



Computational Molecular Science

2019

Warwick, 27-29 March 2019

Organisers:

Dr. G.C.Sosso & Dr. R.J. Maurer

27-29 March 2019
University of Warwick, UK

The Computational Molecular Science (CMS) meeting has been running for more than a decade, and on this occasion will feature five sessions encompassing a diverse array of disciplines, from machine learning to simulations of soft and biological matter, from quantum chemistry methods to energy materials and interfaces.

- **Session 1:** *Simulations of Soft and Biological Matter*. Keynote speaker: Adrian Mulholland (The University of Bristol, UK)
- **Session 2:** *Density Functional Theory - Methods and Applications*. Keynote speaker: Kieron Burke (The University of California - Irvine, USA)
- **Session 3:** *Energy Materials and Interfaces*. Keynote speaker: Giulia Galli (The University of Chicago, USA)
- **Session 4:** *Advances in Quantum Chemistry*. Keynote speaker: Frank Neese (MPI Kohlenforschung, DE)
- **Session 5:** *Machine Learning*. Keynote speaker: Alexandre Tkatchenko (The University of Luxembourg, LU)
- **Future Perspectives:** Alessandro Troisi (The University of Liverpool, UK)

Computational
Molecular
Science

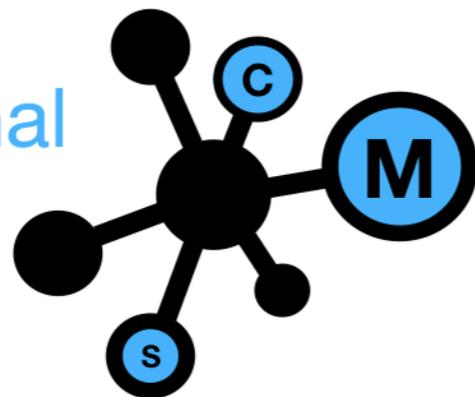


Table of contents

- Page 2. Important information
- Page 3. Campus map
- Page 4. Programme
- Pages 5-6. Session 1: *Simulations of Soft and Biological Matter*
- Pages 7-9. Session 2: *DFT - Methods and Applications*
- Pages 10-11. Session 3: *Energy Materials and Interfaces*
- Pages 12-14. Session 4: *Advanced Quantum Chemistry*
- Pages 15-16. Session 5: *Machine Learning*
- Page 16. *Future perspectives*.
- Pages 18-58. Poster abstracts
- Pages 59,60. Participants list
- Page 61. Sponsors

Organisers:

Dr. Gabriele C. Sosso : g.sosso@warwick.ac.uk
Dr. Reinhard J. Maurer : r.maurer@warwick.ac.uk

Important information

Arrival:

- Travel directions to the University of Warwick can be found at: https://warwick.ac.uk/fac/sci/chemistry/news/events/cms2019/how_to_get_there/
- An interactive map of the Warwick campus can be found at: <https://warwick.ac.uk/about/visiting/maps/interactive/>
- If traveling by car, please do register for your car parking permit at: <https://carparking.warwick.ac.uk/events/cms-2019> - **until March 20th** at the very latest.
- Upon arrival, please report to the registration desk.
 - If arriving on March 26th, the registration desk will be located in the Students' Union building, ground floor (see map on the next page) from 15:00 to 18:30.
 - If arriving on March 27th or later, the registration desk will be located in the Oculus building, ground floor (see map on the next page) from 8:30 to 9:30.
- On Tuesday 27th at 18:30 there will be a welcome reception at the Dirty Duck (see map on the next page) with dinner and drinks.

Accommodation:

- Your room will be located in the Arthur Vick Hall (see map on the next page). You will be provided with a key or key card which will give you access to your bedroom and entry door to the accommodation block.
- Bedroom keys will be available to collect from 15:00 to 21:45 at the Conference Reception (a dedicated stand located in the Students' Union building).
- If you plan to arrive after 21.45, please contact Conference Reception to arrange late key collection wcpreception@warwick.ac.uk or +44(0)2476 528910.
- The location of key collection after 21:45 is from the Gatehouse ([see the interactive campus map](#)).
- Bedrooms are to be vacated by 09:30 on your day of departure. Luggage and belongings should be removed by that time. If required luggage can be stored in the Left Luggage facility in Conference Reception until departure.
- On the day of departure, keys can be left at Conference Reception (in the Students Union building), Rootes Restaurant (in Rootes Building) or one of the boxes situated in the entrance hall of each accommodation block.

Dietary requirements:

- Every meal offers a vegetarian option. We would be happy to accommodate any particular dietary requirement: in order to do so, please do let us know (by emailing the organisers) **until March 11th** at the very latest.

Meals:

Breakfast will be served on March 27th, 28th and 29th from 7:00 to 9:00 in the Rootes Restaurant (Rootes building, see map on the next page). Refer to the programme [page 5 of this booklet] for the location where lunch and dinner will be served on each day.

Posters:

Each poster contribution has been numbered within this booklet. Please do position your poster (A0 format, portrait) on your (numbered) board on March 27th any time before the start of the poster session (19:30 of the same day) - in the Oculus building, 1st floor. Posters should be taken off on March 28th - afternoon, until 16:00 at the very latest.

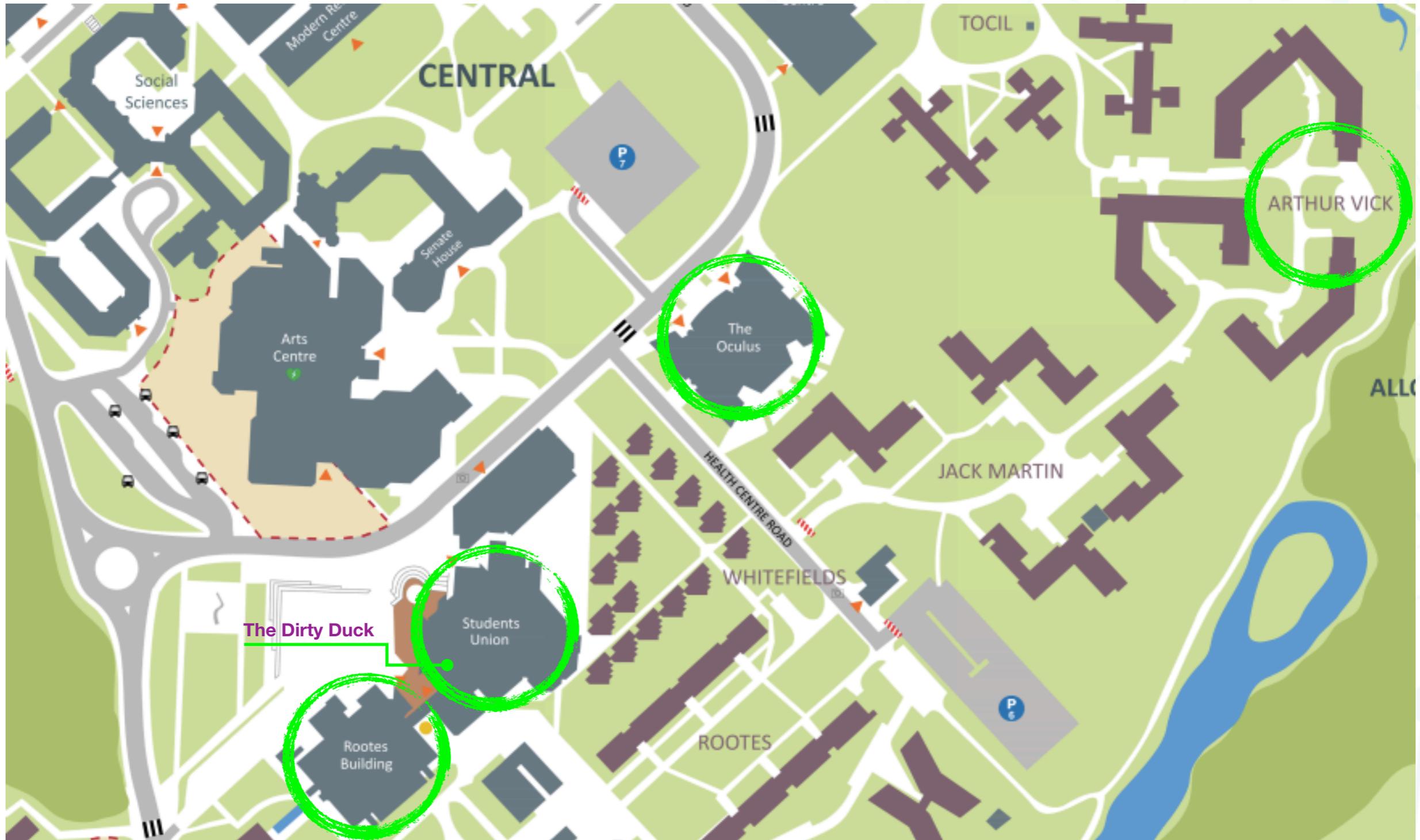
Community board:

Close to the registration desk, you will find a community board where you can put forward job ads, conferences/meetings/workshops announcements, mailing lists, software, and broadly speaking anything of relevance to the computational molecular science community. Feel free to send to the organisers some material beforehand - you are also very welcome to contribute to said board at any time during the meeting.

If in doubt:

If you have any questions and/or if you would be in need of anything at all, please report to the registration desk or get in touch with the organisers.

Campus map (<https://warwick.ac.uk/about/visiting/maps/interactive/>)



Programme

Tuesday 26 March

- 15:00 – 18:30
Registration (Student Union Building)
- 18:30 - 22.00
Dinner & Drinks (at the Dirty Duck - Students Union building)

Day 1 - Wednesday 27 March

- 8.50 - 9.00
Opening Remarks
- Session 1: Simulations of Soft and Biological Matter**

Chaired by Rebecca Notman

- 9.00 - 10.00
Keynote Lecture: Adrian Mulholland
- 10.00 - 10.30
Invited Speaker: Christine Peter
- 10.30 - 11.00
Coffee break
- 11.00 - 11.30
Invited Speaker: Andela Saric
- 11.30 - 12.00
Invited Speaker: Michele Vendruscolo
- 12.00 - 12.20
Contributed talk: Stefano Serapian
- 12.30 - 14.00
Lunch [Rootes restaurant - Rootes Building, 1st floor]

Session 2: DFT - Methods & Applications

Chaired by Nicholas Hine

- 14.00 - 15.00
Keynote Lecture: Kieron Burke
- 15.00 - 15.30
Invited Speaker: Aron Walsh
- 15.30 - 16.00
Coffee break
- 16.00 - 16.30
Invited Speaker: David O'Regan
- 16.30 - 17.00
Invited Speaker: Chris Skylaris

- 17.00 - 17.20
Contributed talk: Elizaveta Suturina
- 17.20 - 17.40
Contributed talk: Micaela Matta
- 17.40 - 18.10
Session 1 – reprise! Invited Speaker: Syma Khalid
- 18.30 - 19.30
Dinner & drinks (buffet) [Oculus building]
- 19.30 - 22.00
Poster session & drinks [Oculus building, 1st floor]

Day 2 - Thursday 28 March

Session 3: Energy Materials and Interfaces

Chaired by David Quigley

- 9.00 - 10.00
Keynote Lecture: Giulia Galli
- 10.00 - 10.30
Invited Speaker: Mariana Rossi
- 10.30 - 11.00
Coffee break
- 11.00 - 11.30
Invited Speaker: Fernanda Duarte
- 11.30 - 12.00
Invited Speaker: Livia Bartok-Partay
- 12.00 - 12.30
Invited Speaker: Aaron Kelly
- 12.30 - 14.00
Lunch [Rootes restaurant - Rootes Building, 1st floor]

Session 4: Advanced Quantum Chemistry

Chaired by Scott Habershon

- 14.00 - 15.00
Keynote Lecture: Frank Neese
- 15.00 - 15.30
Invited Speaker: Felix Plasser
- 15.30 - 16.00
Coffee break
- 16.00 - 16.30
Invited Speaker: Fred Manby

- 16.30 - 17.00
Invited Speaker: Elena Besley
- 17.00 - 17.20
Contributed talk: Bora Karasulu
- 17.20 - 17.40
Contributed talk: Venkat Kapil
- 17.40 - 18.00
Contributed talk: Liam Wilbraham
- 19.30 - 22:00
Conference Dinner [The Chancellor Suite - Rootes Building, 2nd floor]
- 22:00 - 00:00
Drinks [Panorama Bar - Rootes Building, 2nd floor]

Day 3- Friday 29 March

Session 5: Machine Learning

Chaired by James Kermode

- 9.00 - 10:00
Keynote Lecture: Alexandre Tkatchenko
- 10.00 - 10.30
Invited Speaker: Christoph Ortner
- 10.30 - 11.00
Coffee break
- 11.00 - 11.30
Invited Speaker: Anatole von Lilienfeld
- 11.30 - 12.00
Invited Speaker: George Booth
- Future Perspectives**
- 12.00-13.00
Keynote Lecture: Alessandro Troisi
- 13.00 - 13.05
Closing Remarks
- 13.00 -14.00
Lunch [Rootes restaurant - Rootes Building, 1st floor]

Session 1: Simulations of Soft and Biological Matter

Prof. Adrian Mulholland
University of Bristol
adrian.Mulholland@bristol.ac.uk

Keynote Lecture, 9:00-10:00

Multiscale modelling of enzyme activity and inhibition for biocatalysis and drug development

Drug action is inherently a multiscale problem, connecting chemical changes at the molecular level with macroscopic biological changes [1]. Multiscale simulation methods have the potential to contribute to drug development by connecting models at different scales and to analyse the connections across scales, e.g. how changes on one scale lead to changes at another. Molecular simulation methods of various types are now capable of modelling processes ranging from biochemical reactions to membrane assembly, and offer increasing predictive power. Simulations can provide effective ‘computational assays’ of biological activity [2]. For example, classical molecular dynamics (MD) simulations can allow predictions of substrate binding, and reveal and predict dynamical changes associated with thermoadaptation and temperature optima of enzyme catalytic activity [3]. Increasingly, simulations are contributing to the design and engineering both of natural enzymes and of *de novo* biocatalysts [4]. Different types of application require different levels of treatment, which can be effectively combined in multiscale models to tackle a range of time- and length-scales, e.g. to study drug metabolism by cytochrome P450 enzymes [5], combining coarse-grained and atomistic molecular dynamics simulations, and combined mechanics/molecular mechanics (QM/MM) methods. QM/MM modelling can identify mechanisms of catalysis in biosynthesis and antibiotic resistance, for example [6]. Projector-based embedding techniques allow highly accurate correlated ab initio QM methods to be applied in QM/MM calculations [7]. Multiscale simulation schemes also now allow QM/MM methods to be applied to free energy simulations to study e.g. protein-ligand binding [8]. Together with enhanced sampling simulations, QM/MM methods can help identify causes of drug resistance e.g. to targeted covalent inhibitors such as the lung cancer drug osimertinib [9] and the mechanism-based β -lactamase inhibitor clavulanate [6].

References: [1] R.E. Amaro & A.J. Mulholland *Nature Reviews Chemistry* 2, 0148 (2018). [2] D.J. Huggins et al. *WIREs Computational Molecular Science* (2018) DOI: 10.1002/wcms.1393. [3] M.W. van der Kamp et al. *Nature Communications* 9, Article number: 1177 (2018). [4] J.R. Anderson et al., *Nature Communications* 8 358 (2017). [5] R. Lonsdale et al. *PLoS Comput Biol.* 10:e1003714 (2014). [6] R.A. Fritz et al. *Biochemistry* 57, 3560-3563 (2018). [7] X. Zhang et al. *Royal Soc. Open Sci.* 5,171390. (2018). [8] S. Halder et al. *J. Chem Theory Comput.* 14, 6093-6101 (2018). [9] D. Callegari et al. *Chemical Sci.* 9, 2740-2749 (2018)

Prof. Christine Peter
University of Konstanz
christine.peter@uni-konstanz.de

Invited Talk, 10:00-10:30

Scale-bridging in simulations of configurational landscapes of protein-protein interactions

Simulations have become an important complement to experimental structural biological approaches since they provide a molecular-level view on structural ensembles and dynamics of conformational transitions or aggregation processes on ns to ms timescales. In recent years, multiscale simulation methods that combine classical atomistic and coarse grained levels of resolution have gained popularity in the biomolecular simulation community. While the coarse grained level extends the accessible length and timescales compared to an all-atom model, a systematic link to an atomistic level of resolution allows to maintain information from a more accurate representation. In the talk I will present an example how such a multiresolution approach in combination with advanced analysis methods can be used to investigate and characterize the structural variability of multidomain proteins and protein conjugates. I will show how dimensionality reduction can be employed to characterize the sampling of free energy landscapes of such multidomain systems and to assess the consistency of the sampling in models at different levels of resolution. These methods are optimally suited to identify, compare, and classify relevant conformational states and to guide the interpretation of the simulations with respect to experimental data.

Dr. Andela Saric
University College London
a.saric@ucl.ac.uk

Invited Talk, 11:00-11:30

Minimal coarse-grained models for biological assembly

Protein assembly into reversible nano- and mesoscale aggregates generates the molecular machinery of life. When protein aggregation takes place in an uncontrolled and irreversible manner, however, severe pathologies can occur, such as neurodegenerative diseases. Due to their multiscale nature, such processes are challenging to resolve with current experimental techniques, and are too complex for detailed computer simulations. Coarse-grained computer simulations, rooted in soft matter and statistical mechanics, can be of great help in determining how functional protein assemblies operate, and how pathological ones might form. Here I will first discuss the use of minimal coarse-grained model in elucidating the functional assembly of mechanosensitive membrane channels and membrane-remodelling filaments. Then I will present a combined molecular dynamics-genetic algorithms scheme to design membrane-remodelling structures of desired functions.

Prof. Michele Vendruscolo
University of Cambridge
mv245@cam.ac.uk

Invited Talk, 11:30-12:00

Principles of protein structural ensemble determination

Achieving a comprehensive understanding of the behaviour of proteins is greatly facilitated by the knowledge of their structures, thermodynamics and dynamics. This information can be provided in an effective manner in terms of structural ensembles. A structural ensemble can be obtained by determining the structures, populations and interconversion rates for all the main states that a protein can occupy. I will describe how the well-established principles of protein structure determination should be extended to the case of protein structural ensembles determination.

These principles concern primarily how to deal with conformationally heterogeneous states, and with experimental measurements that are averaged over such states and affected by a variety of errors. I will address some conceptual problems in the determination of structural ensembles and define future goals towards the establishment of objective criteria for the comparison, validation, visualization, and dissemination of such ensembles.

Dr. Stefano Serapian
University of Bristol
stefano.serapian@bristol.ac.uk

Contributed Talk, 12:00-12:20

Atomistic Simulations of the Catalytic Behaviour of a Ketoreductase Towards Small-molecule and Natural Substrates

Stefano A. Serapian and Marc W. van der Kamp
School of Biochemistry, University of Bristol, United Kingdom.
Centre for Computational Chemistry, University of Bristol, United Kingdom

Actinorhodin ketoreductase (actKR) is one of the enzymes involved in the biosynthesis of the antibiotic actinorhodin. In nature, actKR binds to an acyl carrier protein (actACP), which unsheaths a phosphopantetheinylated octaketide chain into its active site. Here, it is selectively cyclised between carbons C7 and C12 and, subsequently, its C9 ketone is reduced to an alcohol via reductive hydride transfer from a NADPH cofactor, and H⁺ abstraction from a catalytic tyrosine. In vitro, reengineered actKR variants have shown promise for the stereoselective reduction of small ketones.[1] For example, whilst wild-type (WT) actKR only reduces the bicyclic aliphatic ketone trans-1-decalone (1) to trans-1-decalol (2) with mild stereoselectivity (S-2:R-2 ratio = 3.5:1); the P94L mutant is far more selective towards S-2 (as indicated by assays of the reverse reaction); and V151L actKR entirely reverses its preference in favour of R-2. Here, we employ a range of highly efficient simulation protocols to rationalise the stereoselectivity of actKR variants towards 1 (modelling both its enantiomers).[2] Using classical molecular dynamics (MD; to assess preferred prochiral binding poses), MM/PBSA (to quantify binding affinity), and semiempirical quantum/classical (QM/MM) MD with umbrella sampling (to examine reaction barriers), we find that stereocontrol in V151L and P94L actKR is asserted by different combinations of these factors. Thus, all these factors should be considered in designing enzyme stereospecificity. We further use protein-protein and -ligand docking in conjunction with MD to study the interaction of actKR with actACP, exploring octaketide cyclisation and reduction. Our work highlights the crucial role played by atomistic simulations in understanding (bio)catalysis, often providing crucial insight that experimental work is not able to give.

References: [1] Korman TP et al., *Biochem.* 2008, 47, 1837. 2. Serapian SA, van der Kamp MW, submitted, DOI: 10.26434/chemrxiv.7358663.v1

Session 2: DFT - Methods and Applications

Prof. Kieron Burke
UC Irvine
kieron@uci.edu

Keynote Lecture, 14:00-15:00

Density functional theory: Basics, progress, and challenges

In this talk, I will explain some basic elements of DFT, and review progress in the field in recent years. I will attempt to cover both the breadth of recent applications and the depth of insight needed to make progress. I will show areas where progress has been made, and challenges where progress has been slow. The specific cases highlighted will be from areas I am working in. All recent work is available from <http://dft.uci.edu/publications.php#publications>.

Prof. Aron Walsh
Imperial College London
a.walsh@imperial.ac.uk

Invited Talk, 15:00-15:30

Life and times of an electron in a perovskite solar cell

During the course of its lifetime, a photoexcited electron in a solar cell experiences many adventures, from its birth in the form of a hot exciton, through its cooling phase, transport, and collection to generate a current. The variation in length- and time-scales of these processes requires a range of techniques and models to be employed. I will present our latest understanding of perovskite solar cells including the role of lattice vibrations, molecular rotations, and crystal defects [1-4]. This draws from studies using a variety of simulation techniques including density functional theory, GW theory, molecular dynamics and Monte Carlo. The predicted temporal behaviour has been validated through a combination of neutron scattering, time-resolved vibrational spectroscopy, and kinetic measurements of the current-voltage response of operating solar cells. Finally, outstanding challenges and the need for methodological developments for the description of soft semiconductors will be outlined.

References: [1] "Atomistic origins of high-performance in hybrid halide perovskite solar cells", *Nano Letters*, 14, 2584 (2014). [2] "Self-regulation mechanism for charged point defects in hybrid halide perovskites", *Angewandte Chemie Int. Ed.* 54, 1791 (2015). [3] "Slow cooling of hot polarons in halide perovskite solar cells" *ACS Energy Letters* 2, 2647 (2017). [4] "Dynamic symmetry breaking and spin splitting in metal halide perovskites" *Physical Review B* 98, 085108 (2018).

