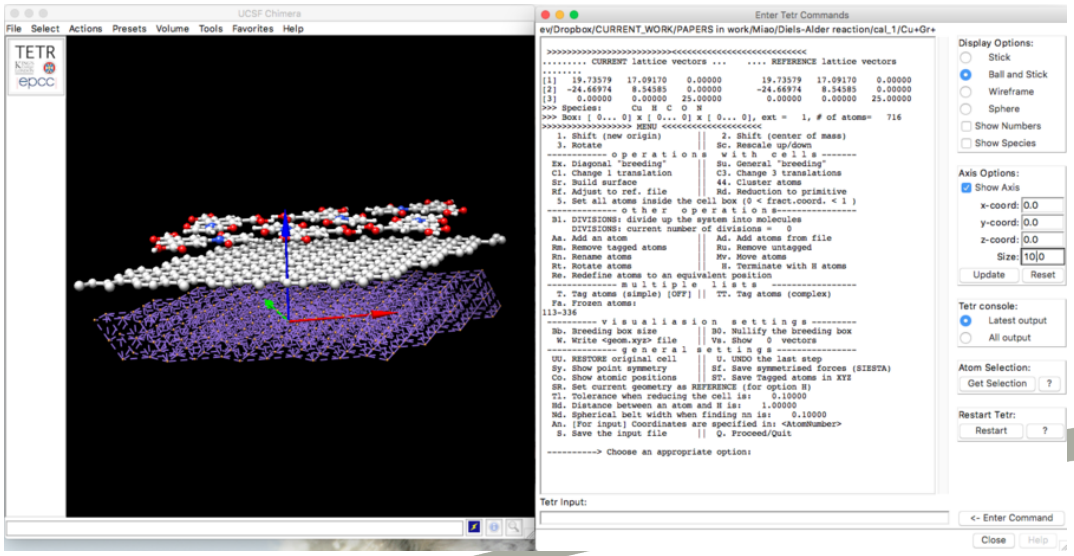
Support for Users

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

- Tools & Usability
  - Feedback from tutorials:
    - building an input is hard!
  - CP2K input GUI
  - USCF Chimera plugins for TETR and LEV00





https://www.cp2k.org/tools:tetr

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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 / toolchain
  - Vibrational Initialisation for MD (West & Estreicher, 2006, PRL)

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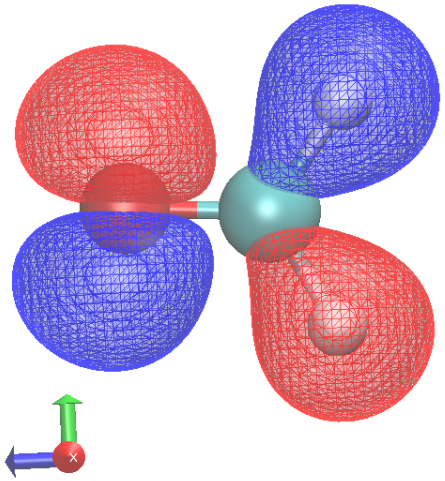
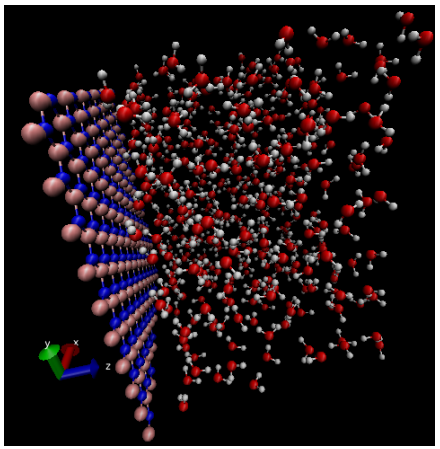
Support for Developers



- External funding
  - Three 12 month funded projects from ARCHER eCSE
  - LR-TDDFT with Hybrid Functionals/ADMM (2015-2016)
    - 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 (2016-2017)
  - CP2K performance improvements (2015-2017)
    - 3.6x speedup for GAPW calculations
    - 10% speedup and GBs memory saving for load-imbalanced systems



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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 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 future user meetings

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Community Involvement

- Interested in contributing to development?
  - ARCHER eCSE is now closed… but opportunities from PRACE, EPSRC…
    - 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/K038583/2) 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 iain.bethune@stfc.ac.uk

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Acknowledgements

- EPSRC (EP/K038583/2)