Prof. David O'Regan
Trinity College Dublin
david.o.regan@tcd.ie

Invited Talk, 16:00-16:30

Towards an automated self-correction protocol for approximate DFT: facile first-principles Hubbard U and Hund's J parameters for arbitrary subspaces

Glenn Moynihan (1), Edward B. Linscott (2), Okan K. Orhan (1), Gilberto Teobaldi (3,4), Daniel J. Cole (5), Michael C. Payne (2), and David D. O'Regan (1)
(1) *School of Physics, CRANN and AMBER, Trinity College Dublin, Ireland* (2) *Cavendish Laboratory, University of Cambridge, United Kingdom* (3) *Stephenson Institute for Renewable Energy and Department of Chemistry, The University of Liverpool, United Kingdom* (4) *Beijing Computational Science Research Center, China* (5) *School of Natural and Environmental Sciences, Newcastle University, United Kingdom.*

In electronic structure methods based on the correction of approximate density-functional theory (DFT) for systematic inaccuracies, Hubbard U parameters may be used to quantify and amend the self-interaction error (SIE) ascribed to selected subspaces. In order to enable the accurate, computationally convenient calculation of U by means of DFT algorithms that locate the ground-state without any diagonalisation, such as in linear-scaling DFT+U [1], we introduce a linear-response formulation for U in terms of the fully-relaxed constrained ground-state density [2]. Expressing the total energy of self-consistent DFT+U in terms of a constrained search over ground-state densities and external DFT+U parameters that satisfy a self-consistency condition, we relegate U parameters to the status of auxiliary variables. This enables the full comparability, conceptually and numerically, of effectively self-corrected DFT energies, such as when external parameters such as ionic positions are changed [3]. Our ground-state tracking linear-response framework also addresses the open question of self-consistency over U in DFT+U. We show that the simplest self-consistency scheme is necessary and sufficient for DFT+U to correct the total energy for SIE under idealized one-electron conditions [3]. For multi-electron systems such as transition-metal oxides (including closed-shell ones), we extend the framework to enable straightforward first-principles calculations of the Hund's exchange parameter J, which we find to be critically important [4]. We also demonstrate successful first-principles U and J corrections for oxygen 2p orbitals.

References: [1] D. D. O'Regan, N. D. M. Hine, M. C. Payne, and A. A. Mostofi, *Phys. Rev. B* 85, 085107 (2012). [2] D. D. O'Regan and G. Teobaldi, *Phys. Rev. B* 94, 035159 (2016). [3] G. Moynihan, G. Teobaldi, and D. D. O'Regan, arXiv:1704.08076 (2017). [4] E. B. Linscott, D. J. Cole, M. C. Payne and D. D. O'Regan, *Phys. Rev. B*, accepted, arxiv:1802.09048 (2018).

Prof. Chris-Kriton Skylaris
University of Southampton
C.Skylaris@soton.ac.uk

Invited Talk, 16:30-17:00

Simulations of platinum nanoparticle catalysts with large-scale Density Functional Theory

First-principles quantum mechanical calculations based on Density Functional Theory (DFT) are free of empirical parameters and can thus provide a very accurate description of properties and processes of materials and molecules. However, the computational effort of conventional DFT scales with the third power in the number of atoms and limits the size of the calculations to no more than a few hundred atoms. To perform DFT calculations with thousands of atoms and enable the study of complex materials we have developed the ONETEP program [1] which is based on a linear-scaling reformulation of DFT in a way that retains the same high level of accuracy as conventional cubic-scaling methods. While the original linear-scaling DFT theory applies only to insulators, our new developments [2,3] have allowed us to extend it to metallic systems opening the way for a host of technologically relevant applications. I will present our recent large-scale simulations of Pt nanoparticles with ONETEP towards applications in catalysis. The adsorption of oxygen on Pt nanoparticle catalysts controls the oxygen reduction reaction (ORR) which is the rate-determining step in fuel cell operation. We have investigated how this process is affected by the size, support [4] and coverage [5] of the nanoparticle. While most studies make use of idealized structures such as extended surfaces or regular polyhedral nanoparticles, we have been able to work with real 3D nanoparticle structures obtained from high-precision electron microscopy. We find significant differences between experimental structures and idealised geometries and we use electronic and geometric descriptors to assess the performance of potential catalysts and to determine the optimum nanoparticle size and shape [6].

References: [1] C.K. Skylaris, P. D. Haynes, A. A. Mostofi and M. C. Payne. *J. Chem. Phys.* 122 (2005) 084119. [2] A. Ruiz-Serrano, and C.-K. Skylaris. *J. Chem. Phys.* 139 (2013) 054107. [3] J. Aarons, and C.-K. Skylaris. *J. Chem. Phys.* 148(2018) 074107. [4] L. G. Verga, J. Aarons, M. Sarwar, D. Thompsett, A. E. Russell and C.-K. Skylaris. *Phys. Chem. Chem. Phys.* 18 (2016) 32713. [5] L. G. Verga, J. Aarons, M. Sarwar, D. Thompsett, A. E. Russell, and C.-K. Skylaris. *Faraday Discuss.* 208 (2018) 497. [6] J. Aarons, L. Jones, A. Varambhia, K. E. MacArthur, D. Ozkaya, M. Sarwar, C.-K. Skylaris, and P. D. Nellist. *Nano Lett.* 17 (2017) 4003.

Dr Elizaveta Suturina
University of Bath
e.suturina@bath.ac.uk

Contributed Talk, 17:00-17:20

Paramagnetic shift and nuclear relaxation enhancement: synergy of ab initio methods and spectroscopy

Nuclear magnetic resonance (NMR) spectroscopy is a powerful analytical tool, which is largely undervalued when it comes to paramagnetic metal complexes. Fast nuclear relaxation often makes it impossible to record 2D NMR spectra needed for assignment, leaving 1D spectra of large non-symmetric molecules incomprehensible. However, the paramagnetic shifts and nuclear relaxation rates contain valuable information on electronic structure and dynamic properties of the system, and this information can be extracted from NMR spectra with the help of quantum chemistry. In this communication I will present semi-automatic assignment procedure for 1D NMR spectra that fits both shift and relaxation data, and its application to various metal complexes. [1-3] The following topics will be addressed: (1.) the limits of the point-dipole approximation for the hyperfine tensor prediction and importance of spin delocalisation in the context of lanthanide complexes as well as mono- and polynuclear transition metal complexes, (2.) the role of the magnetic susceptibility anisotropy in paramagnetic NMR, (3.) extraction of spin Hamiltonian parameters from variable temperature NMR, (4.) comparison of the magnetic susceptibility computed by SOC-CASSCF (Spin-Orbit Coupled Complete Active Space Self-Consistent Field) and extracted from variable temperature NMR.

References: [1] Beyond Bleaney's Theory: Experimental and Theoretical Analysis of Periodic Trends in Lanthanide Induced Chemical Shift, EA Suturina, K Mason, CFGC Geraldes, I Kuprov, D Parker, *Angew. Chem.*, 2017, 56, 12215. [2] Rationalisation of anomalous pseudo-contact shifts and their solvent dependence in a series of C₃-symmetric lanthanide complexes, M Vonci, K Mason, EA Suturina, AT Frawley, SG Worswick, I Kuprov, D Parker, EJM McInnes, NF Chilton, *JACS*, 2017, 139, 14166. [3] Lanthanide-induced relaxation anisotropy, EA Suturina, K Mason, CFGC Geraldes, NF Chilton, I Kuprov, D Parker, *PCCP*, 2018, 20, 17676.

Dr Micaela Matta
Northwestern University
matter.micaela@gmail.com

Contributed Talk, 17:20-17:40

Design and Morphology Tuning of Polymer Donors and Non-Fullerene Acceptors for Organic Photovoltaics

Micaela Matta, Thomas J. Aldrich, Steven M. Swick, Ferdinand Melkonian, Kevin L. Kohlstedt, Antonio Facchetti, Tobin J. Marks, George C. Schatz
Northwestern University, Chemistry Department, USA

Organic bulk-heterojunction (BHJ) solar cells made of polymeric donors and small molecule non-fullerene acceptors (NFA) are in the spotlight due to their record-high efficiencies. [1] We studied the role of side chains in mediating intermolecular π -stacking and aggregation in a series of PBTZF4 polymer donors [2] with increasingly long alkyl chains. Insight from molecular dynamics (MD) simulations connect the single polymer chain behaviour to its aggregation, BHJ domain formation, and ultimately device efficiencies. We also studied the effects of fluorination [3], end-group conjugation extension [4] and side-chain length [5] in a series of novel ITIC-derived acceptors. We used electronic structure methods and MD simulations to investigate how changes in the acceptor molecular structure influence both electronic properties and solid state packing.

References: [1] Hou, J. et al. Nat. Mater., 17, 119–128 (2018). [2] Wang, G. et al., in preparation. [3] Swick, S. M. et al. Proc. Natl. Acad. Sci. U. S. A. 2018, 115 (36), E8341–E8348. [4] Aldrich, T. J. et al. J. Amer. Chem. Soc., submitted. [5] Matta, M. et al., in preparation.

Syma Khalid
University of Southampton
S.Khalid@soton.ac.uk

Session 1 – reprise! Invited Speaker, 17:40-18:10

Focusing the Computational Microscope on the Cell Envelopes of Gram-negative Bacteria

A protective cell envelope surrounds Gram-negative bacteria such as *E. coli*, providing a selective gateway connecting the interior of the cell to the external environment. We employ molecular dynamics simulations, at multiple levels of resolution, to reveal the details of covalent and non-covalent interactions of proteins, lipids, and sugars within the cell envelope to gain insights into how these molecules function individually, and also together as a whole. We use data from experimental methods such as X-ray, NMR and cryoEM structures from our structural biology colleagues, and combine them with molecular models that represent the *in vivo* environment of the bacterium to study their dynamics. The data from our simulations allows to make ‘molecular movies’, I will show some of these movies in my talk to highlight some of our recent results. We have used coarse-grain models based on cryoEM data to reveal the differences in correlation between protein and lipid motion as a function of membrane and protein type. More recently we have built an atomistic model of the *E. coli* cell wall, and have explored the interactions of inner and outer membrane proteins with the peptidoglycan that comprises the wall.

References: [1] Hsu PC, Samsudin F, Shearer J, Khalid S, (2017) “It Is Complicated: Curvature, Diffusion, and Lipid Sorting within the Two Membranes of Escherichia coli.” J Phys Chem Lett. 8 (22), 5513-5518. [2] Samsudin F, Boags A, Piggot TJ, Khalid S. (2017), “Braun’s Lipoprotein Facilitates OmpA Interaction with the Escherichia coli Cell Wall”. Biophys J 113 (7) 1496-1504. [3] Boags A, Hsu PC, Samsudin F, Bond PJ, Khalid S (2017). “Progress in Molecular Dynamics Simulations of Gram-Negative Bacterial Cell Envelopes.” J. Phys Chem Lett. 8 (11) 2513-2518.

Session 3: Energy Materials and Interfaces

Prof. Giulia Galli
University of Chicago
gagalli@uchicago.edu

Keynote Lecture, 9:00-10:00

Materials for energy: the interface is still the device

We present the results of hybrid density functional and many body perturbation theory calculations aimed at characterizing charge transfers at heterogeneous interfaces between photo-absorbers, catalysts and water, and between nanoparticles used in electronic devices. We discuss the importance of considering realistic structural models at the atomistic level in order to predict the efficiency of solar energy conversion processes.

Dr. Mariana Rossi
Fritz Haber Institute of the Max Planck Society
rossi@fhi-berlin.mpg.de

Invited Talk, 10:00-10:30

Addressing the nuclear and electronic structure of weakly bonded interfaces

Weakly bonded systems composed by organic constituents are ubiquitous in nature and nowadays also in technological applications. In particular, the use of organic components interfaced with inorganic materials offers the possibility of enhancing the efficiency and versatility of devices. One aspect that hinders advances in this field is the lack of understanding about how the electronic and atomic degrees of freedom cooperate or compete to yield the desired interface properties. From a theoretical perspective, addressing these systems involves efforts in finding the relevant structural motifs, evaluating their dynamical evolution and evaluating the associated electronic properties. These tasks are especially challenging in these systems due to the large conformational space they can explore at finite temperatures, and the inherent anharmonicity of their intra and intermolecular interactions. In this talk, I will discuss our recent efforts to address the challenges mentioned above, based on density functional theory and ab initio molecular dynamics simulations. I will present strategies for conformational space sampling of organic/inorganic interfaces, techniques to include anharmonicity in vibrational fingerprints, and our recent methodological developments that allow the inclusion quantum nuclear effects in high-dimensional systems using path integral molecular dynamics.

Dr. Fernanda Duarte
University of Oxford
fernanda.duarte@chem.ox.ac.uk

Invited Talk, 11:00-11:30

Computational Modelling at the Interface of Asymmetric Catalysis and Supramolecular Chemistry

Intermolecular forces are being increasingly recognised as crucial factors determining selectivity in numerous catalytic processes. Excellent examples include asymmetric hydrogen-bonding and counteranion-directed catalysis. In parallel, new possibilities of supramolecular catalysis have also been demonstrated using multicomponent assemblies. Despite these promising results, a molecular understanding of these interactions in condensed-phase and their influence in the reaction outcome remains challenging. In this talk I discuss some of the inherent challenges involved in the quantitative characterization of these interactions in solution and our ongoing work to overcome them. I will present examples in the area of asymmetric catalysis and supramolecular chemistry, which have provided us with deeper understanding on the critical influence of non-covalent interactions for reactivity and selectivity.

Dr Livia Bartok-Partay
University of Reading
l.bartokpartay@reading.ac.uk

Invited Talk, 11:30-12:00

L.B. Partay, N. Bernstein, R.J.N. Baldock, A.P. Bartok, G. Csanyi

In recent years we have been working on adapting a novel computational sampling technique, called nested sampling, to study the potential energy surface of atomistic and molecular systems (JPC B 114, 10502 (2010)). Nested sampling automatically generates all the relevant atomic configurations, unhindered by high barriers, and one of its most appealing advantages is that the global partition function can be calculated very easily as a simple post-processing step, thus thermodynamic properties become accessible. Nested sampling explores the potential energy surface starting from the high energy region, hence no prior knowledge of the potentially stable structures is needed. This means that unlike other methods, nested sampling may be fully automated, allowing high-throughput calculations of phase transformations and phase diagrams of different materials. The method has been used to calculate phase diagrams of metals (PRB 93, 174108 (2016)), nanoparticles (Scientific Reports, (2018) 8:9150) and molecular systems are being explored.

Prof. Aaron Kelly
Dalhousie University
aaron.kelly@dal.ca

Invited Talk, 12:00-12:30

Nonequilibrium Charge and Energy Transport at the Nanoscale

Recently developed approaches for simulating nonequilibrium quantum dynamics in nanoscale systems will be discussed. The feature unifying these methods is the statistical ensemble of trajectories that is employed in order to construct observables and transport properties for real-time nonadiabatic quantum processes, such as charge and energy transfer. We will explore the performance of selected techniques of this type in a variety of scenarios, including exciton transport, polaron formation, charge separation at donor-acceptor interfaces, and heat transport through molecular junctions.

Session 4: Advanced Quantum Chemistry

Prof. Frank Neese
Max Planck Institut für Kohlenforschung
frank.neese@kofo.mpg.de

Keynote Lecture, 14:00-15:00

Correlated wavefunction based ab initio methods for Chemistry

The talk will discuss the opportunities (and limitations) for the applying post Hartree-Fock single- and multireference methods to chemistry. The examples will be taken from catalysis, transition metal chemistry, magnetism, biochemistry and material science. It hopefully will become apparent that the application of high-level wave function based methods alongside or as an alternative to Density Functional Theory is now possible in a routine fashion.

Dr Felix Plasser
Loughborough University
f.plasser@lboro.ac.uk

Invited Talk, 15:00-15:30

Understanding ionic and covalent wavefunction character without valence bond theory

The excited states of alternant hydrocarbons such as naphthalene are usually divided into two different classes denoted covalent and ionic states. The characterisation of ionic and covalent character is quite cumbersome requiring specialised valence-bond-theory based protocols despite the fact that the distinction has existed since the early days of quantum chemistry [1]. This is particularly troublesome as the ionic/covalent character has a strong but hard-to-pin-down impact on commonly used electronic structure methods. It is the purpose of this talk to address the issue of ionic and covalent wavefunction character from an entirely new perspective. The wavefunctions are represented in terms of electron and hole quasiparticles [2,3] and correlations between them are visually represented in real space [4]. Using this prescription, a natural distinction between ionic and covalent character arises, that does not have any explicit reference to valence-bond theory: covalent and ionic states are represented by dynamic electron-hole avoidance and enhanced overlap, respectively. This observation opens a new perspective on this long-standing problem in quantum chemistry.

References: [1] R. Pariser, J. Chem. Phys. 24, 250 (1956). [2] F. Plasser, M. Wormit, and A. Dreuw, J. Chem. Phys. 141, 024106 (2014). [3] S. A. Boppler, F. Plasser, M. Wormit, and A. Dreuw, Phys. Rev. A 90, 052521 (2014). [4] F. Plasser, submitted for publication.

Prof Fred Manby

Invited Talk, 16:00-16:30

University of Bristol
fred.manby@bristol.ac.uk

Tim Wiles, Zack Williams, Fred Manby
School of Chemistry, University of Bristol, United Kingdom

Density functional theory remains an extraordinarily powerful tool in computational molecular science. Many of the difficulties with the approach arise from self-interaction errors, which in turn arise from the approximate exchange-correlation functional used. A large part of the self-interaction error comes from the inexact cancellation between the self-interacting part of the Coulomb energy (which is calculated exactly) and of the exchange energy (which is approximated). Here we discuss a new type of correlation functional that has, amongst its various benefits, one interesting and unexpected one: it works alongside a very large portion of exact exchange, thus leading to density-functional approximations that show exceptionally little self-interaction error.

Professor Elena Besley
University of Nottingham
elena.Besley@nottingham.ac.uk

Invited Talk, 16:30-17:00

The notion that "like charges repel and opposite charges attract" is familiar to everyone but electrostatic attraction between like-charged objects is also possible due to their mutual polarization. A problem of fundamental and general interest is how electrostatic interactions are influenced by the presence of a polarizable medium, for example water. We overview a comprehensive theory [JCP 133, 024105 (2010); JCP 140, 074107 (2014)], with universal relevance to the electrostatic properties of closely interacting particles of arbitrary size and charge [Perspective Article, PCCP 18, 5883 (2016)], which has been extended recently to modelling electrostatic interactions in solvents [JCTC 14, 905 (2018)] and ionized medium [JCP 145, 084103 (2016)]. These developments contribute to the design of thin films and surface assemblies with novel properties. We find that the nature of electrostatic interaction is determined by how polarizable the particle and surface are as compared to the medium. The findings allow a comprehensive understanding of electrostatic particle-particle and particle-surface interactions in many areas of Science, ranging from Coulomb fission of charged clusters [JCP 146, 164302 (2017); J. Phys. Chem. A 117, 3877 (2013)] to aerosol growth in planetary atmospheres [Icarus 291, 245 (2017)]. Experimental studies undertaken by Whitesides [Nat. Mater. 2, 241 (2003); Soft Matter 8, 9771 (2012); JACS 136, 13348 (2014)] relating to electrostatic self-assembly have been the subject of our dynamic computer simulations, where the consequences of changing the charge and the dielectric constant of the materials concerned have been explored. Our simulations on the assembly of polymer particles subjected to tribocharging successfully reproduce many of the observed patterns of behaviour. We extend this study further to explore the significance of electrostatic interactions for the fabrication of binary nanoparticle superlattices.

Dr. Bora Karasulu
University of Cambridge
bk393@cam.ac.uk

Contributed Talk, 17:00-17:20

Solid-Solid Interfaces in all Solid-State Li-ion Batteries: Insights from ab initio Modelling

Bora Karasulu 1, James P. Darby 1, Clare P. Grey 2, and Andrew J. Morris 3
1 Dept. of Physics, Univ. of Cambridge, UK 2 Dept. of Chemistry, Univ. of Cambridge, UK 3 School of Metallurgy and Materials, Univ. of Birmingham, Birmingham, UK

All solid-state batteries (ASSBs) can potentially mitigate the safety issues known for conventional Li-ion batteries, and provide enhanced energy densities, by replacing the organic electrolyte solutions with solid inorganic equivalents. Mechanical and (electro)chemical incompatibilities between the ASSB solid components, however, lead to high resistances, curtailing the Li-ion transport at their interfaces [1]. In this talk, we introduce a high-throughput ab initio modelling approach towards the rational design of electrolyte/electrode interfaces in ASSBs. First, we obtain phase diagrams of sulfide-based electrolytes with diverse compositions, phases, vacancies and doping using the Ab Initio Random Structure Searching (AIRSS) method [2]. Next, the stable and low-lying metastable phases are screened for their ionic conductivity using ab initio molecular dynamics simulations. Finally, diverse surfaces of the selected electrolyte phases are interfaced with the surfaces of electrodes or other interfacial (e.g. solid electrolyte interphase, SEI) layers to determine the stable combinations using an automated procedure (INTERFACER). The devised approach will be demonstrated in action for a collection of interfaces, e.g. Li-P-S electrolytes with LiCo₂, Li-metal electrodes and alike.

References: [1] C. George, et al. Chem. Mat. 28, 7304-10 (2016); M. Butala et al. Chem. Mat., 29,3070-82 (2017) [2] C. J. Pickard, R. J. Needs, PRL 97, 045504 (2006); Medeiros et al., ACS Nano, 11, 6178-6185 (2017).

Mr Venkat Kapil
EPFL Lausanne
venkat.kapil@epfl.ch

Contributed Talk, 17:20-17:40

Accurate and efficient molecular dynamics with nuclear quantum effects: Using density functional theory to accelerate wavefunction methods

Venkat Kapil, Joost VandeVondele, Michele Ceriotti
Laboratory of Computational Science and Modelling, EPFL Lausanne, Switzerland, Swiss National Supercomputing Centre (CSCS), Zürich, Switzerland.

The development and implementation of increasingly accurate methods for electronic structure calculations mean that, the sampling procedure used to compute thermodynamic properties has become the bottleneck to reach the ultimate level of accuracy. The computational cost of performing molecular dynamics remains large, due to the need of evaluating the energetics of several tens of thousands of configurations. Furthermore, to account for the quantum nature of light nuclei, the overhead is typically a factor of ten to hundred times larger, making it prohibitive when combined with advanced electronic structure methods. Here, we present how multiple time step integrators [1] can be used in the context of ab initio molecular dynamics to dramatically reduce the cost of statistical sampling, while describing inter-particle interactions at high levels of electronic structure theory [2,3]. Furthermore, we show by it is possible to drive the overhead of modelling nuclear quantum effects virtually to zero [2], by performing multiple time stepping in imaginary time [4]. This is demonstrated for a combination of MP2 and semi-local density functional theory using our implementation in i-PI, the universal force engine.

References: [1] Tuckerman et. al Journal of Chemical Physics, 97, 1990 (1992) [2] Kapil et. al Journal of Chemical Physics, 144, 054111 (2016) [3] Kapil et. al Journal of Physical Chemistry C, 122 (22), pp 6048-6054 (2018) [4] Markland, Manolopolous Journal of Chemical Physics, 129, 024105 (2008) [5] Kapil et. al Computer Physics Communication (2018) [10.1016/j.cpc.2018.09.020]

Dr. Liam Wilbraham
University College London
l.wilbraham@ucl.ac.uk

Contributed Talk, 17:40-18:00

Enabling the Exploration of Copolymerisation Space with Machine Learning

(1) Liam Wilbraham, (2) Reiner Sebastian Sprick, (3) Kim Jelfs, (1) Martijn Zwijnenburg
(1) *Department of Chemistry, University College London, United Kingdom.* (2) *Department of Chemistry and Materials Innovation Factory, University of Liverpool, United Kingdom.* (3) *Department of Chemistry, Imperial College London, United Kingdom.*

Conjugated polymers are an important class of materials. Their optoelectronic properties, as well as the ease of tuning their properties through co-polymerization, underpins their application in many areas. The ease of generating new materials through co-polymerization, however, also means that only a fraction of all possible materials has been explored experimentally. In an effort to enable the computational exploration of the property space spanned by a large number of binary copolymer compositions, we train a neural network to accurately predict their optical and electronic properties, using a tiered data generation strategy.[1] As a result, we resolve the property space spanned by 350,000 synthesizable copolymers and extract insight that would otherwise be unattainable from smaller datasets. Rather than focus on the neural network model itself, we concentrate on what can be done with the data it generates. By identifying general features of the homo and copolymer property space, we outline how simple models are able to relate the properties of specific copolymers to the homopolymers of their constituent monomers. Further, as an example of how such large volumes of data permit the data-driven testing of common materials design strategies, we consider the commonly-employed hypothesis that copolymerisation of donor and acceptor monomers can result in copolymers with a lower optical gap than their related homopolymers. Our results not only lend context and understanding to this hypothesis, but propose a heuristic to predict promising combinations of monomers for which this behaviour is likely to be observed. Finally, through a “topographical” analysis of the co-polymer property space, we show how this machine learning facilitates the identification of dominant monomers in specific regions of property space that may be amenable to a variety of applications.

References: [1] L. Wilbraham et. al. ChemRxiv, 2018, doi: 10.26434/chemrxiv.7446014.v1.

Session 5: Machine Learning

Alexandre Tkatchenko
University of Luxembourg
alexandre.tkatchenko@uni.lu

Keynote Lecture, 9:00-10:00

Machine Learning (R)evolution in Chemistry and Physics

Learning from data has led to paradigm shifts in a multitude of disciplines, including web, text and image search, speech recognition, as well as bioinformatics. Can machine learning enable similar breakthroughs in understanding (quantum) molecules and materials? The main challenges are the disproportionately large size and intricate structure of chemical space, estimated to contain 10^{60} molecules even when only counting small organic drug-like candidates. Aiming towards a unified machine learning (ML) model of quantum interactions, I will discuss the potential and challenges for using ML techniques in chemistry and physics. ML methods can not only accurately estimate molecular properties of large datasets, but they can also lead to new insights into chemical similarity, aromaticity, reactivity, and molecular dynamics. However, to do so one needs to carefully unify spatial and temporal physical symmetries with purpose-designed ML methods. While the potential of machine learning for revealing insights into complex quantum-chemical systems is high, many challenges remain. I will conclude my talk by discussing these challenges.

Prof. Christoph Ortner
University of Warwick
C.Ortner@warwick.ac.uk

Invited Talk, 10:00-10:30

Interatomic Potentials from Linear Polynomial Fits

I will report on our initial experience in constructing interatomic potentials (IPs) for materials using a basis of symmetric polynomials. Our approach adapts the methods of Bowman and Braams in two fundamental ways: adapting their methods to be suitable for materials systems using a body-order expansion and cut-off mechanisms while retaining systematic improvability; supplying the linear regression with regularisation procedures in order to obtain “transferrable” potentials that are suitable for a wide range of modelling scenarios.

Prof. Anatole von Lilienfeld
University of Basel
anatole.vonlilienfeld@unibas.ch

Invited Talk, 11:00-11:30

O. Anatole von Lilienfeld

Many of the most relevant chemical properties of matter depend explicitly on atomistic and electronic details, rendering a first principles approach to chemistry mandatory. Alas, even when using high-performance computers, brute force high-throughput screening of compounds is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of chemical space, i.e. all compositional, constitutional, and conformational isomers. Consequently, efficient exploration algorithms need to exploit all implicit redundancies present in chemical space. I will discuss recently developed statistical learning approaches for interpolating quantum mechanical observables in compositional and constitutional space. Results for our models indicate remarkable performance in terms of accuracy, speed, universality, and size scalability.

Dr George Booth
King's College London
george.booth24@gmail.com

Invited Talk, 11:30-12:00

From Green functions to wave functions for correlated quantum chemistry

George Booth, Max Nusspickel, Oliver Backhouse, Edoardo Fertitta
King's College London, UK

Electronic structure theories of quantum chemistry built around (dynamical) Green's functions or (static) wave functions are generally considered very different in origin. However, can we switch between the two, and build a zero temperature, wave function theory which identically reproduces the same results of Greens function theory? We show that this is indeed possible, and develop a novel, wave function based, zero temperature renormalized perturbation theory, which scales with only MP2 cost, but able to deal with moderate correlation strengths and bond breaking. This reimagining of Greens function theory as wave functions can be extended to embedding theories, where the dynamic coupling is replaced by a static approach with a substantially reduced computational cost. This opens paths to new classes of electronic structure theory in a range of quantum many-body problems.

Future Perspectives

Prof. Alessandro Troisi
University of Liverpool
a.troisi@liverpool.ac.uk

12:00-13:00

Computational Molecular Science: the Next 20 Years.

This lecture will use examples from all the talks of the conference and the speaker's own work to look at the future of computational molecular science. It will be about questions more than answers with more time than usual left for discussion. Where do we go from here? How do we blend hot new fashion and fundamental technical developments? What interactions with experimental science are the most and least effective? Should we be involved with the development of new hardware (from HPC to quantum computers)? Are we too self-referential? How can CMS retain centrality in science (from research projects to high profile publications)?

CMS 2019

Computational
Molecular
Science



Posters

Poster n. 1 - Nicholas Hine
University of Warwick
n.d.m.hine@warwick.ac.uk

Excited state calculations and theoretical spectroscopy of complex nanomaterials using Linear-Scaling Density Functional Theory

N. D. M. Hine (1), J. Aarons (1), D. J. Cole (2), P. D. Haynes (3), J.-H. Li (4), M. A. Turner (1), T. J. Zuehlsdorff (4)
(1) *Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom* (2) *School of Chemistry, Newcastle University, Newcastle upon Tyne NE1 7RU, UK* (3) *Department of Materials, Imperial College London, London, UK* (4) *TCM Group, Cavendish Laboratory, J. J. Thomson Avenue, Cambridge, UK*

Linear-scaling approaches to density functional theory (LS-DFT) employing an efficient local orbital representation of the density matrix have made great progress in enabling ground state properties of large and complex systems. They have been less frequently used for excited states, partly because of the difficulty of representing unoccupied Kohn-Sham states of extended systems using localised orbitals. Within the ONETEP LS-DFT code, we have addressed the issues using a combination of in situ optimisation of orbitals for unoccupied states [1] and Linear-Response Time Dependent DFT (LR-TDDFT) [2] to study excitations. The newly-enabled calculations of excited states of chromophores in realistic environments make it possible to reach convergence of environmental influences as a function of the size of the region studied quantum mechanically [3], and to accurately predict properties such as solvatochromic shifts deriving from solvent-solute interactions [4,5]. We have also applied these methods to other complex systems including pigment-protein systems such as the Fenna-Matthew-Olson Complex [6,7], and the potential energy surfaces of photoexcited reactions in DNA [8]. Recent advances include development of functionality for excited state forces.

[1] L. E. Ratcliff et al, *Phys Rev B* 84 165131 (2011). [2] T. J. Zuehlsdorff et al, *J. Chem. Phys.* 139, 064104 (2013). [3] T. J. Zuehlsdorff et al, *J. Chem. Theory Comput.* 12, 1853 (2016). [4] T. J. Zuehlsdorff et al, *J. Chem. Phys.* 146, 124504 (2017). [5] M. A. Turner et al, *J. Phys. Chem. A* in press (2019). [6] D.J. Cole et al, *J. Phys. Chem. Lett.* 4, 4206 (2013). [7] A. S. Fokas et al, *J. Phys. Chem. Lett.* 8, 2350 (2017). [8] J.-H. Li, *J. Phys. Chem.* 122, 11633 (2018).

Poster n. 2 - Hui Yang
Imperial College London
hui.yang@imperial.ac.uk

Highly Anisotropic Thermal Transport in lithium battery electrodes from first-principles

Hui Yang, Jia-yue Yang, Aron Walsh
Department of Materials, Imperial College London

The Faraday Institution brings together scientists on research projects to reduce battery cost, weight, and volume; to improve performance and reliability, and to boost UK's transition to electric vehicles in near future. Lithium-ion battery emerges as a versatile and efficient candidate. $\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$ (NMC, $x + y + z = 1$) is the state-of-the-art option of cathode materials for high-capacity Li-ion batteries in the electric vehicle applications. Thermal stability of the electrodes is a key issue for the safe operation of Li-ion batteries. Thus, our study starts from the thermal property of the singly doped ones. The supercell models are built in the Vienna Ab-initio Simulation Package (VASP). An open source package, Phonopy, is used for phonon dispersion calculations. Based on the phonon structure, thermal properties are calculated using the quasi-harmonic approximation. We found LiCoO_2 has highly anisotropic thermal conductivity. Our first-principle modelling provides a theoretical foundation on understanding of the physicochemical properties of energy materials.

Poster n. 3 - Ivan Scivetti
Science and Technology Facilities Council
ivan.scivetti@stfc.ac.uk

Electrostatics at metallic surfaces: an old standing density functional problem

Ivan Scivetti, Alin M. Elena, Mats Persson, Ivan Runggers
Daresbury Laboratory, Sc. Tech. Keckwick Lane, Daresbury, WA4 4AD, Warrington, UK. Surface Science Research Centre and Department of Chemistry, University of Liverpool, Liverpool L69 3BX, UK. Department of Applied Physics, Chalmers University of Technology, SE-412 96 Goteborg, Sweden. National Physical Laboratory, Hampton Road, Teddington, TW11 0LW, UK.

Almost fifty years ago, the seminal work of N.D. Lam and W. Kohn [1] on metallic surfaces revolutionised the field of surface science, and made of computational research based on Density Functional Theory (DFT) an invaluable tool to support experiments. Nowadays, most DFT simulations of surfaces are routinely conducted using periodic boundary conditions (PBCs) together with the slab approximation and the pseudo-potential method. Since metals screen any perturbation within a range of approximately 2 Angstroms, only few atomic layers are often considered for the slab models, and this choice is mainly restricted by the amount of atoms that can be included in the simulation. Surprisingly, despite the enormous amount of DFT work over the years, it appears there are no reported studies of how the electrostatic response of bare metallic slabs depends on the constraints imposed by PBCs, nor how results might be affected by the thickness of the modelled slabs. Understanding this complex interplay is crucial towards the development of robust semi-classical approaches to circumvent, for example, the well-known limitation of fractional charge transfer at interfaces [2,3]. To this purpose, we apply a new DFT methodology [2] to evaluate the electrostatic response of the low-index facets of lithium. Via detailed computations of neutral and charged slabs with different number of atomic layers, we investigate the electrostatics beyond linear response. Analysis of key response parameters allow us not only to revise the range of validity of standard approximations but also to provide an alternative view of the connection between the quantum response and classical electrostatic models.

[1] Lang N D and Kohn W. Phys. Rev. B 1970, 1(12) 4555-4568; 1971, 3(4) 1215-1223; 1973, 7(8) 3541-3550. [2] Scivetti I and Persson M. Journal of Physics: Condensed Matter 25 355006 (2013). [3] Souza A M, Rungger I, Pemmaraju C D, Schwingenschloegl U and Sanvito S. Phys. Rev. B 88(16) 165112 (2013).

Poster n. 4 - Tom Hardcastle
University of Leeds
cp14tejh@leeds.ac.uk

Platonic Solids: Ab initio prediction of crystal morphologies.

Tom Hardcastle, Andrew Scott
University of Leeds

Over the past 20 years, considerable progress has been made in the field of crystal structure prediction, allowing many solid state properties of compounds to be predicted prior to synthesis. As these methods improve, the difficulties associated with the prediction of solid state properties are less attributable to a poor understanding of the solid state geometric structure and energetic properties. As prediction of the bulk energetics and geometries improves, the influence of particle surfaces becomes a more significant source of error when attempting to predict solid state properties. As a result, an improved a priori understanding of the surface effects and relative surface expressions becomes more important. In this work, crystal morphologies of molecular crystals are predicted using attachment energies calculated with density functional theory, and compared with morphologies predicted with BFDH, molecular mechanics, and experimental morphologies where available. Additionally, a rapid method of predicting crystal morphologies by exploiting the anisotropy of the electron density is explored and its advantages and limitations discussed. Each method performs reasonably well at predicting major facets, however fall short of consistent reproduction of experimental crystal morphologies. This is due to the significant influence of growth conditions on experimental morphologies; the need for more advanced predictive techniques that go beyond a simple structure-morphology relationship is highlighted.

Poster n. 5 - Miroslav Suruzhon
University of Southampton
M.Suruzhon@soton.ac.uk

Automation of relative protein-ligand binding free energy calculations and performing large-scale high-throughput studies

Miroslav Suruzhon (a), Russell Viner (b), Ian Wal (c), Richard Ward (d) and Jonathan W. Essex (a)

(a) School of Chemistry, University of Southampton, Southampton, UK (b) Syngenta, Jealott's Hill, Bracknell, UK (c) GlaxoSmithKline, Stevenage, UK (d) Medicinal Chemistry, Oncology, IMED Biotech Unit, AstraZeneca, Cambridge, UK.

There are many variables in every molecular dynamics (MD) simulation, the choice of which is often subjective. For example, in a protein simulation, one has to specify a starting crystal structure, amino acid protonation states, thermostat / barostat coupling constants, and many others. Changing each one of these initial conditions and parameters may produce a different result for any calculated thermodynamic property. Despite some recent investigative work[1-3], this variance is currently mostly unknown, calling the robustness of many MD simulations into question. Even though investigating the effect of varying these parameters is computationally possible, protein-ligand binding free energies require careful manual system set-up, which greatly limits the feasibility of high-throughput studies. Since the time needed for system preparation is currently comparable to the time required for the whole simulation, one needs a tool that attempts to automate this lengthy and somewhat non-trivial process. Although there are existing tools that attempt this task, they have limited capabilities, and a fully-integrated freely available tool which provides an environment to automate the whole process from reading a raw protein crystal structure to writing a simulated trajectory, is still yet to be made. Here we report the creation of such a tool by integrating a variety of specialised Python-based packages in order to achieve this task. To begin to explore the sensitivity of free energy calculations to simulation conditions, we present the results of using this tool to study relative protein-ligand binding free energies as a function of the initial crystal structure of the protein.

[1] J. Chem. Theory Comput. 2018, 14, 2867-2880. [2] J. Chem. Theory Comput. 2018, 14, 6127-6138. 3. J. Chem. Theory Comput., 2018, 14, 5567-5582.

Poster n. 6 - Ben Hourahine
The University of Strathclyde
benjamin.hourahine@strath.ac.uk

DFTB+ : delivering post GGA accuracy at tight-binding costs for 100k atoms

Ben Hourahine, Bálint Aradi

SUPA, Department of Physics, University of Strathclyde, John Anderson Building, 107 Rottenrow, Glasgow, G1 1XJ BCCMS, Universität Bremen, TAB Building, Entrance 1 A, 3rd floor, Am Fallturm 1, 28359 Bremen, Germany

Modern self-consistent density functional tight binding (DFTB) can match the thermochemistry of GGA density functional theory to chemical accuracy [1], or efficiently include hybrid functionals [2] and post-DFT methods [3] in both the ground and excited state, all while maintaining a minimal basis. The DFTB+ [4] code became open source in 2017 and continues to develop. This presentation will introduce recent extensions that are about to become available in the DFTB+19.1 release. These include: Non-equilibrium Green's function boundary conditions for self-consistent electronic transport under bias, rapid transmission calculations and semi-infinite structure simulations [5]. Range-separated hybrid functionals for the ground and excited state [2]. Access to the ELSI [6] electronic structure solvers for high performance parallel calculations, including several low and linear order scaling methods. GPU accelerated solutions using the MAGMA solvers. A well defined API for integration with other codes, including QM/MM coupling with polarisable classical models.

1. A. Dominguez, B. Aradi, T. Frauenheim, V. Lutsker, JCTC 9 4901 (2013) 2. V. Lutsker, B. Aradi, and T. A. Niehaus, J. Chem. Phys. 143, 184107 (2015); J. J. Kranz, M. Elstner, B. Aradi, T. Frauenheim, V. Lutsker, A. D. Garcia, T. A. Niehaus, JCTC, 13 1737 (2017) 3. T.A. Niehaus, M. Rohlfing, F. Della Sala, A. Di Carlo, and T. Frauenheim, Phys. Rev. A71, 022508 (2005). 4. B. Aradi, B. Hourahine, and Th. Frauenheim, J. Phys. Chem. A, 111 5678 (2007). 5. A. Pecchia and A. Di Carlo, Rep. Prog. Phys.67, 1497 (2004). 6. V. Yu et al., Comput. Phys. Commun. 222, 267 (2018).

Poster n. 7 - Kimberly Bowal
University of Cambridge
klb83@cam.ac.uk

The formation and growth of carbonaceous particles in a flame environment

Kimberly Bowal, Laura Pascazio, Jacob W. Martin, Markus Kraft

Carbonaceous particles, known as soot, are by-products of incomplete combustion that negatively impact combustion devices, human health and the environment. There is a strong desire to mitigate these undesired effects through the use of clean fuels or redesign of combustion devices. This requires detailed knowledge of the complex chemical and physical processes involved in the formation and growth of soot particles, such as the transition between gas phase molecules to solid particles. The interactions between curved polycyclic aromatic hydrocarbon molecules (cPAHs) and ions are believed to play a significant role in soot formation (Martin et al., Proc. Combust. Inst, 2018). Recently, we have developed an intermolecular potential (curPAHIP) that is able to capture the properties and interactions of cPAHs and have explored the ion-induced nucleation behaviour of the smallest cPAH corannulene (Bowal et al., Combust. Sci. Technol., In Press). This work suggests that cPAH-ion interactions are indeed significant in heterogeneous nucleation, although this has not yet been explored for systems representative of a flame environment. This work uses an advanced form of molecular dynamics to explore the nucleation and particle growth of soot-representative cPAHs. Well-tempered metadynamics is able to determine the thermodynamic stability of atomic and molecular systems and maps the potential and free energy surfaces of the system considered, providing the possible free energy minima configurations and the energy barriers between them. This sheds light on whether cPAH-ion interactions are significant enough to form stable clusters at flame temperatures, and provides insight into further details including the nucleation rate, critical nucleus size, and particle morphology of young soot particles. These results provide valuable information for soot formation and growth and can be used to expand the current soot models.

Poster n. 8 - Alexandru Moldovan
University of Leeds
pmaam@leeds.ac.uk

The Interfacial Interactions between Faceted Organic Crystals: An in-silico & Atomic Force Microscopy Study

A. A. Moldovan (1*), A. Bayly (2), R. Hammond (2) and S. Connell (3)

1 -Complex Particulate Products and Processes (CP3) Central Doctoral Training (CDT), School of Chemical and Process Engineering, University of Leeds, UK 2-School of Chemical and Process Engineering, University of Leeds, UK 3 -School of Physics, University of Leeds, UK

The formulations of pharmaceutical products have historically been a time and resource extensive endeavour [1]. Excipients are used in formulations to enhance product performance and/or improve manufacturability. The compatibility between the active pharmaceutical ingredient (API) and the excipients used plays a critical role in the final product performance. The ability to pre-screen API-Excipient compatibility in-silico would allow formulators to make a more informed decision on the experimental studies to be carried out thus reducing the development time and resources required to get a molecule from discovery to product. Atomic force microscopy (AFM) is being used to measure the adhesive force between defined crystal planes of acetaminophen. These faceted surfaces will also be measured against a range of excipients. AFM studies [2] have been previously carried out using colloidal probes and coated cantilevers, however, there is a lack of fully faceted crystals adhesion data. For the in-silico approach, a molecular mechanics (MM) framework has been developed to calculate the interfacial interactions between faceted organic crystals. By focusing on facet-specific interactions both computationally and experimentally, energetics associated with the surface chemistry can be identified. A surface compatibility ranking system has been developed allowing relative comparisons to be made between adhesive and cohesive forces.

[1] Taylor, D. The Pharmaceutical Industry and the Future of Drug Development. In *Pharmaceuticals in the Environment*; 2015; pp 1-33. [2] Jones, M. D.; Buckton, G. Comparison of the cohesion-adhesion balance approach to colloidal probe atomic force microscopy and the measurement of Hansen partial solubility parameters by inverse gas chromatography for the prediction of dry powder inhalation performance. *Int. J. Pharm.* 2016, 509 (1-2), 419-430 DOI: 10.1016/j.ijpharm.2016.06.002.

Poster n. 9 - Jakub Janowiak
University of Leeds
pm11j@leeds.ac.uk

Melting point prediction using message passing neural networks based on molecular and crystal structures

Jakub Janowiak, Elaine Martin, Richard Marchese-Robinson, Ilenia Giangreco, Andrew Maloney

Melting point (MP) is an important property as it can be used to predict solubility and identify "brick dust" compounds, where the solubility is limited by the intermolecular interactions within the crystal structure. Two questions considered in this work were: (1) can message passing neural networks be used to construct a melting point prediction model; and (2) can the performance of the model be improved by including crystal structure information? Message Passing Neural Networks (MPNN) have been successfully applied to predict a range of endpoints, from bioactivity to optoelectronic properties. They use a number of recurrent layers to produce a fixed-length representation of a graph from which property predictions can be inferred. In this work, MPNNs are applied that incorporate molecular structure and intermolecular interaction information to predict MP. Melting point is a solid state specific property, but due to data limitations, current prediction models do not utilise any crystal information. In this work MP data from the Cambridge Structural Database (CSD), a repository of small-molecule organic and metal-organic crystal structures, where each MP is associated with a specific crystal structure forms the basis of the analysis. We focused on single component crystals, of which there are 51,617 with associated MP values. The range of values for MPs and heavy atom count (molecular size) was -187 to 570 C and 2 to 672 respectively. This dataset allowed us to develop models that consider molecular information and also include crystal information. The model developed using only molecular information achieved a Root Mean Squared Error (RMSE) of 29.2 C on the internal validation subset, which is an improvement on the typical values of > 30 C achieved for models reported in the literature. An improvement of approximately 1 C was observed in models that also utilised crystal information (RMSE = 28.3 C).