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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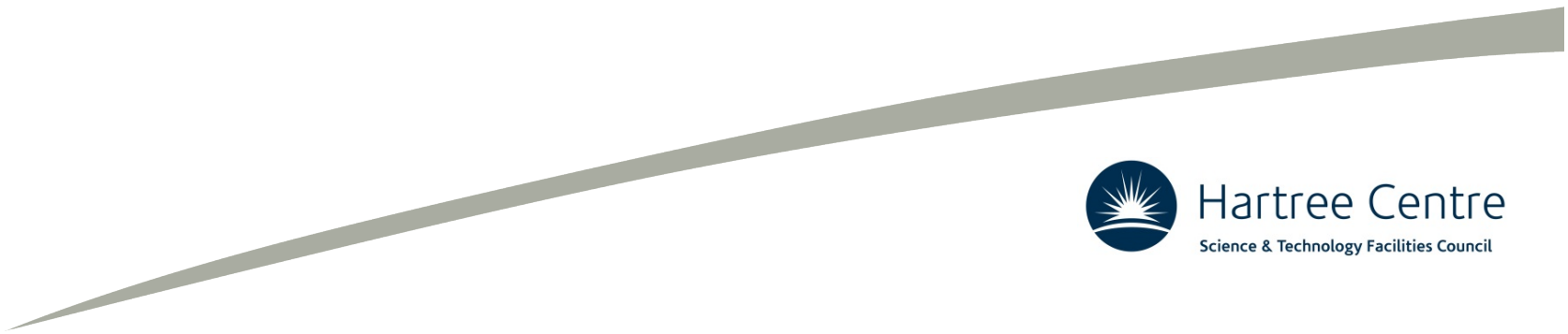

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Lightning talks

- 3 minute summaries of research using CP2K:
  - Stephen Cox, University of Cambridge
  - Matthew Krzystyniak, STFC
  - David Benoit, University of Hull
  - Natalia Martsinovich, University of Sheffield

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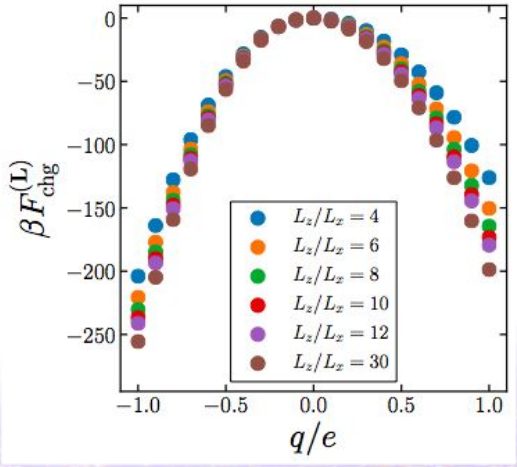
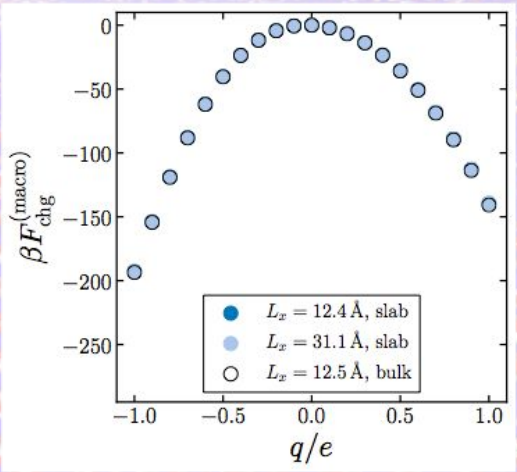
Interfacial ion solvation: Obtaining the thermodynamic limit from molecular simulations

- Potential future user of CP2K.
- Using the constant *D* ensemble to probe the statistical mechanics of electrolyte solutions.
- Hoping to investigate acidity of liquid/solid interfaces in future [see e.g. Zhang & Sprik, PRB **94**, 245309 (2016) and Sayer, Zhang Sprik JCP **147**, 104702 (2017)].
- Recent work on finite size effects in slab geometry…
- **Cox and Geissler arXiv:1801.00810 (2018).**





simple finite size correction.

related to polarization fluct's/response at interface.

disambiguates contributions of surface potential in solvation.