Poster n. 10 - Daniel Corken
Warwick University
daniel.corken@warwick.ac.uk

A first-principles description of transient NO ion formation on Au(111)

D. M. Corken, Nicholas D.M.Hine, R. J. Maurer
Warwick University

Gaining a fundamental understanding of the interactions of molecules on metal surfaces is essential for the development of novel heterogeneous catalysts. An interesting feature of gas-surface reactions at metal surfaces is that the Born-Oppenheimer approximation breaks down. Vibrationally excited and translationally hot molecules can transfer energy to the electrons of a metal via excitation of electron-hole pairs (EHP). [1] In the case of NO on Au(111), this nonadiabatic energy loss is believed to stem from the transient generation of charged ion species at the surface. [2] A computationally feasible and accurate description of such a molecule-metal charge-transfer state represents a challenge and several methods have been proposed. One of the main challenges to modelling charged molecules on metal surfaces is that DFT tends to overly-delocalise charge. Meaning the true charge on the molecule is underestimated. Here we present our approach to this problem. We use linear expansion-Delta-Self-Consistent-Field Density Functional Theory (le Δ SCF-DFT) [3] to model the anionic resonance of NO on Au(111). The le Δ SCF-DFT method enforces the electronic configuration of reference molecular states while solving the Kohn-Sham equations self-consistently, enabling us to localise charge on the molecule. By comparison to experiment and other models, we assess the methods' ability to describe the ground and excited-states during molecular scattering. We further explore avenues to extract nonadiabatic couplings and to construct model Hamiltonians based on this method.

[1] A. M. Wodtke, J. C. Tully, and D. J. Auerbach, *Int. Rev. Phys. Chem.* 23, 513 (2004) [2] B. Gergen, H. Nienhaus, W. H. Weinberg, and E. W. McFarland, *Science*. 294, (2001) [3] R. J. Maurer and K. Reuter, *J. Chem. Phys.* 139, 014708 (2013)

Poster n. 11 - Abhishek Khedkar
Warwick University
abhishek.khedkar@rub.de

Active Space Selection and Inspection Scheme based on perturbation Theory (ASSIST)

Abhishek Khedkar, Michael Roemelt

1. *Department of Theoretical Chemistry, Ruhr University Bochum, Bochum, Germany* 2. *Max-Planck-Institute for Coal Research, Mülheim an der Ruhr, Germany*

Efficient and robust approximations to the full configuration interaction (Full-CI) method such as the density matrix renormalization group (DMRG) and the Full-CI quantum Monte-Carlo (FCIQMC) algorithm allow for multi-configurational self-consistent field (MC-SCF) calculations with large active spaces. This opens up the possibility to treat large and complex systems that were previously untractable but at the same time, it calls for an efficient and reliable active space selection as the choice of how many electrons and orbitals enter the active space is critical for any multireference calculation. In this work, we propose an Active Space Selection and Inspection Scheme based on perturbation Theory (ASSIST)[1] that follows a 'bottom-up' strategy and utilizes a set of quasi-natural orbitals together with sensible thresholds for their occupation numbers. The required quasi-natural orbitals are generated by diagonalizing the virtual and internal part of the one-electron reduced density matrix that is obtained from strongly contracted n-electron valence perturbation theory (SC-NEVPT2) on top of a minimal active space calculation. Self-consistent results can be obtained when the proposed selection scheme is applied iteratively. Here we present the initial applications on two benchmark systems indicate the capabilities of ASSIST and the strengths and limitations are critically discussed.

[1] Abhishek Khedkar, Michael Roemelt. (2018) Manuscript submitted for publication

Poster n. 12 - Mohamed Ali al-Badri
King's College London
mohamed.al-badri@kcl.ac.uk

Super-exchange mechanism and quantum many body excitations in the archetypal hemocyanin di-Cu oxo-bridge

Mohamed Ali al-Badri,¹ Edward Linscott,² Antoine Georges,³ Daniel J. Cole,⁴ and Cédric Weber¹

¹ *King's College London, Theory and Simulation of Condensed Matter (TSCM), Strand, London WC2R 2LS, United Kingdom,*

² *Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom,*

³ *Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France,*

⁴ *School of Natural and Environmental Sciences, Newcastle University, Newcastle upon Tyne NE1 7RU, United Kingdom.*

We perform first-principles quantum mechanical studies of dioxygen ligand binding to the hemocyanin protein. Electronic correlation effects in the functional site of hemocyanin are investigated using a state-of-the-art approach, treating the localised copper 3d electrons with cluster dynamical mean field theory (DMFT) for the first time. This approach has enabled us to account for dynamical and multi-reference quantum mechanics, capturing valence and spin fluctuations of the 3d electrons. Our approach predicts the stabilisation of a quantum entangled di-Cu singlet in the London-Heitler limit, with localised charge and incoherent scattering processes across the oxo-bridge, that prevent long-lived charge excitations. This suggests that the magnetic structure of hemocyanin is largely influenced by the many-body corrections.

Poster n. 13 - Harry Morgan
University of Oxford
harry.morgan@chem.ox.ac.uk

Pressure-induced structural transitions in vanadium oxyhydrides, Sr₂VO₃H and Sr₂V₂O₅H₂

Harry W. T. Morgan, Dihao Zeng, John E. McGrady
Physical and Theoretical Chemistry Laboratory, University of Oxford South Parks Road Oxford OX1 3QZ

Aims The high-pressure structural and electronic behaviour of the low-dimensional vanadium oxyhydrides Sr₂VO₃H and Sr₃V₂O₅H₂ was investigated computationally in conjunction with experimental methods. Pressure studies of these Ruddlesden-Popper derivatives allow us to probe of the nature of metal-hydride bonding in extended solids. **Methods** Periodic Density Functional Theory (DFT) calculations as implemented in the Vienna Ab Initio Simulation Package (VASP) were used to calculate total enthalpies and density of states (DOS) of the oxyhydrides at a range of pressures. **Results** Enthalpy calculations at a range of pressures, complemented by powder diffraction studies, reveal structural phase transitions in both phases akin to the B1-B2 transition observed in binary halides and oxides. These low-dimensional structures show strongly anisotropic compressibility along the lattice vectors owing to the dramatically different characters of the V-O, V-H and Sr-O bonds. The structural transition can be shown to change the Sr-O bonding only, leaving the vanadium local environment unaffected. This transition has no significant influence on the electronic structures of the crystals, and no electronic transition is observed at experimentally accessible pressures; DFT reveals that this is because the low-dimensional crystal structures are able to absorb the applied pressure without significant changes to the V-O bonding. **Conclusion** This study has revealed that these low-dimensional oxyhydrides respond to pressure in such a way as to minimize the effect on the vanadium bonding character and thus do not undergo pressure-driven electronic phase transitions at accessible pressures. They are able to do this as a result of the extreme anisotropy of their crystal structures. Ongoing investigation into the related cobalt phase will indicate whether this behaviour is common to all transition metals.

Poster n. 14 - Emiliano Poli
ICTP Trieste
epoli@ictp.it

On the Origins of the Charging of Water at Hydrophobic Interface.

Emiliano Poli, Ali Hassanali
The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy.

Aqueous interfaces are ubiquitous in nature and technological applications. Numerous physical, chemical and engineering processes occur at interfaces involving water and hydrophobic surfaces. Despite long study, many issues remain highly controversial regarding the properties of water at hydrophobic interfaces. One noteworthy system in this regard is the air-water interface. In particular, the origins of the surface charge of water, remains highly controversial [1-5]. In this work we investigate the electronic properties of the air-water interface using state-of-the-art linear scaling DFT methods [6] allowing us to model systems consisting of over thousands of atoms. We examine how the charge transfer at the surface is rooted in topological properties of the water network such as coordination defects and water wires. These results are then discussed within the broader framework of water near hydrophobic interfaces such as oil (i.e. dodecane), and solid surfaces (i.e. graphene). The differences and common trends between these systems are analysed in order to highlight the atomistic origin of the behaviour of water surfaces with respect to various hydrophobic interfaces of variable hydrophobicity. In particular, the role of both classical electrostatics and quantum mechanical effects like charge transfer, polarization and exchange, are examined with respect to the water interface configurations in contact with different hydrophobic surfaces.

[1] R. Vacha, V. Buch, A. Milet, J. Devlin, P. Jungwirth, *Phys. Chem. Chem. Phys.*, 9, 4736 (2007). [2] J. K. Beattie, A. M. Djerdjev, *Angew. Chem., Int. Ed. Engl.*, 43, 356 (2004). [3] T. L. Tarbuck, S. T. Ota, G. L. Richmond, *J. Am. Chem. Soc.*, 128, 14519 (2006). [4] K. N. Kudin and R. Car, *JACS*, 130, 3915 (2008) [5] R. Vácha, S. Roke et al., *JACS*, 133, 10204 (2011) [6] C. K. Skylaris, P. D. Haynes, A. A. Mostofi, M. C. Payne, *J. Chem. Phys.* 122, 084119 (2005)

Poster n. 15 - Eleanor Jayawant
University of Warwick
E.Jayawant@warwick.ac.uk

Combined MD and NMR approach to characterise structures of cyclic oxetane-modified peptides

E. Jayawant, A.M. Dixon and R. Notman
Department of Chemistry, University of Warwick, Coventry CV4 7AL, United Kingdom

Peptide-based drugs combine some of the advantages of larger biologic therapeutics with those of small molecule drugs, but they still have poor permeability and metabolic stability. Cyclic peptides have huge therapeutic potential as they are able to overcome some of the disadvantages of their linear counterparts, although they remain challenging to make. Recent research involved the development of a new type of peptide bond isostere, in which the carbonyl of the amide bond is replaced with a 3-aminooxetane unit [1]. Incorporation of an oxetane heterocycle into the backbone of a linear peptide increases the efficiency of macrocyclisation. The formation of a β -turn (as observed by long-range NOE interactions) in the backbone about the oxetane modification is thought to bring the termini of the peptide closer together, making cyclisation by chemical means feasible for short peptides [2]. However, the structure and characteristics of cyclic oxetane-modified peptides (cOMPs) are still poorly understood. Using a combination of molecular dynamics (MD) simulations and NMR experiments, the structure and dynamics of a cOMP and an unmodified parent pentapeptide were assessed. The oxetane modification has a drastic impact on the chemical shifts and intra-molecular NOE peaks observed using 2D NMR techniques compared to the unmodified parent peptide. NOE-derived distance restraints were estimated from inter-residue NOE peaks, and were incorporated as time-averaged restraints in a series of MD simulations. This MD with NMR refinement was used to generate representative model structures which illustrate the similarities and differences between the modified and unmodified cyclic backbones. The cOMP appears more rigid compared to the unmodified parent, and an additional intra-peptide hydrogen bond is observed [2]. Unrestrained MD simulations were also performed - the simulations with NMR refinement show good agreement compared to the unrestrained ones. This allows for the possibility of screening novel oxetane-modified peptides *in silico* and assessing their potential as therapeutics prior to synthesis.

[1] N. H. Powell et al., *Chem. Comms.*, 50, 8797 (2014)

[2] S. Roesner et al., *Chemical Science*, Advance Article (2019)

Poster n. 16 - Søren Meldgaard
Aarhus University, Denmark
sm@phys.au.dk

Machine learning enhanced global optimization by clustering local environments

Søren A. Meldgaard, Esben L. Kolsbjerg, Björk Hammer

Accurate prediction of catalytic activity relies on realistic underlying atomic models of the catalyst and substrate. However, as systems increase in size and complexity the task of determining the geometry of the catalyst becomes increasingly difficult. In this work [1] we show how to speed up global optimization of structures using machine learning methods. To represent the structures we introduce the auto-bag feature vector that combines: i) a local feature vector for each atom [2], ii) an unsupervised clustering of such feature vectors for many atoms across several structures, and iii) a count for a given structure of how many times each cluster is represented. During global optimization searches, accumulated structure-energy relations of relaxed structural candidates are used to assign local energies to each atom using supervised learning. The usefulness of the method is demonstrated in basin hopping [3] searches for 19-atom structures described by single- or double-well Lennard-Jones type potentials and for 24 atom carbon structures described by density functional theory. In all cases, utilizing the local energy information derived on-the-fly enhances the rate at which the global minimum energy structure is found.

[1] Meldgaard et al, *Journal of Chemical Physics*, 149, 134104 (2018) [2] J. Behler, M. Parrinello, *Phys. Rev. Lett.*, 98, 146401 (2007) [3] D. Wales, J. Doye, *The Journal of Physical Chemistry A*, 101, 5111 (1997)

Poster n. 17 - Henrik Lund Mortensen
Aarhus University, Denmark
hlm@phys.au.dk

Intelligent prediction of atomistic structures with reinforcement learning

Esben L. Kolsbjerg, Thomas L. Mathias S. Jörgensen, Henrik L. Mortensen, Sören A. Meldgaard, EJacobsen, Knud H. Sørensen, and Björk Hammer

We introduce an atomistic structure learning algorithm (ASLA) that utilizes a convolutional neural network to build atomistic structures atom by atom. The algorithm takes no prior data or knowledge on atomic interactions, but has access to inquire a first-principles quantum mechanical program for physical properties of any structure it may build. Using reinforcement learning, the algorithm accumulates knowledge of chemical compound space for a given number and type of atoms and effectively stores in the neural network the blue print for the optimal structural arrangement of the atoms for a given target property. With ASLA it is possible to transfer knowledge between similar problems. We demonstrate this feature by first obtaining knowledge on a simple, pristine graphene problem and subsequently reusing this knowledge to solve a complex graphene grain boundary problem, which includes a defect. The advantage of this feature is, that the simple problem may be computationally cheap to learn with no prior knowledge, compared to the complex problem. Using layerwise relevance propagation [1] we show that ASLA learns local 'rules' from the simple system, such as the well-known honeycomb pattern of pristine graphene. These rules are then applied to the complex system, giving a head-start compared to solving the complex system from scratch.

[1] Bach, Sebastian, Binder, Alexander, Montavon, Gregoire, Klauschen, Frederick, Muller, Klaus-Robert, and Samek, Wojciech. "On Pixel-Wise explanations for Non-Linear classifier decisions by Layer-Wise relevance propagation." PLoS One, 10(7):e0130140, 10 July 2015.

Poster n. 18 - David McDonagh
University of Southampton
dm1m15@soton.ac.uk

David McDonagh, Robert Shaw, Staszek Welsh, Jonathan Shearer, Lee Steinberg, William Glass
University of Southampton, University of Sheffield, University of Oxford

Argon is an interactive molecular dynamics simulator that teaches concepts in computational chemistry to people of all ages. Users can form crystals and watch phase changes, push and pull atoms, explore commonly used atomic potentials, or even make their own to create new kinds of interactions. Real-time updates of the Maxwell-Boltzmann distribution, the kinetic and potential energy, and the atomic radial distribution provide instant feedback to changes made, introducing concepts in an intuitive way. This outreach project is a collaboration between PhD students in Oxford, Southampton, and Sheffield, and has been taken across the country to science festivals, research showcases, and a variety of STEM events aimed at everyone from young children to undergraduates. Here we summarise some of the key features of the app with iPad and laptop demonstrations, and highlight how it has been used to teach chemistry to different age groups.

Poster n. 19 - Mirko Vanzan
University of Padova
mirko.vanzan@phd.unipd.it

A multiscale computational approach to investigate small gold nanoclusters optical features in solution

Mirko Vanzan and Stefano Corni
Department of Chemical Sciences, University of Padova

Nowadays, the study of thiolate-protected gold nanoclusters is of the most promising and exciting research field in nanoscience. The intrinsic quantum confinement effects given by the small dimension of the metallic core, gives them unique properties in terms of optical, magnetic and catalytic features.¹ Among all gold-based nanoclusters, $[\text{Au}_{25}(\text{SR})_{18}]^0$ (R = organic ligand) received the most extensive attention^{2,3}. Our work has the purposes of elucidate how the optical features of the $[\text{Au}_{25}(\text{SR})_{18}]^0$ changes with respect to the charged form and to understand how different ligands can affect the equilibrium distances (and thus the optical features) of various nanoclusters systems in solution. Time Dependent Density Functional Theory (TDDFT) simulations were performed on two X-Ray Diffraction (XRD) resolved structures of $[\text{Au}_{25}(\text{SR})_{18}]^0$ finding that different orientations of the organic ligands (coming from different nanoclusters structures) gives different equilibrium geometries and a sensible modification of the inner metallic kernel structure and polarizability. Metadynamics simulations were also performed on $[\text{Au}_{25}(\text{SCH}_2\text{CH}_3)_{18}]^0$, $[\text{Au}_{25}(\text{SC}_{16}\text{H}_{33})_{18}]^0$ and $[\text{Au}_{25}(\text{SCH}_2\text{CH}_2\text{Ph})_{18}]^{-1}$ double clusters systems. The results show a tendency in forming cluster aggregates in the long chain substituted nanoclusters system. Surprisingly, the Coulomb repulsion among nanoclusters in $[\text{Au}_{25}(\text{SCH}_2\text{CH}_2\text{Ph})_{18}]^{-1}$ system are well screened by the solvent and we recover a near cluster configuration minimum in the free energy profile. Finally, the free energy profile of the short chained nanoclusters pair is almost flat, indicating that no aggregations naturally occur here.

References

- (1) Chakraborty, I.; Pradeep, T. *Chem. Rev.* 2017, *117*, 8208–8271.
- (2) Heaven, M. W.; Dass, A.; White, P. S.; Holt, K. M.; Murray, R. W. *J. Am. Chem. Soc.* 2008, *130*, 3754–3755.
- (3) Dainese, T.; Antonello, S.; Gascòn, J. A.; Pan, F.; Perera, N. V.; Ruzzi, M.; Venzo, A.; Zoleo, A.; Rissanen, K.; Maran, F. *ACS Nano* 2014, *25*, 3904–3912.

Poster n. 20 - Martin Lea
University of Warwick
m.lea@warwick.ac.uk

Creating Versatile Photoswitches: Shedding Light on Design Parameters of Hemithioindigos

Martin Lea, Vasilios Stavros, and Reinhard J. Maurer
University of Warwick

The ability to reversibly modify the properties of a material in response to external stimuli is fundamental for the design of novel functional materials. Being able to manufacture and control this ability at the molecular level could lead to the realization of the next generation of nanomaterials for sensors and optoelectronics. Achieving an understanding of how chemical modifications can be used to augment or even inhibit switching will enable intuitive component design for the fabrication of tailor-made, light responsive materials and interfaces. An emerging class of photoswitching molecules Hemithioindigos (HTIs) exhibit promising photoisomerization properties which can be tuned through means of chemical functionalization. Here we present a joint first-principles-based computational and spectroscopic experimental study, wherein we identify the key design parameters of HTIs that enable its switching capabilities. We investigate how these parameters are modified through the influence of functional groups. On the basis of our findings, we propose molecules with a propensity for successful switching across various applications.

Poster n. 21 - Orestis Ziogos
University College London
o.ziogos@ucl.ac.uk

Computational studies of tetracene derivatives for organic electronics applications

Orestis G. Ziogos, Jochen Blumberger
Department of Physics and Astronomy University College London London WC1E 6BT, U.K.

Polyaromatic hydrocarbon (PAH) molecules are currently considered as a promising materials family for organic electronics applications [1]. An interesting PAH category includes the so-called cata-condensed PAHs, i.e. molecules made up by the fusion of benzene rings in such a way as not having a common carbon atom to three rings. A molecule belonging to this category is tetracene, a known hole-conducting material, which in its tetra-phenyl substituted form - the so-called rubrene molecule - has already surpassed amorphous silicon in device performance [2]. Our computational studies focus on organic molecules similar to tetracene, capable of hole transfer in their condensed phase. To be more precise, two families of materials are examined: pi-isoelectronic to tetracene molecules and tetracene derivatives with various non-aromatic peripheral functionalization [3]. Charge transfer capabilities are probed via the calculation of hole charge transfer integrals at the molecular dimer level using a plethora of computational methods [4,5], thus providing a critical overview of the quantitative results obtained by each method. Moreover, distinct structure-property relations are established, elucidating the effect of molecular morphology and substitution to the charge transfer mechanism.

[1] J. Wu, W. Pisula and K. Müllen, *Chem. Rev.* 2007, 107, 718. [2] C. Reese and Z. Bao, *Materials Today* 2007, 10, 20. [3] C. Kitamura et al. *Chem. Eur. J.* 2010, 16, 890-898. [4] A. Kubas, F. Gajdos, A. Heck, H. Oberhofer, M. Elstner, J. Blumberger, *Phys. Chem. Chem. Phys.* 2015, 17, 14342. [5] Z. Futera and J. Blumberger, *J. Phys. Chem. C* 2017, 121, 9677-19689.

Poster n. 22 - Raphael Chantreau Majerus
University of Warwick
R.Chantreau-Majerus@warwick.ac.uk

Investigating reaction rates using the Reaction Path Hamiltonian

Raphael Chantreau Majerus, Scott Habershon
University of Warwick, Department of Chemistry

The Reaction Path Hamiltonian was first derived in 1980, by Miller, Handy and Adams. They had derived a classical Hamiltonian for a reacting molecular system based on the principle that the reaction valley describes all mechanistic and dynamic steps accompanying a chemical reaction. The original Reaction Path Hamiltonian was formulated considering a number of assumptions. Firstly that the reaction valley is considered harmonic and can be described by a mass-weighted projected force constant matrix at each point. Secondly, in order to simplify the Reaction Path Hamiltonian, rotations of the reaction complex are excluded by assuming zero angular momentum. By using the Reaction Path Hamiltonian, one can ideally get insight into qualitative features of reaction mechanism and reaction dynamics such as vibrationally adiabatic potential, energy dissipation during the course of the reaction, translational-vibrational energy transfer during the course of the reaction. With respect to the project, the objective is to construct a Reaction Path Hamiltonian for a given reaction using information obtained through a climbing image nudged elastic band calculation in order to avoid the disadvantages of transition state searching. Once the Reaction Path Hamiltonian has been constructed using the Hessian, the rate of reaction of a given reaction can be investigated. An ensemble of trajectories that cross the dividing surface are obtained by sampling initial positions and momenta from the Boltzmann distribution on the dividing surface. Each initial condition is then propagated forward and backward in time using Hamilton's equations from the Reaction Path Hamiltonian and information can be gathered about the rate.

Poster n. 23 - Stela Makri
University of Warwick
S.Makri@warwick.ac.uk

A Preconditioning scheme for Minimum Energy Path finding methods

Stela Makri, Christoph Ortner, James R. Kermode

In transition state theory, the study of thermally activated transitions between energy minima is achieved by finding transition paths connecting the minima. These paths provide information on the energy barrier and reaction rates of the system without going through long and expensive simulations. To find them, current techniques use steepest descent-like minimisation to relax a discretised initial guess. However, steepest descent typically gives slow convergence rates in the presence of ill-conditioned potentials. I will be presenting how to reduce the condition number of the potential of an arbitrary system and improve the convergence speed and robustness of transition path finding methods, using a preconditioning scheme. Our key assumption is that the cost of constructing a preconditioner is much smaller than the cost of computing the potential; for density functional theory the cost of single point evaluations is much more expensive than the computation of a preconditioner and thus the proposed approach improves computing times significantly. We have developed a preconditioning scheme, where the preconditioner acts as a coordinate transformation of the discrete images along the path to aid the ill-conditioning in the transverse direction. We are currently developing a preconditioning scheme that considers the interactions between the images as well. Finally, we are working towards a preconditioning scheme for finding energy barriers in quantum molecular - mechanical molecular models.

Poster n. 24 - Christopher Penschke
University College London
c.penschke@ucl.ac.uk

Christopher Penschke, Angelos Michaelides
Department of Physics and Astronomy, University College London, Gower Street, London, WC1E 6BT, United Kingdom

Titanium dioxide (TiO₂) is one of the industrially most relevant materials and, consequently, a vast number of studies can be found in the literature [1-3]. In many applications, the adsorption of small molecules like water or carbon monoxide is a critical step, and understanding how to tune binding energies could facilitate optimization of catalytic and technological processes. It is well known that lattice expansion increases reactivity of metal surfaces [4], but it is not understood if and how this effect extends to metal oxides. In order to understand the effect of lattice strain on adsorption, various catalytically and/or environmentally relevant small molecules were adsorbed on different rutile-type metal oxides. Despite sharing the same crystal structure, the oxides differ in many properties, such as equilibrium lattice parameters and electronic structure, and display large variations in binding energies. Nevertheless, strain affects most molecule-oxide interactions in a similar way, with lattice expansion resulting in a stronger molecule-surface binding. This is especially pronounced for water adsorption on TiO₂, and expansive strain additionally facilitates water dissociation. The extent to which the adsorption energy varies with strain is dependent on the molecule and metal cation, but the general trends discussed in this work may provide crucial insights for an important class of materials.

[1] U. Diebold, Surf. Sci. Rep. 48, 53 (2003). [2] M. A. Henderson, Surf. Sci. Rep. 66, 185 (2011). [3] C. L. Pang, R. Lindsay, G. Thornton, Chem. Rev. 113, 3887 (2013). [4] M. Mavrikakis, B. Hammer, J. K. Nørskov, Phys. Rev. Lett. 81, 2819 (1998).

Poster n. 25 - James Brixey
University of Warwick
j.brixey@warwick.ac.uk

Modeling the scattering of cracks in diamond at single atom impurities

James Brixey [1,2], James Kermode [1]

[1] *Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry CV4 7AL, United Kingdom* [2] *Diamond Science & Technology CDT, Materials & Analytical Sciences, University of Warwick, Coventry CV4 7AL, United Kingdom*

Diamond is commonly used as an industrial cutting implement and in drill bits due to its extreme hardness. However, it undergoes catastrophic brittle fracture, with the macroscopic material response determined by breaking of individual bonds [1]. Single atom defects can even lead to crack deflection, e.g. in silicon [2]. This work targets the idea that similar single atom defects in diamond, such as substitutional nitrogen, the nitrogen vacancy, may lead to crack scattering in diamond. Addressing this requires a diamond model coupling quantum mechanical (density functional theory) and empirical potentials [3]. Preliminary results for the multiscale model of crack propagation along the (111) cleavage plane, intersecting with point defects, will be presented. Since it is possible to control the nature [4] and density [5] of point defects, we envisage our work will suggest practical strategies for the manufacture of more durable industrial diamonds.

[1] Bitzek et al., *International journal of Fracture* 191(1): 13-30, (2015) [2] Kermode et al., *Nature Communications* 4, 2441 (2013) [3] Bernstein et al., *Reports on Progress in Physics*, 72, 026501 (2009) [4] Jelezko and Wrachtrup, *phys. stat. sol. (a)* 203, No. 13 [5] Kanda and Watanabe, *Diamond and Related Materials* 8 (1999)

Poster n. 26 - Harry Tunstall
The University of Warwick
h.tunstall@warwick.ac.uk

Towards a General-Purpose Interatomic Potential for Silicon Carbide

Harry Tunstall, James Kermode, Gabriele Sosso
The University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, UK

SiC is a prototypical material for high temperature applications (e.g aerospace, automotive and thermoelectric) involving complex microscopic processes typically inaccessible to experiments [1]. To gain insight into the functional properties of e.g. SiC nanostructures, computationally expensive quantum mechanical methods such as density functional theory (DFT) must be employed. This is because less computationally demanding methods are almost always not accurate enough. In fact, similar to Si and C alone, various empirical interatomic potentials have been developed for SiC, such as Tersoff or Stillinger-Weber [2,3]. These potentials are designed to reproduce specific features of the material, at the expense of transferability to a wider range of functional properties. The aim of this project is to build a general purpose interatomic potential for SiC (e.g using machine-learning regression starting from a DFT dataset of representative configurations [4,5]). As a first step towards achieving this goal we here report a comparative study of the performance of currently available models for SiC [2,3,6], focussing in particular on the structural properties of the liquid phase.

[1] I. Aharonovich and M. Toth, *Nat. Phys.* 10, 93 (2014). [2] J. Tersoff, *Phys. Rev. B* 39, 5566 (1989). [3] P. Vashishta, R. K. Kalia, A. Nakano, and J. P. Rino, *J. Appl. Phys.* 101, 1 (2007). [4] A. P. Bartok, J. Kermode, N. Bernstein, and G. Csanyi, *Phys. Rev. X* 8, 41048 (2018). [5] G. C. Sosso, V. L. Deringer, S. R. Elliott, and G. Csányi, *Mol. Simul.* 44, 866 (2018). [6] L. Pastewka, A. Klemenz, P. Gumbsch, and M. Moseler, *Phys. Rev. B* 87, 1 (2013).

Poster n. 27 - Connor Box
University of Warwick
connor.box@warwick.ac.uk

Simulation of electronic friction effects in ultrafast chemical dynamics at metal surfaces: Understanding the successes and failures of ab-initio methods

Connor Box, Reinhard J. Maurer
Department of Chemistry, University of Warwick, Coventry, CV4 7AL, UK

The coupling of molecular adsorbate motion with hot electrons in a metal substrate represents a breakdown of the Born-Oppenheimer approximation with measurable consequences. An accurate theoretical description of how these hot-electron effects modify the reaction dynamics of molecules on metals will be essential to utilize light-matter interaction in catalysis. The electron-phonon coupling between adsorbate vibrations and hot electrons are efficiently described in a density functional theory-based molecular dynamics with electronic friction (MDEF) approach, where electronic friction forces act on atoms within a Langevin framework. [1] Several methods have been proposed to describe electronic friction; however, more work remains to be done to provide a transferable and accurate description of experimental findings. In this work, we present our efforts towards pushing beyond the current limitations of the MDEF method. We explore the consequences of existing approximations in MDEF calculations for the frequently studied carbon monoxide adsorbed Cu(100). [2] We systematically assess the importance of substrate motion, vibrational anharmonicity, and mode coupling in comparison with recently published many-body perturbation theory results [3] to guide future directions of method development.

[1] M. Askerka, R. J. Maurer, V. S. Batista and J. C. Tully, *Phys. Rev. Lett.*, 2016, 116, 115432. [2] R. J. Maurer, M. Askerka, V. S. Batista and J. C. Tully, *Phys. Rev. B*, 94, 115432 [3] D. Novko, M. Alducin and J. I. Juaristi, *Phys. Rev. Lett.*, 120, 156804.

Poster n. 28 - Siva Chiriki
Aarhus University
sivachiriki@phys.au.dk

Role Model Regularization for Accelerating Atomic Structure Search

Siva Chiriki
Department of Physics and Astronomy, Aarhus University, Denmark.

In order to speed up the atomic structure search for chemical compounds, we have developed role model regularization (RM-reg) method within the frame work of density functional tight binding theory (DFTB) using evolutionary algorithm. The method is to demonstrate the speed up the finding global minima (GM) of anatase TiO₂(001) surface reconstruction with increasing number of layers. The present method consists of feature space relaxation by minimizing role model distance followed by DFTB relaxations. The key development in this method is different strategies for the selection of some of the atomic environments as role models (RM's) and relaxation strategies of few atoms within the feature space. This allows the GO search to escape meta stable states in configurational space and hence speed up the GO search. The results based on the GM search of anatase TiO₂(001) surface indicates that the method outperforms with increasing number of layers compared to the cluster regularization method [*J. Chem. Phys.*,148, 241734 (2018)] as benchmark.

Poster n. 29 - Berk Onat
University of Warwick
B.Onat@warwick.ac.uk

Analyses on Structural Representations of Molecules in Machine Learning

Berk Onat, James R. Kermode
School of Engineering, University of Warwick, Coventry, United Kingdom

Machine Learning has been gaining considerable attraction in materials science, chemistry and biology as the need to extract and classify the information of materials and molecules increases as a result of the large amount of theoretical and experimental data that is now available. For more than a decade, classification of molecules has been studied according to chemical and biological properties, and as the structural point of view, their construction based on many-body expansions, e.g. bonds, angles and dihedrals. However, these approaches have been complemented recently with efficient structural representations based on the atomic configurations such as Behler-Parrinello symmetry functions (SF) [1], Smooth Overlap of Atomic Positions (SOAP) [2] and Many-Body Tensor Representation (MBTR) [3] in machine learning approaches. A common approach is to identify the similarities of the molecules or in other words the differences of them for classification or regression. While these representation methods are based on mapping of the structural information of the molecules to hyper-dimensional spaces, research on how they are effective and sensitive on their choices of representations is very limited so far. In this presentation, we will discuss the classification of representations and how one can examine their sensitivity to changes in atomic configurations using large datasets. We will also present our results on the analyses of the performance of various representations of materials on bulk and molecular datasets extracted from NOMAD European Centre of Excellence archive.

[1] J. Behler and M. Parrinello, PRL 98, 146401 (2007). [2] A.P. Bartok, R. Kondor, and G. Csanyi, PRB 87, 184115 (2013). [3] H. Huo, M. Rupp, arXiv 1704.06439, (2017).

Poster n. 30 - Wilke Dononelli
Aarhus University
wd@phys.au.dk

CCSD(T) Embedding for Molecules and Metal Nanoparticles

Wilke Dononelli (a,b), Björk Hammer (a) and Thorsten Klüner (b)
a) Theoretical Chemistry, Carl von Ossietzky University Oldenburg, Germany b) Department for Physics and Astronomy, Aarhus University, Denmark

Calculating energies and properties with chemical accuracy is one of the goals of quantum chemistry. Unfortunately, methods that lead to highly accurate results are often computationally demanding. Therefore, embedding methods have become popular approaches e.g. for calculating PES of adsorbed molecules on oxide surfaces or partial optimization of molecular structures containing thousands of atoms. The general idea of such embedding techniques is to describe a subsystem at a high level of theory (e.g. CCSD(T)) and embedded it in an extended region, which can be described at a lower level of theory like DFT or force fields. In a recent study, we calculated CCSD(T) adsorption energies on metal nanoparticles (NPs) of varying sizes [1]. We were able to show that it is possible to calculate adsorption energies and activation barriers for different sizes of NPs at the CCSD(T) level of theory by using ONIOM as a QM/QM' embedding scheme and discussed the results with respects to full CCSD(T) and DLPNO-CCSD(T) energies for small 13 atom metal NPs [2]. Another way of calculating energies at higher levels of theory is using either the method of increments (see e.g. ref [3,4]) or a simpler similar approach (without usage of localized molecular orbitals from an all electron calculation), the many body expansion (MBE). The advantage of using a MBE is that total energies for a given system can be summed from a pre-calculated database or can be estimated e.g. with neural networks [5]. In our new approach we are trying to use a MBE in the framework of the before mentioned QM/QM' embedding scheme [1] in order to overcome some problems related to neglecting the overall electronic structure of a system when using the MBE.

[1] W. Dononelli and T. Klüner; Faraday Discuss. 208(2018) [2] R. Arrigo et. al, Faraday Discuss. 208(2018) [3] H. Stoll, Phys. Rev. B 46(1992) [4] E. Voloshina, Phys. Rev. B 85(2012) [5] K. Yao et. al., J.Chem.Phys. 146(2017)

Poster n. 31 - Harry Jenkins
Cardiff University
JenkinsHJ1@Cardiff.ac.uk

Identifying Design Principles for Solid State QM/MM Embedded Cluster Modelling

Harry Jenkins, Andrew Logsdail
Cardiff Catalysis Institute, Cardiff University

The current most popular computational method in modelling surface reactions is periodic planewave density functional theory (DFT) [1]. Periodic DFT is both expansive in its functionality, and easy to use. However, there are still some major limitations. For instance, the preferred basis representation of planewaves is inefficient for high-level hybrid-DFT approaches for isolated catalytic chemistry. In addition, periodic surface models cannot be used to model charged defects due to technical incompatibilities when trying to include any compensating background charge. As an alternative, hybrid quantum- and molecular-mechanical (QM/MM) modelling can be coupled with an embedded cluster approach, which combines the high accuracy of QM modelling, with the high efficiency of MM modelling (MM), all in an aperiodic model that reproduces the bulk environment [2]. However, the uptake of QM/MM in the solid-state community is limited by the bespoke nature of the model configuration, which typically requires empirical tuning to achieve accuracy comparable to the periodic DFT approaches. In this work, we present our progress in outlining systematic design principles for QM/MM models, based initially on work using MgO. This has been pursued using the ChemShell [3] software package, with FHI-aims [4] used to perform DFT calculations, using both popular GGA approaches, compared to periodic DFT, and high-level exchange-correlation functionals (PBE0). The focus of the work is understanding how cluster design principles, such as partitioning of the QM-region affect the accuracy of measurable results. Our overall aim is to deliver an automated approach to cluster construction, with objective justification for each step involved.

[1] Becke, J. Chem. Phys. 140, 18A301 (2014) [2] Groenhof, Methods in Molecular Biology, Ch.3 (2013) [3] Sherwood et al., J. Mol. Struct. (Theochem.) 632, 1 (2003) [4] Blum et al., Computer Physics Communications 180, 2175-2196 (2009)

Poster n. 32 - Matthew Turner
University of Warwick
m.turner.1@warwick.ac.uk

Determination of Secondary Species in Solution Through Pump-Selective Transient Absorption Spectroscopy and Explicit-Solvent TDDFT

Matthew Turner
University of Warwick chemistry and physics department

The measured electronic excitations of a given species in solution are often a composite of the electronic excitations of various equilibrium species of that molecule. It is common for a proportion of a species to deprotonate in solution, or form a tautomeric equilibrium, producing new peaks corresponding to the electronic excitations of the new species. One prominent example is alizarin in methanol, which at different temperatures, and in solutions with differing pH, has an isosbestic point between the two dominant excitations at 435 nm and 540 nm. The peak at 435 nm has been attributed to alizarin; the peak at 540 nm, however, more likely results from a species in equilibrium with alizarin. In this work, we were able to use both experimental and computational techniques to selectively examine electronic properties of both alizarin and its secondary species in equilibrium. This was achieved through use of transient electronic absorption spectroscopy, following selective photoexcitation of a specific species in equilibrium. The resulting transient electronic absorption spectra were compared to the known transient absorption spectra of potential secondary equilibrium species. The ground state absorption spectra associated with each species in equilibrium were predicted using linear-scaling Time-Dependent Density Functional Theory with an explicitly-modelled solvent and compared to the experimental result. This evidence from both techniques combines to suggest that the excitation at 540 nm arises from a specific monoanionic form of alizarin.

Poster n. 33 - Malthe Bisbo
University of Warwick
mkb@phys.au.dk

Automated structure determination accelerated with machine learning

M. K. Bisbo, B. Hammer
Department of Physics and Astronomy, Aarhus University

Knowing the exact atomic configuration of chemical systems is a prerequisite for calculating their chemical properties, making automated structure determination an important field. When using density functional theory (DFT), current search methods are however limited in either thoroughness or to relatively small systems because of the large number of expensive DFT calculations required. Inspired by the current popularity of machine learning, we propose a surrogate based search method that relies on machine learning to reduce the required number of DFT calculations by orders of magnitude. The majority of current search methods rely on locally relaxing new candidate structures with DFT, which requires multiple DFT calculations for each candidate. We use a Gaussian Process regression (GPR) [1] model as a cheap surrogate model of the potential energy surface, and train it on the fly using all DFT energies accumulated during the search. Throughout the search all local relaxations [2] are performed using this cheap surrogate model, and single DFT calculations are only made for especially promising surrogate-relaxed candidates. To quantify how promising new structures are, we take into account both the energy and uncertainty predicted by the GPR model as a means to balance exploration and exploitation in the search [3]. The superior performance compared to a standard GA is exemplified on the recently discovered SnO₂(110)-(4x1) reconstruction [4] and the anatase TiO₂(001)-(1x4) reconstruction, for which the complexity of the problem is varied by increasing the number of bulk layers included in the search.

[1] A. P. Bartók, M. C. Payne, R. Kondor, and G. Csányi, Phys. Rev. Lett. 104, 136403 (2010). [2] E. G. del Rio, J. J. Mortensen, K. W. Jacobsen, arXiv: 1808:08588 (2018) [3] M. S. Jörgensen, U. F. Larsen, K.W. Jacobsen, B. Hammer, J. Phys. Chem. A 122, 1504 (2018) [4] L. R. Merte et al, Phys. Rev. Lett. 119, 096102 (2017)

Poster n. 34 - Martina Stella
CEA Grenoble
m.stella@imperial.ac.uk

Towards a systematic multi-scale method for TADF-based OLED materials in the BigDFT code

Martina Stella (1), Laura Ratcliff (1), Luigi Genovese (2)
1) Imperial College London, UK, 2) INAC, CEA Grenoble, France

Thermally activated delayed fluorescence (TADF) represents a promising mechanism for the design of the next generation of OLEDs. The need for substituting the expansive transition metal-based materials with fully organic ones, has boosted research in the electronic structure of these materials. TADF emission is based on inverse inter-system crossing from triplet state to singlet states. Extensive characterisation of these states has shown that such excitations cannot be simply categorised as charge-transfer or local excitation but are described by a mixture of these two processes. As a result of such intricate electronic structure, modelling of TADF requires a methodology able to provide high accuracy while explicitly including environmental effects. We aim to develop a multi-scale approach within the BigDFT code where we combine the needed accuracy with the ability of treating big systems, which would allow one to go beyond implicit models. BigDFT is designed to run on parallel architectures and can treat large systems while ensuring high, controllable precision. As a first step towards a robust methodology, we assess the performance of TDDFT and CDFT methods for model systems using both cubic and linear scaling approaches.

[1] Daubechies wavelets for linear scaling density functional theory, S Mohr, LE Ratcliff, P Boulanger, L Genovese - The Journal of chemical physics, 2014. [2] Fragment approach to constrained density functional theory calculations using Daubechies wavelets, LE Ratcliff, L Genovese, S Mohr, T Deutsch - The Journal of chemical physics, 2015.

Poster n. 35 - João Morado
School of Chemistry, University of Southampton
J.Morado@soton.ac.uk

Study of the Conformational Dynamics of Small Molecules with Pharmaceutical Relevance

João Morado [1], Richard Ward [2], Paul Mortensen [3], Marcel Verdonk [3], Jon Essex [1], Chris Skylaris [1]

[1] School of Chemistry, University of Southampton, Southampton, United Kingdom [2] IMED Oncology, AstraZeneca, Cambridge, United Kingdom [3] Astex Pharmaceuticals, Cambridge, United Kingdom

All processes in living organisms rely on molecular organization and recognition events. Molecular recognition is highly influenced by the conformational changes that occur before and upon binding. This phenomenon is of uttermost importance in drug design because, in general, a molecule that binds a protein becomes less mobile, and the resulting loss in configurational entropy opposes the attractive enthalpy force that drives binding. The observed decrease of conformational flexibility upon binding leads to the emergence of ligand pre-organization as a strategy for structure-based drug design, in which the flexibility of potential ligands is restricted so that they benefit from a lesser entropic penalty during complexation. We are interested in controlling the pre-binding molecular organization of small molecules with pharmaceutical relevance. As a first step towards this goal, we present a study of the conformational dynamics of compound 26, which is a non-peptidic, orally bioavailable and efficacious low nM antagonist of both cIAP1 and XIAP. In order to study its conformational dynamics, we performed molecular dynamics simulations in implicit and explicit solvent. We also ran replica exchange with solute scaling simulations in order to address the convergence of the standard molecular dynamics simulations and overcome the problem of quasi-ergodicity. Finally, we used the DASH dihedral clustering algorithm to identify the main observed conformations and performed principal component analysis to characterize the collective movements responsible for the observed dynamics. The aim of these simulations was to corroborate NMR and X-Ray data, which indicate that the molecule is possibly pre-organized in solution via "hydrophobic collapse" into a conformation similar to the one observed in the protein-ligand complex. The results obtained support the experimental data and give new insights about state populations and collective molecular movements of compound 26.

Poster n. 36 - Victor L. Do Nascimento
University of Southampton
vdn1m17@soton.ac.uk

Topological and Energetic Characterization of Organic Hydrate Crystal Structures and Novel Structure Prediction Method Development.

Victor L. Do Nascimento

Crystal structure prediction (CSP) has seen many advancements over the recent years, as can be observed by comparing successive CSP blind tests [1]. Nonetheless, high-degree-of-freedom systems comprising highly flexible molecules and those with multiple components remain a challenge. In conjunction with this, crystal water absorption and hydrate formation is a widespread phenomenon, often occurring during storage and as a side-effect of manufacturing processes, which can have adverse effects on drug formulation, such as lowering bioavailability [2]. It is thus of interest to be able to predict hydrate crystal formation and its relative stability within a computationally tractable time. Current works concerned with hydrate crystal structure prediction show that current energy models employed are sufficiently robust to correctly reproduce the geometry and relative stability among hydrate stoichiometries though these calculations have required full CSPs to be carried out for expensive multicomponent crystals [3-5]. Here we present current work carried out in understanding the role played by water in stabilizing crystals, together with looking at the topology of water environments in stable hydrate structures. We combine this information in present efforts at generating hydrates from the inexpensive single component landscape generation coupled with anisotropic lattice expansion and Monte-Carlo water insertion.

1. Reilly, A. M. et al. *Acta Crystallogr. Sect. B Struct. Sci. Cryst. Eng. Mater.* 72, 439-459 (2016). 2. Khankari, R. K. & Grant, D. J. W. *Thermochimica Acta* 248, (1995). 3. Braun, D. E., Karamertzanis, P. G. & Price, S. L. *Chem. Commun.* 47, 5443 (2011). 4. Braun, D. E. & Griesser, U. J. *Front. Chem.* 6, 31 (2018). 5. Hulme, A. T. & Price, S. L. *J. Chem. Theory Comput.* 3, 1597-1608 (2007).

Poster n. 37 - Kjell Jorner
AstraZeneca UK
kjell.jorner@astrazeneca.com

Reaction prediction with hybrid mechanistic and machine learning models

Kjell Jorner, Tore Brinck, Per-Ola Norrby, David Buttar
Kjell Jorner, David Buttar: Early Chemical Development, Pharmaceutical Sciences, IMED Biotech Unit, AstraZeneca, Macclesfield, United Kingdom
Tore Brinck: Applied Physical Chemistry, Department of Chemistry, CBH, KTH Royal Institute of Technology, Stockholm, Sweden
Per-Ola Norrby: Early Product Development, Pharmaceutical Sciences, IMED Biotech Unit, AstraZeneca, Gothenburg, Sweden

Machine learning models are increasingly used to predict chemical reactivity. General models aim to treat all chemical reactions and are trained on patent data and databases of published reactions [1]. Reaction-class models instead aim to achieve higher accuracy for a specific reaction type of special interest [2]. At AstraZeneca, we are developing predictive models for use in drug development and route design [3, 4]. Reaction prediction has the potential to both accelerate the drug discovery process as well as aid the development of efficient processes for drug manufacturing. While models with lower accuracy can be tolerated in drug discovery, where the goal is diversity, demands in route design are higher as the goal is optimizing yields, selectivity and reaction conditions. We are now developing high-accuracy models for predicting the outcome of nucleophilic aromatic substitution, one of the most important reaction classes in the pharmaceutical industry. To reach the required accuracy, we use a hybrid mechanistic and machine learning approach. By including calculated transition states from quantum chemistry, smaller data sets are needed to train the model [5]. Machine learning models are trained on a relatively small set of physical meaningful descriptors [6] together with the approximate activation energies. The resulting model will be incorporated into a black-box tool accessible to experimental process chemists through a web interface.