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'Electron-volt Neutron Spectroscopy: One Atom at a Time'

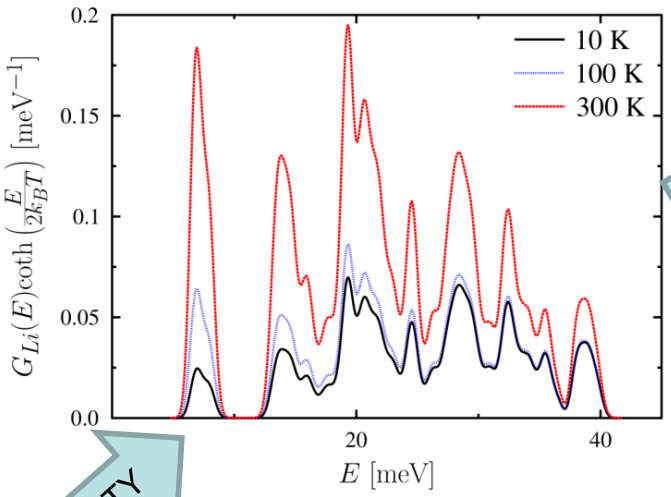
Matthew Krzystyniak

ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK

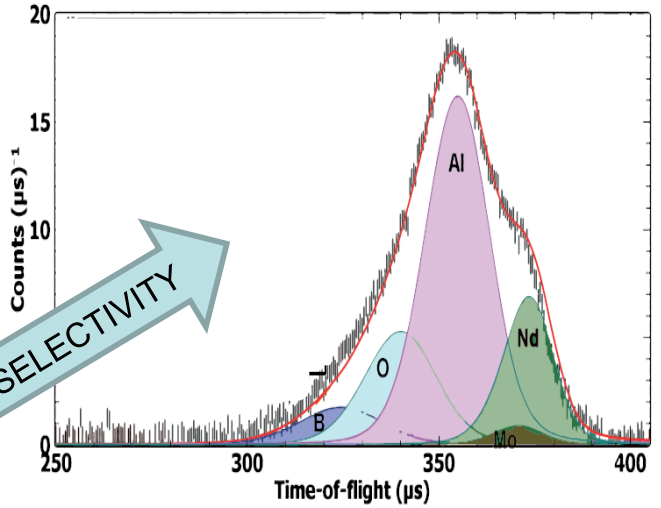
Mass-selective neutron Compton spectroscopy

No coupling constant weighting as PVDOS and cross section are separate parameters!

In many respects, an ultimate ab initio benchmarking tool!



MASS SELECTIVITY

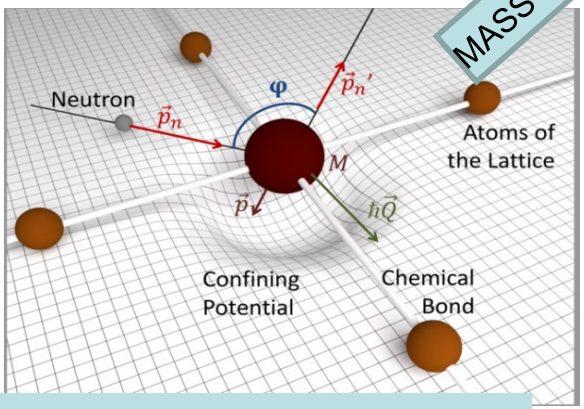


MASS SELECTIVITY

$$width\_M^2 \sim \int_0^\infty E \cdot G_M(E) \cdot coth\left[\frac{E}{2kT}\right] \cdot dE$$

first moment of the pVDOS!