[1] Schwaller et al. arXiv:1811.02633 [2] Ahneman et al. Science. 2018, 360, 186.
[3] Tomberg et al. J. Org. Chem. 2018, DOI: 10.1021/acs.joc.8b02270 [4] Rosales et al. Nat. Catal. 2018. DOI: 10.1038/s41929-018-0193-3. [5] Zhang et al. Comput. Mater. 2018, 4, 25 [6] Brinck et al. J. Phys. Chem. A 2016, 120, 10023.

Poster n. 38 - Berk Onat
University of Warwick
B.Onat@warwick.ac.uk

Determination of Interatomic Voids Between Molecules Using Voronoi S-Networks

Berk Onat (1, 2), Narjes Ansari (3), Ali Hassanali (3), Gabriele C. Sosso (2)
1. School of Engineering, University of Warwick, Coventry, United Kingdom
2. Department of Chemistry, University of Warwick, Coventry, United Kingdom
3. Condensed Matter and Statistical Physics, ICTP, Trieste, Italy

Voronoi tessellation has been extensively used to investigate the atomic configurations in material science, chemistry, biology and to understand the order-disorder packing, neighbouring in atomic structure and complex system analyses in wide range of materials and molecules. Although it is an effective method to partition the space according to the given atomic configuration, the method has limitations on capturing the interatomic space when material consists of multi-species with different van der Waals radii. Variable radii in the method leads sphere-cutting through the Voronoi edges and hence misses the desired space determination. To tackle this problem, S-Networks of Euclidean Voronoi diagrams are utilised. Voronoi S-Networks are constructed on the equidistant boundaries away from the van der Waals surfaces. This lets one to identify the available voids between the atoms accurately. In this presentation, we will give the details of the algorithm to build the S-Networks and our code implementation on how to determine the voids using these networks. Furthermore, we will present our results on the identification of the voids in supercooled water based on molecular dynamics simulations.

Poster n. 39 - Gareth Richings
University of Warwick
g.richings@warwick.ac.uk

MCTDH on-the-fly: Efficient grid-based quantum dynamics without pre-computed potential energy surfaces

Gareth W. Richings, Christopher Robertson, Scott Haberson

Recent advances in the field of theoretical quantum dynamics have made the study of molecules of non-trivial size feasible. However, the bottleneck in terms of effort is the construction of the potential energy surface (PES) on which the nuclear wavefunction evolves. In order to minimise effort, and make methods usable by non-experts, the PES should ideally be constructed on-the-fly, that is while the nuclear dynamics is proceeding. As quantum dynamics is inherently non-local, this is an issue. One solution is the DD-vMCG method which uses Gaussian functions as the basis of the nuclear wavefunction, allowing a local harmonic expansion of the PES around the centres of the Gaussians to be calculated from which a global representation of the PES can be formed. This method suffers from numerical difficulties in the dynamics due to the non-orthogonality of the basis and requires the expensive calculation of energy gradients and Hessians. In this work we present a recently developed method to integrate construction of the PES, on-the-fly, using Kernel Ridge Regression (KRR) with grid-based quantum dynamics methods, in particular the MCTDH method.[1] These well developed dynamics methods use orthonormal basis functions whilst the KRR expansion of the PES only requires the evaluation of electronic energies. In addition to allowing dynamics on a single PES, the KRR expansion has been allied with pragmatic diabatisation schemes,[2,3] and hence the method can also cope with dynamics on multiple, non-adiabatically coupled PESs. Along with a description of the method, including recent, significant improvements to the method's efficiency, illustrative results will be presented showing the method's efficacy.

[1] G.W. Richings, C. Robertson, S. Habershon, J. Chem. Theory. Comput., 2018, DOI: 10.1021/acs.jctc.8b00819 [2] G.W. Richings and G.A. Worth, J. Phys. Chem. A, 2015, 119, 12457 [3] C. Robertson, et al., J. Comp. Chem., 2018, DOI: 10.1002/jcc.25764

Poster n. 40 - Christopher Robertson
University of Warwick
c.robertson@warwick.ac.uk

Novel Path-Integral Approximations Using the Thermal-Symmetric Time-Correlation Function

Dr. Christopher Robertson, Dr. Scott Habershon

In recent years a number of Monte-Carlo (MC), short-time Path integral strategies (1,2,3) have been devised to calculate complex-symmetrised quantum-correlation function between two operators. The so-called 'sign problem' when evaluating the phase component using MC makes the integral difficult to converge for long euclidean-times. We present two novel approaches which successfully overcome the sign problem. The first replaces the phase of the correlation function by an approximate function which has only positive components and can therefore be included into the sampling function, obviating the sign-problem all together. The second converts the TCF into a joint density of states (JDOS) representation for which the JDOS can be calculated using the Wang-Landau Algorithm. The approximations are shown to work satisfactorily for 1D $x^n(0) x^n(t)$ correlation functions with different model system potential and which can be extended to a larger number of degrees of freedom.

(1) Goran Krilov, Eunji Sim, and B. J. Berne, JChemPhys, 114, 1075 (2001); (2) Monteferrante, M., Bonella, S., Ciccotti, G, JChemPhys, 133, 16, 164104, (2010) (3) Rota, R., Casulleras, J., Mazzanti, F., et al., JChemPhys 142, 11, 114114 (2015)

Poster n. 41 - Germain Clavier
SIMATLAB
germain.clavier@uca.fr

Germain Clavier, Alain Dequidt, Benoit Latour, Etienne Munch, Benoit Schnell, Patrice Malfreyt

SIMATLAB/TIM - Institut de Chimie de Clermont-Ferrand (ICCF) - UMR 6296, Bâtiments Chimie 3 à 7, Campus Universitaire des Cézeaux, 24 avenue Blaise Pascal TSA 60026, CS 60026, 63178 AUBIERE Cedex France Manufacture Française de Pneumatiques MICHELIN, Centre de Ladoux, 23, place des Carmes, 63040 Clermont-Ferrand, France

Polymeric materials are widely used in the industry for their wide variety of properties. For the industry, the making of interesting materials and their study is often time and resource consuming. Molecular simulation is a way to easily understand and predict some interesting properties of polymeric systems, such as mechanical properties, but macromolecular time and length scales are often out of reach for molecular dynamics simulations. Simplifying the molecular models using a coarse-grained approach allows to extend the size of the systems as well as the timescales. Yet depending on the coarse-graining method, some properties are better retained from the molecular level than others. We propose to compare two coarse-grained force fields for modelling cis-polybutadiene to understand limitations of both methods. The emphasis will be put on how the properties depend on the force fields, as well as on the effect of the degree of coarse-graining and the molecular weight. The force fields were developed using either iterative Boltzmann inversion [1] or Bayesian parametrization [2] and were used to compute static structural properties (radial distribution function, end-to-end vector distribution, density) and dynamical properties (shear modulus, mean-square displacement). We show how some of these results can be related to experimental measurements of mechanical properties.

[1] G. Maurel, F. Goujon, B. Schnell, and P. Malfreyt. Prediction of structural and thermomechanical properties of polymers from multiscale simulations. *RSC Advances*, 5(19):14065-14073, 2015. [2] A. Dequidt and J. G. S. Canchaya. Bayesian parametrization of coarse-grain dissipative dynamics models. *The Journal of Chemical Physics*, 143(8):084122, 2015.

Poster n. 42 - Billal Sohail
University of Warwick
billal.sohail@warwick.ac.uk

Tuning TCNQ adsorption on Ag(100): A joint DFT and experimental study of the role of alkali co-adsorption

Billal Sohail (1), Luke Rochford (2), Phil Blowey (1,3), Phil Woodruff (4), Giovanni Costantini (1), and Reinhard J. Maurer (1)

(1) Department of Chemistry, University of Warwick, UK (2) School of Chemistry, University of Birmingham, UK (3) Diamond Light Source, Didcot, OX110DE, UK (4) Department of Physics, University of Warwick, UK

TCNQ(7,7,8,8-tetracyanoquinodimethane) is a well-established electron acceptor with an innate ability to form conductive organic salts. The application of organic semiconductors on coinage metals is a growing field which lends to the understanding of molecular electronics. A multidisciplinary field which has piqued in recent years due to the variety of applications such as, organic photovoltaics (OPVs), organic field effect transistors (OFETs). TCNQ alone on coinage metal surfaces conforms to a specific geometry with the peripheral cyano groups bent towards the surface; an effect lifted upon co-adsorption with potassium. The work presented is to elucidate the underlying mechanism of charge transfer and dispersion interactions using theoretical and computational efforts. Combining many-body-dispersion-inclusive Density-Functional Theory [1] and experimental techniques such as X-ray standing wave (XSW) data and STM measurements.

[1] Maurer et al., *J. Chem. Phys.*, 143, 102808 (2015)

Poster n. 43 - Daniele Fazzi
University of Warwick
dfazzi@uni-koeln.de

Daniele Fazzi, Simone Fabiano, Fabrizia Negri and Klaus Meerholz

The accurate description of polaronic states in organic conjugated materials is of paramount importance to understand charge and energy transfer mechanisms [1]. Such mechanisms are at the basis of emerging energy-saving applications, as organic thermoelectric devices, electrochemical transistors and bioelectronic applications [2]. Modelling polaronic states in extended conjugated systems (e.g. polymers and organic crystals), is here performed in the frame of Density Functional Theory (DFT) and constrained-DFT (C-DFT) methods. We show how DFT fails in describing the polaronic states, the higher is the electron delocalisation and the extension of the system, thus leading to unstable solutions for the ground state electronic wavefunction [3]. Broken-symmetry and C-DFT methods represent possible strategies to overcome the problem, providing acceptable descriptions for multi-configurational states, otherwise impossible to describe neither with wavefunction based methods nor with hybrid approaches. The case of two different n-type polymers (i.e., naphthalene-diimide donor-acceptor polymer - P(NDI2OD-T2) - and poly-benzimidazobenzophenanthroline - BBL), state-of-the-art materials for organic transistors and thermoelectric devices [3], is here discussed. We show how the molecular structure, the backbone regioregularity and the inter-molecular packing of the chains influence the polaronic properties, in particular the structural relaxations, reorganisation energies, electronic transitions and coupling integrals. Both theoretical and experimental investigations are here compared with the aim to provide an overall picture of the structure-property relationships and charge transport mechanisms in the emerging class of n-type conjugated materials.

[1] Oberhofer H., et al., Chem. Rev. 2017, 117, 10319. [2] Kroon, R., et al., Chem. Soc. Rev. 2016, 45, 6147. [3] Wang, S., et al., Adv. Mater. 2018, 30, 1801898.

Poster n. 44 - Idil Ismail
University of Warwick
Idil.Ismail@warwick.ac.uk

Optimising catalytic design using automated reaction path sampling

Idil Ismail
Department of Chemistry and Centre for Scientific Computing, University of Warwick, Coventry CV4 7AL, United Kingdom.

The automated prediction and construction of catalytic reaction pathways has gained increasing interest over the past decade. However, despite the remarkable advances made in computational chemistry, the complete exploration of all possible reaction paths remains an outstanding challenge, with previous studies finding that such manual, exhaustive explorations to be largely error prone and generally unfeasible [1]. In this work, we employ a novel approach using stochastic graph-based methods to allow for the complete and automated sampling of the potential energy surface (PES) of chemical reactions involving the oxidation of Carbon monoxide using Platinum-based catalysts. Using our conceptual knowledge of chemistry, we employ simple chemical heuristics to improve the efficiency of sampling chemical space by disregarding all chemically irrelevant elementary reactions. The development of such unbiased methods will allow for unprejudiced discoveries in molecular reactivity, with the potential to uncover previously unknown chemical intermediates and mechanisms. The catalytic oxidation of Carbon monoxide molecules over Platinum nano-particle catalysts is investigated using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) and the ReaxFF forcefield [2]. The results of these simulations will help to identify the complete dynamic process of reaction mechanisms, providing atomic scale insights in enumerating all chemically sensible reaction paths that give rise to Carbon dioxide. This will in turn provide us with the necessary information to help inform a better strategy to optimise catalytic design in order to maximise product selectivity and increase the overall yield.

Poster n. 45 - Samuel Hall
University of Warwick
s.hall.4@warwick.ac.uk

Revealing spectroscopic signatures of molecule-metal interaction: A computational core-level spectroscopy study.

Samuel J Hall and Reinhard J Maurer
Department of Chemistry, University of Warwick

Core-level spectroscopy, both x-ray absorption (XAS) and photoemission (XPS), represents an immensely important tool for the characterisation of complex hybrid organic-inorganic interfaces. The information on these interactions is often hidden in a convolution of spectroscopic signatures that is affected by initial state effects (e.g. chemical bonding) and final state effects (e.g. molecule-metal charge-transfer and hybridisation) alike. First-principles simulation of core-level spectra enables us to disentangle these effects and offers a systematic assessment of varying molecule-metal interaction strength and its spectral manifestation. On the examples of small conjugated organic molecules and aromatic carbon nanostructures at single-crystal metal surfaces such as Cu(111), Ag(111), and Pt(111), we investigate the signatures of molecule-metal bonding by simulating near-edge X-ray absorption fine-structure (NEXAFS) and XPS spectra. Calculations were carried out using dispersion-inclusive Density Functional Theory calculations using the transition potential method. [1,2] Using orbital-projection techniques, we are able to provide a full spectral decomposition in terms of initial and final states. In combination with a charge and structure analysis, we arrive at a detailed picture of how molecular composition and metal reactivity affect core-level spectra.

[1] K. Diller, R. J. Maurer, M. Müller and K. Reuter, *J. Chem. Phys.*, 146, 214701, (2017). [2] L. Triguero, L. G. M. Petterson and H. Ågren, *Phys. Rev. B*, 58, 8097, (1998).

Poster n. 46 - Zdenek Futera
University College London
z.futera@ucl.ac.uk

Calculation of Electric Currents in Multi-Heme Protein Junctions

Zdenek Futera(1), Xiuyun Jiang(1), Jan B. D. Elsner(2), Jochen Blumberger(1,3)
(1) Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom (2) University of Cambridge, Robinson College, Grange Road, Cambridge CB3 9AN, United Kingdom (3) Institute for Advanced Study, Technische Universität München, Lichtenbergstrasse 2 a, D-85748, Garching, Germany

Multi-Heme proteins such as STC or MtrF are membrane proteins facilitating long-range electron transfer (ET) across cell membrane in metal-reducing bacteria [1]. We used classical molecular dynamics (MD) together with electronic-structure calculations based on density functional theory (DFT) to show that in native environment the conducted electrons are transferred by incoherent hopping between the heme cofactors. Kinetics of the ET is significantly enhanced by presence of cysteine linkages [2,3,4]. However, recent experimental measurements of current-voltage curves suggested that the ET mechanism changes to coherent electron tunneling in vacuum when the protein is electronically coupled with metal electrodes [5]. Therefore, we performed MD simulations in accurate gold/protein interaction force field [6] to identify adsorption of STC and MtrF between two gold electrodes. By extended DFT calculation on the complete interfacial structure we then identified the conduction channels formed predominantly by delocalized heme iron states. Finally, we applied Landauer formalism to compute I-V curves on investigated junctions using the DFT electronic states corrected for band alignment and discuss the ET mechanism.

References [1] M. Breuer, K. M. Rosso, J. Blumberger, *Proc. Natl. Acad. Sci. USA*. 2014, 111, 611-616. [2] Z. Futera, J. Blumberger, *J. Phys. Chem. C*. 2017, 121, 19677-19689. [3] X. Jiang, Z. Futera, E. Md. Ali, F. Gajdos, G. F. von Rudorff, A. Carof, M. Breuer, J. Blumberger, *J. Am. Chem. Soc.* 2017, 139, 17237-17240. [4] X. Jiang, B. Burger, F. Gajdos, C. Bortolotti, Z. Futera, M. Breuer, J. Blumberger, *Proc. Natl. Acad. Sci USA*. 2018, submitted. [5] K. Garg, M. Ghosh, T. Eliash, J. H. van Wonderen, J. N. Butt, L. Shi, X. Jiang, Z. Futera, J. Blumberger, I. Pecht, M. Sheves, D. Cahen, *Chem. Sci.* 2018, 9, 7304-7310. [6] Z. Futera, J. Blumberger, *J. Chem. Theory Comput.* 2018, submitted.

Poster n. 47 - Lee Steinberg
University of Southampton
ls2m15@soton.ac.uk

Topological Data Analysis of Alanine Dipeptide Conformational Space

Lee Steinberg, Ingrid Membrillo-Solis, Mariam Pirashvili, Jacek Brodzki, Jeremy Frey

The problem of protein folding is often posed as an optimisation of a large number of dihedral angles that minimises the (free) energy. To that end, there have been many attempts to develop general methods for understanding conformational spaces and energy landscapes. Perhaps the most common is the Ramachandran plot [1], a contour plot of the free energy function projected onto two dihedral angles. Although powerful, the Ramachandran plot does not take the topology of the conformational space directly into account. In particular, the circular nature of the dihedral angles naturally induces a toroidal topology, which is not captured by the square nature of the Ramachandran plot. Mathematical and computational developments allow us to apply the area of topological data analysis [2]. In this work, we apply these techniques to the conformational space of a well-studied molecule, alanine dipeptide. Using a representative set of conformers, we show that the toroidal topology is easily recovered. We use these techniques to study the energy landscape itself, and show that we are able to observe the presence of transition states. Finally, we present a perspective as to how these techniques could be applied to more complex molecules, in particular in improving the understanding of their free energy landscapes without complex calculation.

[1] Ramachandran, Ramakrishnan, Sasisekharan, Stereochemistry of polypeptide chain configurations, *Journal of Molecular Biology*, 7, 1963, 95-99 [2] Edelsbrunner, Harer, *Persistent Homology - A Survey*, *Contemporary Mathematics*, 435, 2007, 257-282

Poster n. 48 - Eva Pluharova
University of Southampton
eva.pluharova@jh-inst.cas.cz

Solvent effects on enantioselectivity of a lipase-catalyzed reaction

Zuzana Sochorova Vokacova, Damien Laage, Eva Pluharova

Enzymes are extraordinary catalysts satisfying the needs of living organisms, but their efficiency and selectivity is also appealing for utilizing them in technological applications [1]. Perhaps surprisingly, a wide range of enzymes do not denature and moreover retain catalytic activity in organic solvents. This opens a path for carrying out new unnatural reactions. The change of reaction medium significantly alters enzyme activity, as well as chemo-, regio- and enantioselectivity. Solvent effects on enantioselectivity are complex; different types of enzymes exhibit qualitatively different behavior [2,3] and simple rules for rationalization are still missing. Our aim is to systematically investigate enantioselectivity of a transesterification reaction catalyzed by *Candida antarctica* lipase B in various solvents. First, we examine the detailed nature of the rate-limiting step using QM/MM calculations. Next, we sample the conformational space of the most important reaction intermediate for both enantiomers by classical molecular dynamics simulations and characterize the productive binding modes. The gained molecular level insight will help to understand the puzzling dependence of enantioselectivity on solvent properties.

References [1] A. M. Klivanov, *Nature* 409, 241 (2001). [2] S. Tawaki, A. M. Klivanov, *J. Am. Chem. Soc.* 114, 1882 (1992). [3] Y. Kitamoto, Y. Kuruma, K. Suzuki, T Hattori, *J. Org. Chem.* 80, 521 (2015).

Poster n. 49 - Sunghyun Kim
Imperial College London
sunghyun.kim@imperial.ac.uk

Theoretical Maximum Efficiency of Solar Cells Limited by Non-radiative Recombination

Sunghyun Kim, Ji-Sang Park, Samantha N. Hood and Aron Walsh
Department of Materials, Imperial College London, UK

In photovoltaic materials, photogenerated carriers (electrons and holes) can be annihilated by recombination processes, limiting the performance of solar cell devices. Radiative and Auger recombinations are considered as intrinsic qualities of a material which are unavoidable. In solar cells with low carrier densities, trap-assisted non-radiative recombination process is a dominant mechanism described by Shockley-Read-Hall (SRH) statistics. However, the theoretical maximum efficiency of solar cells, so-called Shockley-Queisser limit, has mainly focused on the radiative recombination due to the difficulty in calculating the thermodynamic limit of non-radiative recombination rate theoretically. In this work, we predict the thermodynamic maximum efficiency of kesterite solar cells ($\text{Cu}_2\text{Zn}(\text{Ge},\text{Sn})(\text{S},\text{Se})_4$) limited by non-radiative carrier recombination mediated by the native point defects using First-principles density functional theory (DFT) calculations. We find that the inert-pair effect in Sn-related defects induces both deep levels and large lattice distortion after the carrier captures. Hence, the sulfur vacancy (V_S), sulfur vacancy-donor complex and Sn antisites (Sn_{Zn}) produce deep levels and large capture cross sections resulting in the low open-circuit voltage and the solar-to-electricity conversion efficiency. Since the thermal equilibrium concentrations of harmful native defects are intrinsic properties of the material, they determine the fundamental limit of solar cell efficiencies.

[1] Kim, S., Park, J.-S. & Walsh, A. Identification of Killer Defects in Kesterite Thin-Film Solar Cells. *ACS Energy Lett.* 3, 496 (2018).

Poster n. 50 - Christopher Miles
University of Warwick
c.miles.1@warwick.ac.uk

Cryopreservation by design: employing long scale molecular simulations to understand the formation of ice in biological matter

Christopher M. Miles, Gabriele C. Sosso

Ice formation accounts for the majority of cellular damage in current cryopreservation procedures. In particular, this damage occurs via the process of ice re-crystallisation: the growth of larger ice crystals at the expense of smaller ones. Despite the fundamental nature of ice nucleation, relatively little is known about the conditions which encourage the process or the extent to which biological matter can act as an ice nucleating agent. Previous studies have shown that cholesterol crystals can promote ice nucleation via the formation of ice-like cages involving both water molecules and the terminal hydroxyl groups of the cholesterol surface. The focus of this project is how model membrane systems can promote the formation of ice, via qualitative observation and quantitative analysis of simulation trajectories. The model membranes in question are lipid bilayers, consisting of varying proportions of DPPC, DMPI and cholesterol. These systems are simulated using molecular dynamic simulations at 233.15 K; in order to probe the existence of pre-critical ice nuclei at the membrane-water interface.