$$partial\ VDOS = G_M(E) \cdot E \cdot coth\left[\frac{E}{2kT}\right]$$



$E \gg$ *binding energy*

$Q \gg$ *inverse interatomic distance*

LD from DFT → BOMD → PIMD

Ab initio modelling difficulty axis

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ISIS

E.A. Milne Centre for Astrophysics

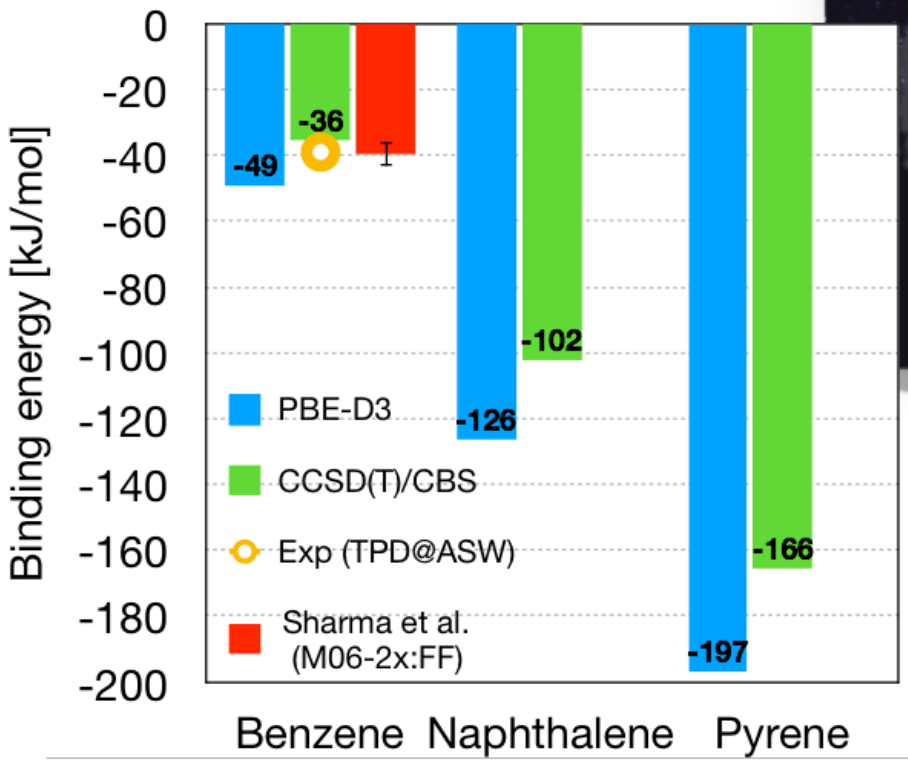
VIPER Transforming Research

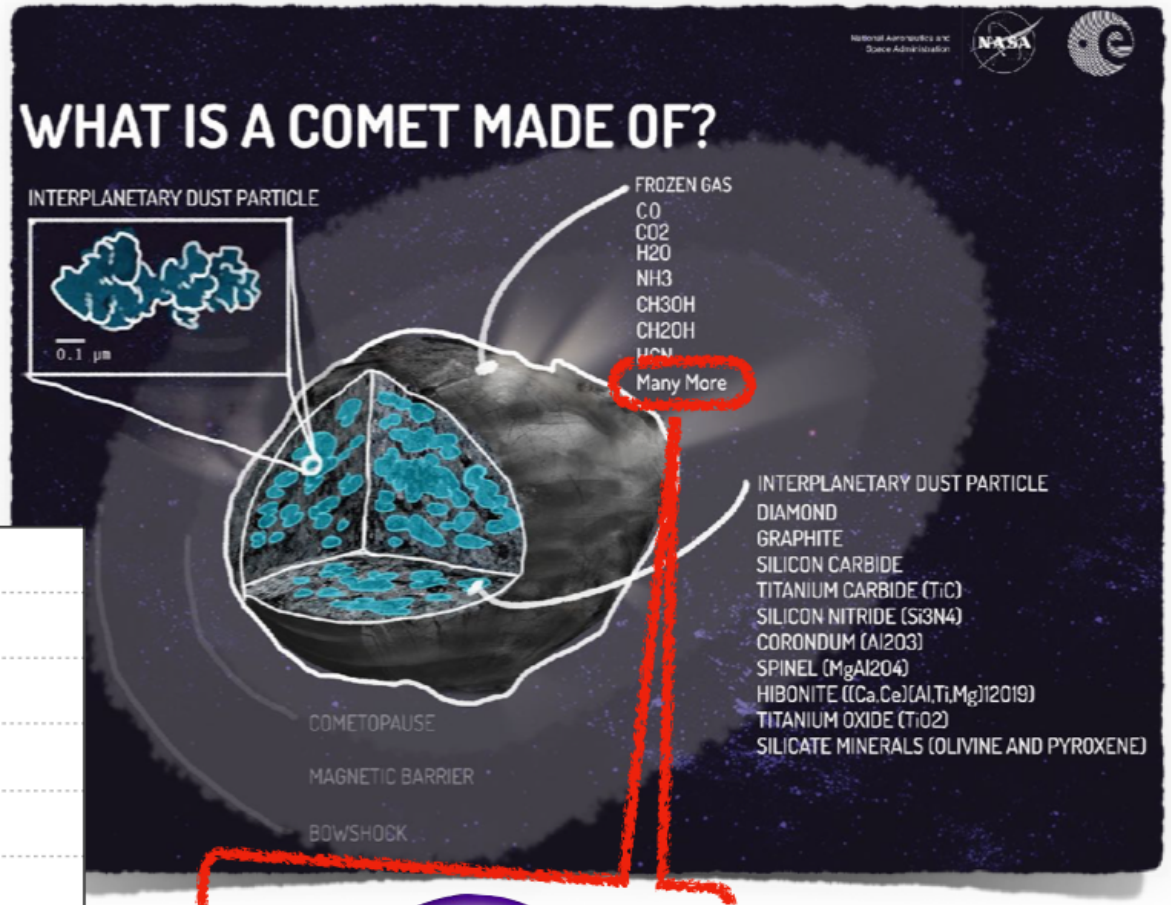
PVSCF

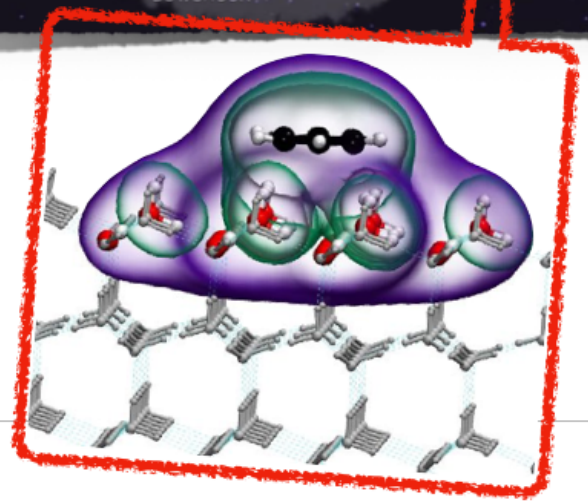
UNIVERSITY OF HULL

Dusty Interstellar Ices