Poster n. 51 - Christopher R. Taylor
University of Southampton
C.R.Taylor@soton.ac.uk

Molecular crystal structure prediction: accurate ranking and flexible exploration

The application of computational chemistry methods to the problem of crystal structure prediction (CSP) has achieved considerable success for a wide range of systems, with significance for pharmaceutical and material design [1]. Our work aims to evaluate the effectiveness of existing CSP methods for such problems, and to refine them or develop improved approaches for more complex systems. We describe the success of traditional periodic DFT for rationalising the formation of 350 experimentally-observed co-crystals, when conventional descriptor-based explanations are not necessarily predictive [2]. We also explore the possibilities of co-crystal CSP in predicting the presence or absence of specific interaction motifs in observed [3] co-crystal families, as well as alternative approaches when standard periodic DFT descriptions of co-crystals fail due to significant charge-transfer effects [4]. More recently, our work has focused on the treatment of molecules with conformational flexibility in the CSP process. Methods have previously been developed in-house for both sampling the conformational degrees of freedom and including them in the crystal structure energy minimization [5]. We are currently using and improving these methods to rationalise the experimental use of low-molecular-weight gels [6] in searching for alternative polymorphs of known systems, with the hope of using CSP to aid in designing a “toolkit” of such gels to allow targeted crystallisation of pharmaceuticals.

- [1] Day, G. M., *Crystallography Reviews*, **2011**, 17 (1), 3–52.
- [2] Taylor, C. R.; Day, G. M., *Crystal Growth & Design* **2018**, 18 (2), 892–904.
- [3] Corpinot, M. K.; Stratford, S. A.; Arhangelskis, M.; Anka-Lufford, J.; Halasz, I.; Judaš, N.; Jones, W.; Bučar, D.-K., *CrystEngComm*, **2016**.
- [4] LeBlanc, L. M.; Dale, S. G.; Taylor, C. R.; Becke, A. D.; Day, G. M.; Johnson, E. R., *Angewandte Chemie International Edition* **2018**, 57 (45), 14906–14910.
- [5] Bygrave, P. J.; Case, D. H.; Gee, T. S.; Day, G. M., *in preparation*.
- [6] Kennedy, S. R.; Jones, C. D.; Yufit, D. S.; Nicholson, C. E.; Cooper, S. J.; Steed, J. W., *CrystEngComm* **2018**, 20 (10), 1390–1398.

Poster n. 52 - David McDonagh
University of Southampton
dm1m15@soton.ac.uk

Machine-Learnt Fragment-Based Energies for Crystal Structure Prediction

David McDonagh, Chris-Kriton Skylaris, Graeme M. Day
University of Southampton

The ability to predict experimentally viable crystal structures using only basic molecular connectivity creates an opportunity for in silico design, where potential materials with desirable properties can be discovered before entering the laboratory. Identifying likely candidates relies on efficiently searching the space of possible structures, and accurately calculating their properties. For organic molecular crystals, anisotropic force fields and dispersion-corrected periodic Density Functional Theory (DFT-D) methods are typically used to calculate geometries and energies of generated structures. Force fields allow for robust sampling of the space of possible crystal structures, although typically at a reduced accuracy compared to more expensive DFT-D approaches. Here we present a method to rapidly improve the accuracy of force field lattice energies by correcting two-body interactions with a higher level of theory in a fragment-based approach, and predicting these corrections with machine learning. By replacing all significant dimer energies with commonly used density functionals and second order perturbation theory, we find substantial improvements in the energy ranking of experimentally known polymorphs compared to other candidate structures across a range of molecules. Relative energies of polymorphs are also found to systematically improve towards known experimental data and more comprehensive models, despite the model only consisting of a single-point energy correction. Predicting two-body interactions with atom-centered symmetry functions in a Gaussian process is found to give highly accurate results with as little as 10% of the data of the higher level of theory, reducing the cost by an order of magnitude. These results suggest this highly parallelisable method can be used to explore the space of possible structures with a fragment-based approach more efficiently, providing a bridge between force fields and DFT-D approaches.

Poster n. 53 - Jolyon Aarons
University of Warwick
j.aarons@warwick.ac.uk

Linear scaling excited state forces within the linear-response time dependent DFT formalism: method and applications

Jolyon Aarons, Tim J. Zuehlsdorff, Nicholas D.M. Hine
University of Warwick University of California, Merced University of Warwick

Recently it has become possible to calculate accurate excited state properties of large model systems in complex environments, up to many 1000s of atoms, with linear scaling time-dependent density functional theory (TDDFT) (J. Chem. Phys. 143, 204107 (2015)). This can be applied to diverse topics such as solvated molecules, nanostructures and biologically inspired molecules, where both the necessary system-size and the number of relevant electronic excitations can be very large. Our approach addresses both problems, and removes the need for explicit representation of Kohn-Sham states, through the use of a minimal, in-situ optimized, local basis representation in terms of which transitions and excitations can be represented as density matrices which can be made sparse. Manipulation of the sparsity pattern of the density matrices also allows us to block unwanted transitions, for example, spurious solvent-solvent excitations in calculations of solvated molecules with many solvent molecules. We now show how this methodological framework may be extended to calculate excited state properties involving derivatives, including forces, while maintaining linear-scaling with system size. We demonstrate this through large-scale calculations on molecules including photo-active dyes, UV protectant molecules, and pigment-protein complexes. Many exhibit photoisomerism, which can be explored using excited state forces and geometry optimizations. Longer-term, the formalism promises the ability to calculate accurate excited state absorption and emission spectra and excited state dynamics for chromophores in complex environments. For example, one can achieve a high degree of convergence of solvatochromic shifts in absorption and emission spectra with respect to model size and number of snapshots, which would be impossible with the computational scaling of traditional approaches to TDDFT.

Poster n. 54 - Mads-Peter Verner Christiansen
Aarhus University
machri@phys.au.dk

*Mads-Peter Verner Christiansen, Björk Hammer
Aarhus University, Denmark.*

Global optimization is a topic of interest in many scientific disciplines. In chemical physics global optimization problems arise e.g. when trying to determine the lowest energy configuration of a collection of atoms. Traditionally a range of methods have been used to solve these problems such as basin hopping and evolutionary algorithms in combination with potential energy surfaces described by time consuming quantum mechanical methods. However, as increasingly difficult problems are proposed new algorithms that can reduce the number of energy evaluations are required. An important tool from the machine learning toolbox is the use of descriptors or features, which are a representation of atomic coordinates that have certain invariances (translational, rotational, permutational) required to teach a model that eg. rotating a molecule does not change the energy. A previous study has shown that information can be obtained from such a feature representation that can be used to improve global optimization algorithms. It was discovered that only certain clusters of points in feature space are present in the global minimum structure, and a so-called 'cluster regularization' scheme was devised in which atoms are moved in order to enforce clustering in feature space [1]. This can be thought of as a perturbation in a basin-hopping scheme or a mutation in an evolutionary algorithm. The movement of atoms according to their features can be represented as a energy minimization where the energy is a function of the atomic features rather than the coordinates directly. In the present work the freedom available when choosing this new energy expression is explored. We find that basing the expression on only a single atom opens new possibilities for use as an accurate perturbation in a global optimization algorithm.

[1] K. H. Sørensen, M. S. Jörgensen, A. Bruix, B. Hammer, "Accelerating atomic structure search with cluster regularization". J. Chem. Phys, 148, 241734, 2018.

Poster n. 55 - Isabelle Heath-Apostolopoulos
University College London
isabelle.hapostolopoulos@gmail.com

Multi-level investigation of optoelectronic properties of polymers

Heath-Apostolopoulos, I. , Wilbraham, L. , Zwijnenburg, M.
Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ U.K.

Given the urgent need for clean, sustainable forms of energy, materials for light-driven processes such as photovoltaic power production and photocatalytic water-splitting have attracted much attention over recent years. Whilst inorganic semiconductors are commonly used for these applications, the search for equally efficient organic polymers is desirable as they have the advantage of being easily tunable, being based on earth-abundant and non-toxic elements, as well as , flexibility and solution processability. Computational insight into the electronic and optical properties of these materials greatly assists the discovery process when compared with purely experimental design of materials. Computational investigations of materials provide the benefit of a) not having to synthesize vast numbers of materials, therefore leading to efficient screening of many materials at once, b) offering a greater understanding of composition, conformation, sequence and geometric isomerism and c) avoiding the need for technically complicated experiments such as (inverse) photoemission spectroscopy. Different computational strategies however, must be taken in order to explore the different facets of polymer discovery. For the high-throughput screening of large numbers of molecules, approximate methods with a reduced computational cost must be employed. This route leads to the elucidation of materials perhaps not yet considered for the desired application and also confirmation of known appropriate materials. These more accurate methods are also useful to validate the use of more cost-efficient methods. For the determination of properties of polymers to a high degree of accuracy, more accurate methods such as DFT, many-body perturbation theory methods and correlated wavefunction methods must be used instead. The increased cost of these methods limits the size of the system being calculated, but leads to more accurately predicted properties. Here we present the application of state of the art semi-empirical (xTB) and quantum chemical based (GW/BSE and EA/IP-EOM-CCSD) methods to explore the relationships between composition, structure and the optoelectronic properties of these materials

Poster n. 56 - Will Gerrard
University of Bristol
will.gerrard@bristol.ac.uk

Rapid NMR Parameter Prediction with Machine Learning

Will Gerrard, Lars Bratholm, Craig Butts, Adrian Mullholland
University of Bristol, School of Chemistry, Cantocks Close, Bristol, BS8 1TS

Modern drug discovery workflows use both experimental and computational nuclear magnetic resonance (NMR) techniques to resolve the structure of drug targets. The best computational techniques use variations on density functional theory (DFT) and require immense computational resources, with single conformer calculations taking over 100 hours. Machine learning methods can predict the DFT NMR parameters for a given molecule in less than a second, with a modest margin of error. So far we have built Kernel Ridge Regression (KRR) algorithms to predict Carbon and Proton chemical shifts as well as 1-bond proton-carbon scalar coupling. The KRR machines are trained using a massive dataset of 2000 DFT optimised structures and DFT calculated NMR parameters. Using a SLATM molecular representation we have achieved accuracy to DFT of 3.2ppm and 0.38ppm for Carbon and Proton chemical shifts (MAD). As a reference, the typical accuracy of DFT to experiment is 2ppm and 0.2ppm for these parameters. We have also achieved an accuracy of 1.78Hz MAD in predicting 1-bond proton-carbon coupling . This compares to a typical DFT error of 2Hz. This means that for many practical purposes, we can replace a ~40 hour DFT calculation with a 0.4 second prediction. Further work is ongoing to develop neural networks and better datasets to improve the prediction accuracy.

Poster n. 57 - Pablo Sanchez-Palencia
Universidad Politecnica de Madrid
p.sanchez-palencia@upm.es

New and efficient in-gap band materials with improved absorption features: The case of V-doped Sn₃Ge₃Ni₈ spinel

P. Sanchez-Palencia (a,b), G. Garcia (a,b), P. Palacios (a,c), J.C. Conesa (d), P. Wahnón (a,b)
(a) *Instituto de Energía Solar, ETSIT, Universidad Politecnica de Madrid (Spain)* (b) *Dept. Tecnología Fotonica y Bioingeniería. ETSIT, Universidad Politecnica de Madrid (Spain)* (c) *Dept. Física aplicada a las Ingenierías Aeronáutica y Naval, ETSIAE, Universidad Politecnica de Madrid (Spain)* (d) *Instituto de Catalisis y Petroleoquímica, CSIC (Spain)*

Currently, there is a considerable interest in the design of new low cost and high efficiency semiconductor materials to be applied in photovoltaic devices. Among different approaches, the power conversion efficiency (PCE) can be increased through the in-gap band (IGB) concept. Thus, the PCE could be improved thanks to two extra sub-bandgap photon absorptions in which the IGB gets involved: from the valence band (VB) to the IGB and from the IGB to the conduction band (CB), in addition to the traditional VB to CB transition. This approach could reach theoretical efficiencies up to 63%. In this work, solid solutions of group 14 nitrides with spinel structure are selected as host semiconductor material. In this sense, those semiconductors are thermally stable materials and suitable for optoelectronic applications. Concretely, Sn₃Ge₃Ni₈ spinel, with a band gap around 2 eV, presents optimal electronic features to host an IGB with the desired properties. The Vanadium doped Sn₃Ge₃Ni₈ is here proposed as a new and promising in-gap band material. With this aim, a detailed analysis of this new material as well as of the host spinel has been carried out using Density Functional Theory (DFT). The bandgap underestimation of traditional DFT methods have been overcome using HSE-06 hybrid functional. Our results, including structural and electronic properties, point out that Vanadium 3d orbitals introduce new electronic states within the gap of the host spinel, which form the intermediate band leading to improved absorption features through the new sub-bandgap transitions.

Poster n. 58 - Fabienne Bachtiger
University of Warwick
f.bachtiger@warwick.ac.uk

Probing the Molecular Structure of Water at the Interface with Homogalacturonan

Bachtiger, Fabienne., Sosso, Gabriele C.,

The ability of a biomolecule to facilitate - or the opposite- inhibit the formation of ice, is of fundamental interest in cryobiology, not least as it can help to achieve the rational design of improved cryoprotectants, i.e. additives that mitigate cellular damage upon the freezing of biological material. By means of classical molecular dynamics (MD), we probe the structure of water at the homogalacturonan (HGB)/ water interface at strong supercooling (230 K). HGB forms the backbone of the RG-II subdomain found in pectin; a complex carbohydrate present within the cell walls of plants. Here we show that HGB exhibits two preferred conformations, conformation A ($\phi=85$ deg, $\psi=140$ deg) and conformation B ($\phi=85$ deg, $\psi=108$ deg), as determined by the torsional angles of the glycosidic linkages. By probing the crystallinity of supercooled water at the interface of each HGB conformation, we investigate the emergence of hydrogen bonds between the pre-critical ice nuclei and the hydrogen-bond acceptor and donor species on HGB. We find that conformation B displays a stronger tendency to form hydrogen bonds if compared to conformation A. However, we demonstrate that both conformations of HGB do not facilitate the formation of pre-critical ice nuclei at the water-HGB interface and are therefore unlikely to act as ice nucleating agents; in agreement with preliminary experimental evidence provided by our experimental collaborators. Our findings indicate that exploring the conformational space of biomolecules in aqueous solutions is key to probe their impact on ice formation in biological matter. Moreover, this work paves the way to the future investigation of the so-called ice recrystallisation inhibition activity of HGB (and RG-II).

Poster n. 59 - Mathias Siggaard Jorgensen
Aarhus University
mj@inano.au.dk

Building atomistic structures with reinforcement learning

Mathias S. Jorgensen, Henrik L. Mortensen, Soren A. Meldgaard, Esben L. Kolsbjerg, Thomas L. Jacobsen, Knud H. Sorensen, and Bjork Hammer
Interdisciplinary Nanoscience Center (iNANO) and Department of Physics and Astronomy, Aarhus University, Denmark

Recently, machine learning has entered the domain of computational chemistry and spiked the development of novel atomistic structure prediction methods, including techniques involving artificial neural networks [1] and kernel methods [2]. A key challenge in predicting new structures is balancing exploration of unknown regions of the energy landscape and exploitation of regions of the landscape known to have promising candidate structures [3, 4]. In the present work, we introduce an atomistic structure learning algorithm that utilizes a convolutional neural network to build atomistic structures atom by atom. Using reinforcement learning, the neural network eventually learns the optimal structural arrangement of atoms for a given number and type of atoms and a given target property. Contrary to stochastic structure search algorithms such as evolutionary algorithms or basin hopping, the knowledge accumulated by the neural network can be transferred to other and more complicated problems, hence saving computational resources. We demonstrate how this transfer learning can be used to search for a graphene grain boundary reported in literature. Furthermore, the chemical compound space of $C_3H_4O_2$ is used to demonstrate the ability of our method to predict compounds containing specific functional groups.

[1] X. Chen, M. S. Jorgensen, J. Li, and B. Hammer, *J. Chem. Theory Comput.*, 14, 3933-3942 (2018). [2] T. L. Jacobsen, M. S. Jorgensen, and B. Hammer, *Phys. Rev. Lett.*, 120, 026102 (2018). [3] M. S. Jorgensen, M. N. Groves, and B. Hammer, *J. Chem. Theory Comput.*, 13, 1486- 1493 (2017). [4] M. S. Jorgensen, U. F. Larsen, K. W. Jacobsen, and B. Hammer, *J. Phys. Chem. A*, 122, 1504-1509 (2018).

Poster n. 60 - Matthew Addicoat
Nottingham Trent University
matthew.addicoat@ntu.ac.uk

Explicit treatment of hydrogen bonds in the Universal Force Field: validation and application for Metal-Organic Frameworks

Matthew A. Addicoat, Damien E. Coupry, Thomas Heine
School of Science and Technology, Nottingham Trent University, Clifton Lane, Nottingham NG11 8NS

A straightforward means to include explicit hydrogen bonds within the Universal Force Field is presented. Instead of treating hydrogen bonds as non-bonded interaction subjected to electrostatic and Lennard-Jones potentials, we introduce an explicit bond with negligible bond order, thus maintaining the structural integrity of the H-bonded complexes and avoiding the necessity to assign arbitrary charges to the system. The explicit hydrogen bond changes the coordination number of the acceptor site and the approach is thus most suitable for systems with under-coordinated atoms, such as many metal-organic frameworks. The approach is validated for the hydrogen bonded complexes in the S22 dataset and then employed for a set of metal-organic frameworks from the ComputationReady Experimental (CoRE) database and several hydrogen bonded crystals including water ice and clathrates. We show that direct inclusion of hydrogen bonds reduces the maximum error in predicted cell parameters from 66% to only 14% and the mean unsigned error is similarly reduced from 14% to only 4%. With the inclusion of hydrogen bonding, the solvent-mediated breathing of frameworks such as MIL-53 is now accessible to rapid UFF calculations, which will further the aim of rapid computational scanning of metal-organic frameworks.

Poster n. 61 - Miguel Rivera
Queen Mary University of London
m.rivera@qmul.ac.uk

Computational Methods for Photochemistry in Molecular Crystals

Miguel Rivera, Michael Dommett, Rachel Crespo-Otero
E1 4NS, London, United Kingdom

Organic molecular crystals hold great promise for optical technologies due to their low cost, lightness and tuneable photochemical properties. Modelling the excited state mechanisms which underlie these properties represents a methodological challenge since they simultaneously require the consideration of nonadiabatic, excitonic and crystallographic factors. Moreover, these system's excited states are typically localised on only a few constituent fragments.[1] For these reasons, finite cluster models can represent a promising alternative to periodic boundary calculations for excited molecular crystals. In this context, we have carried out an investigation of the performance of ONIOM cluster models, using excited state proton transfer crystals as model systems.[2] To correct the erroneous electrostatic potential stemming from a truncated Madelung sum, the electrostatic embedding is modified to include an array of point charges fitted to match the Ewald potential. The Ewald Embedded Cluster (EEC) model was shown to significantly improve the absorption and emission energies obtained from more traditional cluster model.[3] A Python library was developed to carry out the required geometry optimisations, to interface between different electronic structure codes and to prepare crystalline clusters. The FRamewOrk for Molecular AGgregate Excitations (fromage) is freely available online. This poster will introduce the EEC model, its application to a model system and its implementation in fromage.

[1] Arag J. & Troisi, A. Dynamics of the Excitonic Coupling in Organic Crystals. *Phys. Rev. Lett.* 114, 026402 (2015). [2] Dommett, M., Rivera, M. & Crespo-Otero, R. How Inter- and Intramolecular Processes Dictate Aggregation-Induced Emission in Crystals Undergoing Excited-State Proton Transfer. *J. Phys. Chem. Lett.* 6148-6153 (2017). [3] M. Rivera, M. Dommett, R. C. Otero, M. Rivera, M. Dommett and R. Crespo-otero, 2018, under review.

Poster n. 62 - Gergely Juhasz
School of Science, Tokyo Institute of Technology
juhasz@chem.titech.ac.jp

Electrochemical reduction on TiO₂ surfaces and nanoparticles

Gergely Juhasz

The electrochemical reduction of organic acids on anatase TiO₂ electrode has been recently reported by Yamauchi [1]. Such an electrochemical reaction has a potential to produce alcohol products with high selectivity and efficiency, and these products can be used as alternative fuel in carbon neutral cycles. While the reduction was possible for oxalic acid, other acids like acetic acid remains inert and cannot be reduced on the same electrodes. To understand better the factors influencing the redox activity, we studied the absorption and reduction of small molecules on anatase TiO₂ using Density-Functional Based Tight-Binding method (DFTB) [2]. We found that the strong absorption of the anchoring carboxyl group protects it from the reduction, and only the distant group of oxalic acid is electrochemically active. The strong coupling between the electrode conducting band and the frontier orbitals of oxalic acid orbitals show that electron promotion from the electrode to the acid group is indeed possible. We have also extended our calculation to anatase nanoparticles. The calculations showed that the LUMO (conducting band) levels of the nanoparticles are strongly localized around the low coordinated Ti(IV) ions. Since the electrochemical reduction can be promoted via these low energy orbitals, the morphology of the nanoparticles on electrode surface has direct impact on the energetics of electrochemical reduction reaction.

References 1. R. Watanabe, M. Yamauchi, M. Sadakiyo, R. Abe and T. Takeguchi, *Energy Environ. Sci.* 8, 1456 (2015). 2. B. Aradi, B. Hourahine, and Th. Frauenheim., *J. Phys. Chem. A*, 111, 5678 (2007).

Poster n. 63 - Bethan Cornell
King's College London
bethan.cornell@kcl.ac.uk

First Steps towards Unravelling the Working Mechanisms of a BODIPY-based Molecular Rotor for Sensing Viscosity

B. Cornell, I.E. Steinmark, K. Suhling, C. Molteni
King's College London

Fluorescent molecular rotors are molecules with a rotatable part whose fluorescence quantum yield and lifetime are functions of the viscosity and polarity of their local environment. These properties can be exploited to obtain real time imaging of processes involving viscosity changes, which may be signatures of specific diseases. Rotors based on BODIPY have long fluorescent lifetimes and, hence, make excellent probes. However, a detailed description of their working mechanisms at the molecular level has not yet been obtained. We attempt to shed light on these mechanisms by focussing, initially in the gas-phase, on a prototypical rotor: BODIPY-C12, which is composed of a BODIPY-dye core with an attached rotatable phenyl ring. The ground and excited state potential energy surface of BODIPY-C12 in the gas phase were calculated as a function of the rotation of the phenyl ring (with respect to the core), using Density Functional Theory (DFT), Time-Dependent-DFT and the Restricted Open Shell Kohn Sham (ROKS) method. Minimal energy structures in the S_0 state correspond to a twisted geometry. However, in the S_1 state both flat and twisted geometries correspond to energy minima. Furthermore, molecular dynamics simulations at room temperature show a complex motion of the phenyl ring, coupling rotation with swinging and out-of-plane distortion of the BODIPY-core. Data from our simulations are compared with experimental absorption and emission spectra and provide interesting insights into the properties of the BODIPY-C12 molecular rotor

Poster n. 64 - Eszter Szekely
University of Cambridge
es732@cam.ac.uk

Eszter Szekely, Gabor Csanyi
University of Cambridge

The aim of this research is to create new, highly accurate atomic scale models of small molecules, such as water and methane, applicable to simulating their bulk material properties and reactions. The models will be derived using machine learning algorithms (Gaussian Approximation Potentials [1]) from state-of-the-art quantum mechanical calculations on a large database of molecular configurations. The key scientific question is to what extent such "bottom-up" and "parameter-free" models are capable in describing the energetics, thermodynamics, transport properties and reaction kinetics of arbitrary mixtures of such small molecules.