- Do large carbon-rich molecules stick to ice?
- What is their vibrational signal?







900 atoms,
2300 electrons,
PBE-D3/
MOLOPT-TZV2P

David Benoit

Photocatalytic TiO_2/graphene-based charge-transfer interfaces

Peter Gillespie, Natalia Martsinovich
Department of Chemistry, University of Sheffield

The University Of Sheffield.

Research question: Explain the high efficiency of TiO2/reduced graphene oxide photocatalysts

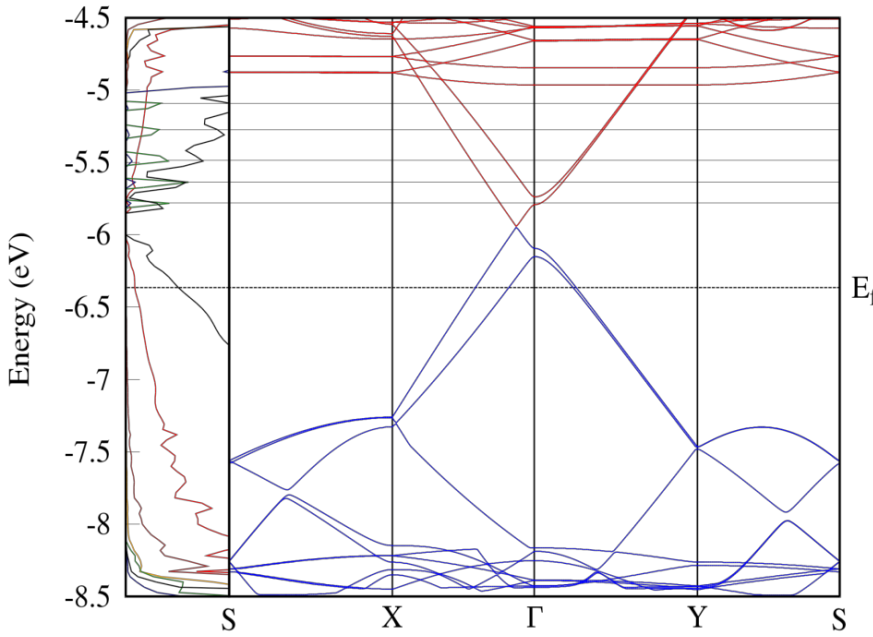
Computational challenges:

- Commensurability => large systems : 180 atoms TiO_2 + 72 atoms C
- Need hybrid functionals to describe TiO_2
- Need dense k-point grid to describe graphene

Our approach:

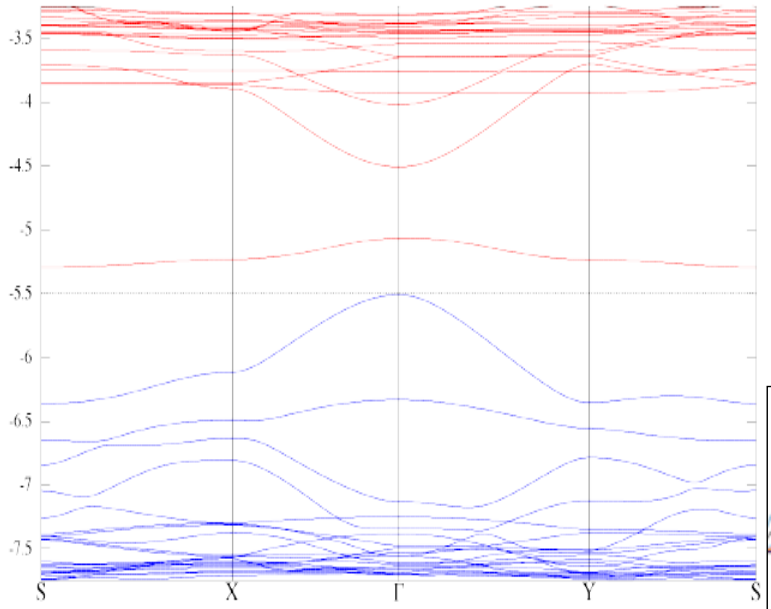
- Geometry optimisation using CP2K (first PBE, then HSE06 using ADMM)
- Electronic structure analysis using CRYSTAL

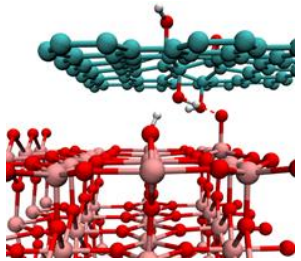
1. TiO_2 (rutile)/graphene



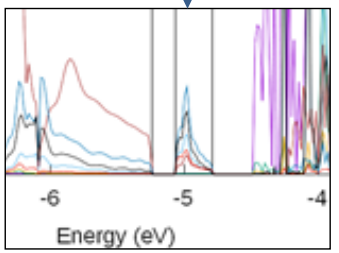
2. TiO_2 (rutile)/reduced graphene oxide (RGO)

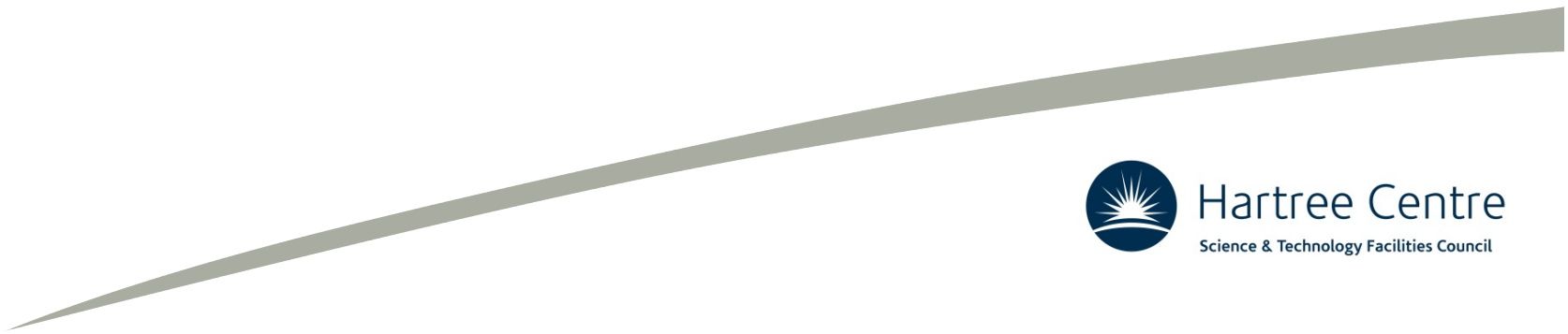
RGO model: C:O ratio =12:1;
4 OH, 2 epoxy groups





DOS





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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 (maybe)!

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