[1] A. P. Bartok, G. Csanyi, *Int. J. Quant. Chem.* 115(16) (2015), code available at: www.libatoms.org

Poster n. 65 - Narjes Ansari
ICTP
nansari@ictp.it

Narjes Ansari, Sebastiano Caravati, Gabriele Cesare Sosso, Alessandro Laio, Ali Hassanali

Herein, we combine a synergy of data-science algorithms to investigate the properties of empty space in liquid water, methane and formamide. We show that the thermodynamics associated with the creation of these voids is distinct from that associated with cavitation classical nucleation theory. All liquids are characterized by small-spherical and large-dendritic shapes with varying relative proportions indicative of a more generic phenomenon which we propose is rooted in percolation of the liquid. This lends itself to a high-dimensional and corrugated free energy landscape modulated by various molecular properties of the liquid. We demonstrate further that the complex shapes adopted by the voids resemble those that small bio-polymers reside in, suggesting that fluctuations in pre-biotic liquids may have an intrinsic conformational bias to host small organic molecules.

Poster n. 66 - Yasmine S. Al-Hamdani
University of Luxembourg
yas.alhamdani@gmail.com

Unravelling the complexity of non-covalent interactions in larger molecular systems

To date, the developments by theoretical chemists and physicists has enabled the accurate prediction of interaction energies in small non-covalently bound systems. This is significant given the intricacy of the quantum mechanical nature of such systems and the need to treat various interactions on a balanced and self-consistent theoretical footing. However, as we apply relatively accurate, but approximate, methods to larger systems, new challenges and uncertainties arise. In particular, the anisotropy and the effects of long-range interactions go beyond what is encountered in small systems. Highly-accurate wavefunction based methods are expected to be reliable methods for predicting larger systems, but there remains a great deal to be understood. We consider whether different wavefunction based methods can predict interaction energies for a set of supramolecular complexes, namely Sedlak's L7 dataset. This includes the stacked coronene dimer among other π - π stacked and biologically relevant complexes. We show that agreement between diffusion Monte Carlo and coupled cluster based approximations is not easily achieved across the data set, with certain complexes being more challenging to establish. A connection is drawn with the performance of a selection of density functional approximations – indicating that certain interactions are yet to be properly accounted for in more approximate but efficient methods.

Poster n. 67 - Mark Driver
University of Cambridge
mdd31@cam.ac.uk

Functional group interaction profile generation for single and multi component solvent systems

Mark D. Driver, Mark J. Williamson, Christopher A. Hunter
Department of Chemistry, University of Cambridge

Scales for hydrogen bond donor and acceptor strength have previously been developed from experimental measurement[1]. The correlation of the donor/acceptor strength to the critical points on the molecular electrostatic potential surface (MEPS) of a molecule has been used to develop the Surface Site Interaction point (SSIP) model of intermolecular interactions. The coarse graining of a MEPS for a molecule produces its characteristic footprint of SSIPs [2]. Consideration of the binding equilibria between all SSIPs of molecules within a phase provides an approach to evaluate the free energy of a molecule within a solution. This is done through summation over all pairwise interactions. This has then been used to calculate solvation properties and free energies of transfer between mixtures[3]. The free energy of interaction between a pair of solute SSIPs in a solvent varies with solute SSIP values. This can be used to generate a Functional Group Interaction Profile (FGIP) for the solvent. The FGIP shows the change in behaviour of the solute-solute interactions graphically. A FGIP could be used to identify which interactions between solutes would promote association within a solvent. This analysis can be performed for single component or multi component solvent systems following a highly automated workflow. This allows exploration of solvent systems, to provide selection criteria before experimental work is undertaken.

[1] Christopher A. Hunter. (2004) Quantifying intermolecular interactions: Guidelines for the molecular recognition toolbox. *Angew. Chem. Int. Ed.*, 43, 5310-5324. doi: 10.1002/anie.200301739. [2] Christian Solis Calero et al. (2013) Footprinting molecular electrostatic potential surfaces for calculation of solvation energies. *PCCP*, 15, 18262-73. doi: 10.1039/c3cp53158a. [3] Christopher A Hunter. (2013) A surface site interaction model for the properties of liquids at equilibrium. *Chemical Science*, 4, 1687-1700. doi: 10.1039/c3sc22124e.

Poster n. 68 - Tahereh Nematiaram
University of Liverpool
tahereh.nematiaram@liverpool.ac.uk

Mining the Cambridge Structural Database for High Mobility Molecular Semiconductors

Tahereh Nematiaram, Daniele Padula, Alessandro Troisi
Department of Chemistry and Materials Innovation Factory, University of Liverpool, Liverpool L69 7ZD, U.K

The Cambridge Structural Database (CSD) is the world largest repository for small organic and organometallic molecules. The CSD represents an invaluable resource for material scientist and crystal engineers. In order to search the database for high-mobility semiconductors, and possibly to design new efficient materials, a repository of organic semiconductors has been derived from the CSD. With particular focus on single-component/identical components structures, the database is reduced to approximately 40 k molecular semiconductors with the electronic gap in the interval of 2-4 eV. Using standard ab-initio calculations we compute the electronic couplings and the nonlocal electron-phonon couplings as two main descriptors for charge mobility. Thus we find many high performance compounds as well as a number of most promising materials that have not yet been considered for an application in organic opto-electronics. Our analysis shows one of the many possible applications of these data and this will open up avenues of research for the future.

Poster n. 69 - Chi Yang Cheng
University of Southampton
c.y.cheng@soton.ac.uk

Fragment Based Discovery of Crystalline Organic Materials

Chi Y. Cheng, Graeme M. Day
University of Southampton

The discovery of innovative and novel materials with favourable properties using chemical intuition alone is both time consuming and costly due to high failure rates in trial and error searches for molecules whose crystal packing leads to favourable properties. The search difficulty is further compounded by the ability of each molecule to form several different stable crystal structures which can also have differing properties from each other. The development of fast and reliable crystal structure prediction methods promises to accelerate the discovery of new materials by allowing candidates for synthesis to be screened computationally and prioritised based on the predicted properties of their predicted crystal structures [1-4]. We now need better methods for suggesting candidate molecules for crystal structure and property prediction. In this research we are therefore working towards the development of a novel fragment based genetic algorithm to search the chemical space and then together with our groups' methods [5] to further search for its crystal packing structures. Using this framework we will be able to discover promising materials for chemical and crystal packing dependent properties such as electron mobilities for organic semiconductors and densities for porous organic crystal solids.

[1]"Functional materials discovery using energy-structure-function maps" *Nature* 543,657(2017) [2]"Predicted energy-structure-function maps for the evaluation of small molecule organic semiconductors" *Journal of Materials Chemistry C*, 5,7574-7584(2017) [3]"Machine Learning for the Structure-Energy-Property Landscapes of Molecular Crystals", *Chemical Science* 9,1289-1300(2018) [4]"Large-Scale Computational Screening of Molecular Organic Semiconductors Using Crystal Structure Prediction", *Chemistry of Materials* 30,4361-4371(2018) [5]"Convergence properties of crystal structure prediction by quasi-random sampling" *Journal of Chemical Theory and Computation*, 12,910-924(2016)

Poster n. 70 - Maximilian Saller
ETH Zurich
maximilian.saller@phys.chem.ethz.ch

On the identity of the identity in nonadiabatic semiclassical dynamics: Would you know 1 if you saw one?

Maximilian A. C. Saller(1), Aaron Kelly(2) and Jeremy O. Richardson(1)
(1) *Laboratory of Physical Chemistry, Swiss Federal Institute of Technology (ETH) Zurich, Zurich, Switzerland* (2) *Department of Chemistry, Dalhousie University, Halifax, Canada*

Many methods relying on semiclassical trajectories aim to simulate nonadiabatic dynamics by mapping the multiple electronic states involved to an extended phase space. This allows them to be applied to large, condensed-phase systems inaccessible to wavefunction based methods, due to the latter's exponential scaling. Yet approaches such as the linearized semiclassical initial value representation (LSC-IVR) fail to quantitatively reproduce exact population dynamics in the long-time limit. We propose a simple modification to these approaches. First any correlation function can be rewritten as a sum, with one element containing the identity. Given then exact knowledge of how the identity operator behaves, instead of computing its value from the semiclassical trajectories, we instead simply set it to one. This straightforward substitution involves no change to the equations of motion, or indeed the algorithm in general, and yet results in a drastic improvement in accuracy over traditional approaches.

Poster n. 71 - Max Veit
EPFL
max.veit@epfl.ch

Max Veit, Sandeep Kumar Jain, Satyanarayana Bonakala, Indranil Rudra, Detlef Hohl, Gabor Csanyi
MV: EPFL, 1015 Lausanne, Switzerland SKJ, SB, IR: Shell Technology Centre Bangalore, Bengaluru 562149, Karnataka, India DH: Shell Global Solutions International BV, Grasweg 31, 1031 HW Amsterdam, The Netherlands MV, GC: Engineering Laboratory, University of Cambridge, Trumpington Street, Cambridge CB2 1PZ

The reliable prediction of the macroscopic properties of molecular liquids requires potential energy surface (PES) models that are not only accurate, but computationally efficient enough to handle large systems and reach long time scales typically inaccessible to explicit quantum-mechanical methods. This work introduces a new approach to the systematic approximation of the first-principles PES of a molecular liquid using the GAP machine learning method [A. Bartók, M. Payne, R. Kondor, and G. Csányi, Phys. Rev. Lett. 104, 136403 (2010)]. By applying machine learning to separately approximate each physical component of the interaction energy in a full many-body framework and with high and controllable accuracy, we can simulate the liquid accurately across a wide range of temperatures and pressures (with the inclusion of quantum nuclear effects) while gaining physical insight into the inner workings of the fluid. Following the recent success of this approach on predicting the equation of state of compressed fluid methane [M. Veit, S. K. Jain, S. Bonakala, I. Rudra, D. Hohl, and G. Csányi, arXiv:1810.10475], I will discuss how this approach can be extended to other molecular liquids with the help of emerging techniques in machine learning potential development, and how these ideas can be applied to other important molecular materials.

Poster n. 72 - Shiyue Yang
University of Southampton
sy1u17@soton.ac.uk

Development of Simulation Methods for Exploring Energy Landscapes of Molecular Crystals

Shiyue Yang, Graeme M. Day
School of Chemistry, University of Southampton, Southampton SO17 1BJ, United Kingdom

Organic crystal structure prediction (CSP) focuses on predicting stable crystal structures of organic molecules, an essential step of which is sampling many points in configurational space. A popular method is to perform a quasi-random sampling of this space, which provides a broad and uniform sampling of candidate crystal structures in the energy landscape [1]. However, such a method can be inefficient in finding the global minimum in lattice energy, which is assumed to be the most likely structure. To improve its efficiency in locating low energy structures, a basin hopping algorithm is utilised where a local relaxation is introduced at every step. Combining both methods by initiating each basin hopping simulation from structures generated by a quasi-random searching method allows for improved sampling compared to each method in isolation. Parameters for basin hopping, including updating strategies, temperature and structure modification metrics are trained to improve the efficiency of convergence of the simulation. The strategy to combine basin hopping and quasi-random searching methods is also discussed, focusing on choices in partitioning the simulation between the two methods. This sampling strategy is applied to single crystal and co-crystal systems, where global searching in conformational space is carried out in multiple space groups. Compared with pure quasi-random searching, the combined strategy shows advantages in locating structures with low lattice energy, especially for co-crystal systems where the dimensionality of the energy landscape makes it difficult to sample thoroughly. These results indicate this method can allow for a more efficient exploration of candidate crystal structures.

[1] "Convergence properties of crystal structure prediction by quasi-random sampling" D. H. Case, J. E. Campbell, P. J. Bygrave and G. M. Day, *Journal of Chemical Theory and Computation*, 12, 910-924 (2016).

Poster n. 73 - Haiyuan Wang
Fritz-Haber-Institut der Max-Planck-Gesellschaft
hwang@fhi-berlin.mpg.de

Critical Interplay of Atomic and Electronic Structure of Strong Electron Acceptors on Semiconductor Surfaces

Haiyuang Wang, Sergey Levchenko, Thorsten Schultz, Norbert Koch, Matthias Scheffler, and Mariana Rossi

In organic-inorganic interfaces, it is necessary to understand how the atomic and electronic degrees of freedom cooperate or compete to yield the desired functional properties. Here, we address this issue first for strong electron acceptors (F4-TCNQ and F6-TCNNQ) adsorbed on H-Si(111). We perform systematic structure searches using density-functional theory with the HSE06 functional augmented by many-body van-der-Waals corrections. The results show that despite their similar composition, F4-TCNQ and F6-TCNNQ adsorb with significantly different geometries and show island formation propensities consistent with Volmer-Weber and Stranski-Krastanov growth modes, respectively. These densely-packed geometries induce a large interface-charge rearrangement, corresponding to a work-function (WF) increase of 1.11 eV for F4-TCNQ and 1.76 eV for F6-TCNNQ. Interestingly, vibrational fluctuations at room temperature produce a wide distribution of WF values, well modeled by a normal distribution with $\sigma=0.17$ eV [1]. We compare these results to the behavior of F6-TCNNQ on MoS₂, where we address the origin of temperature-dependence in the charge transfer. This work is supported by the SFB-951 project.

[1] H. Wang, et al., arXiv:1811.00037 (2018).

Poster n. 74 - Prima Gupta
INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR
priya.gupta1931@gmail.com

Generic AMBER-like Force Field Development for Transition Metal Clusters

Priya Gupta, K S S V Prasad Reddy, Phani Kumar Pentyala, Parag A Deshpande
Quantum and Molecular Engineering Laboratory, Department of Chemical Engineering, Indian Institute of Technology Kharagpur-721302, India.

Nanoclusters are the mono-dispersed particles, generally less than 10 nm in diameter having distinct chemical properties due to their high surface-to-volume ratio, quantum confinement at reduced sizes, and unique geometric and electronic structures [1]. These clusters have been found to catalyze a range of heterogeneous reactions [2]. Studies have been going on to examine the physico-chemical properties of such clusters both experimentally and computationally. Physical properties of such clusters can be determined by Molecular Dynamics for which accurate force field is a pre-requisite. In present study, a new set of force-field parameters have been reported which will aid in the Molecular dynamics and QM/MM studies for transition metal clusters. Existing AMBER force field [3], which is generally employed for the simulation of proteins, nucleic acids and organic molecules, has been taken as the basis for force field development. The parameters for AMBER-like force field equation were fit against an extensive set of quantum data using suitable functional and basis set. Obtained results have been then validated using Molecular dynamics simulations. Keywords: Transition metal clusters, force fields, AMBER

[1] Aiken III, John D., and Richard G. Finke. "A review of modern transition-metal nanoclusters: their synthesis, characterization, and applications in catalysis." *Journal of Molecular Catalysis A: Chemical* 145.1-2 (1999): 1-44. [2] Schmid, Günter. *Clusters and colloids: from theory to applications*. Wiley-VCH, 1994.. [3] Cornell, Wendy D., et al. "A second generation force field for the simulation of proteins, nucleic acids, and organic molecules." *Journal of the American Chemical Society* 117.19 (1995): 5179-5197.

Poster n. 75 - Ljiljana Stojanović
Queen Mary University of London
l.stojanovic@qmul.ac.uk

Propeller-shaped molecules: aggregation quenching vs aggregation induced emission in the solid state

Ljiljana Stojanović and Rachel Crespo-Otero
School of Biological and Chemical Sciences, Materials Research Institute, Queen Mary University of London, Mile End Road, London E1 4NS, UK.

Highly-emissive organic materials found applications in several areas including display technologies, optical communication, biological sensing, and solid-state lasing. One of the main challenges associated with these applications is that aggregation can quench emission due to the stabilisation of $\pi\pi$ and charge transfer states. However, several crystals showing the opposite behaviour has been synthesised. [1] Even though these materials display a weak fluorescence in the gas phase or dilute solution, their emissive response enhances upon aggregation (aggregation induced emission, AIE). Explaining these mechanisms is relevant, due to its potential aid in the design of the new efficient emissive materials. We explored a series of propeller-shaped molecules with contrasting emissive behaviour in the solid state. While TPC shows AIE, TPF is affected by aggregation quenching and TPT displays a weak emission in the solid state. [2] We analysed the excited state relaxation mechanisms of presented molecules in the gas and crystal phase. We believe that this systematic investigation can help understand how to control the role of chemical structure vs crystal packing in AIE.

[1] J. Mei, N. L. C. Leung, R. T. K. Kwok, J. W. Y. Lam, and B. Z. Tang., *Chem. Rev.*, 115(21), 11718–11940, 2015.
[2] H. Nie, K. Hu, Y. Cai, Q. Peng, Z. Zhao, R. Hu, J. Chen, S.-J. Su, A. Qin, and B. Z. Tang, *Mater. Chem. Front.*, 1(6), 1125–1129, 2017.

Poster n. 76 - Yasir Altaf
Victoria University of Wellington, New Zealand
yasir.altaf@vuw.ac.nz

Fluorescence Characteristics of Aminobenzanthrone Dyes

Yasir Altaf, Matthias Lein
The School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand

Benzanthrone and its derivatives are luminophores that emit in the visible region. Due to extended (π) conjugation system, they make excellent donor-acceptor relationship with electron-donating groups to yield efficient chromophoric systems. They find applications in the formation of opto-electronic devices and liquid crystals and this can be attributed to their interesting photophysical and photochemical properties. The aim of the current study is to explore the fluorescence potential of the selected aminobenzanthrone dyes synthesized in a previous experimental study. The computational findings matched well with the experimental results and it was deduced that there occurs an increase in the dipole moment of the molecules when dissolved in a suitable solvent.

Poster n. 77 - Ying-Chih Chiang
School of Chemistry, University of Southampton
yingchihchiang@gmail.com

Relaxation Augmented Free Energy Perturbation (RAFEP)

Ying-Chih Chiang, Christopher Cave-Ayland, Marley Samways, Frank Otto, Jonathan W. Essex

We re-examine the concept of free energy calculation via the single-step free energy perturbation (sFEP) method, which frequently fails to converge due to the problem of insufficient sampling. We find a close resemblance between the operation in sFEP and the Franck-Condon principle in quantum mechanics. The insufficient sampling problem then has a vivid physical interpretation as lacking the subsequent relaxation process after perturbation. Upon augmenting the traditional sFEP with the relaxation process, the new method agrees well with the exact solution for two model systems, shedding new light on the underlying physics in free energy calculations.

Poster n. 78 - Christian Ahart
University College London
ucapca1@ucl.ac.uk

Towards machine learning the dynamics of the hematite/liquid water interface

Christian. Ahart, Jochen. Blumberger

Density functional theory molecular dynamics presents an opportunity for the application of newly developed kernel based machine learning methods. This is driven by a desire to decrease the significant computational cost of these calculations. Through exploiting the redundancies implicit in molecular dynamics trajectories, including the repeated calculation of similar structures, speed ups of orders of magnitude can be expected. Recent work by other groups has demonstrated the potential of such a framework in regards to single component bulk systems [1]. This framework will be extended to an interface between hematite and liquid water. To decrease the errors in the force predictions relative to the hybrid functional HSE, additional information will be provided in the form of the forces at the lower level PBE functional. Supplying this additional information to the machine learning algorithm is likely to be essential to accurately capture the dynamics of such a challenging system. Current work towards machine learning of the forces of bulk water has been promising, with future work extending this to the interfacial system. The application of these techniques in studying the dynamics and charge transfer of the interfacial system will also be discussed, building upon previous work [2].

[1] Botu, V. & Ramprasad, R. *Int. J. Quantum Chem.* 115, 1074-1083 (2015). [2] Von Rudorff, G. F., Jakobsen, R., Rosso, K. M. & Blumberger, J. J. *Phys. Condens. Matter* 28, 394001 (2016).

Poster n. 79 - Samuele Giannini
University College London
samuele.giannini.16@ucl.ac.uk

Atomistic Non-Adiabatic Molecular Dynamics Simulations of Charge Carrier Transport in Organic Materials.

Samuele Giannini (a), Antoine Carof (a), Jochen Blumberger (a)
(a) *Department of Physics and Astronomy, University College London, London WC1E6BT, UK.*

Exciting new technologies such as organic light emitting diodes, photovoltaics and nanoelectronics rely on organic semiconductors. While important progress has been recently made towards theoretical and computational modelling of organic semiconductors (OSs), understanding the charge transport (CT) mechanism in these materials is still very challenging because the parameters determining the dynamics are typically outside the regime of validity of existing theories (e.g. Hopping or Band theories). On the other hand, non-adiabatic molecular dynamics simulation are in principle free of model assumptions permitting an "ab initio" view into the CT mechanism. We have recently developed an efficient decoherence-corrected surface hopping methodology (FOB-SH) which allows us to propagate the coupled electron-nuclear motion in realistic condensed phase systems [1,2]. Here we present the application of FOB-SH to the calculation of room temperature charge mobility for a series of 8 molecular organic crystals [3]. We obtain very good agreement with experimentally measured mobility values over three orders of magnitude successfully bridging the regime where hopping and band models are invalid. We find that the mechanism of transport critically depends on the ratio between electronic coupling and reorganization energy (electron-phonon coupling), V/λ . At small ratios, as found in e.g. naphthalene, the charge carrier is delocalized over no more than 1-3 molecules and diffuses through the crystal via hopping. For values exceeding the critical threshold $V/\lambda > 1/2$, as found in e.g. pentacene, the charge carrier forms a polaron delocalized over 10 or more molecules concomitant with a strong increase in mobility. Implications of our work for the search of new organic materials with high room temperature mobility will be discussed.

[1] A. Carof, S. Giannini and J. B., JCP, (2017) 147, 214113 [2] S. Giannini, A. Carof, and J. B., JPCL, (2018) 9, 3116 [3] S. G. et al, in preparation

Poster n. 80 - Matt Ellis
UCL
ucapell@ucl.ac.uk

Atomistic simulation of charge transfer in non-adiabatic systems using a novel FOB-CTMQC technique.

Matt Ellis, Jochen Blumberger
UCL

Charge transfer in organic molecular systems is difficult to simulate due to only partial delocalisation of the electronic wavefunction across a few sites. This puts transport properties in a difficult regime that can't be fully described by either band theories or hopping theories [1]. A range of techniques have been designed to overcome this, most notably the Trajectory Surface Hopping and Ehrenfest methods. However, they tend to suffer from unphysical overcoherence between the nuclear and electronic subsystems leading to problems such as spurious transfer and too much electronic delocalisation. A coupled-trajectory mixed quantum-classical (CTMQC) method has been proposed to fix this problem which has been shown to provide more accurate results for the electronic populations and decoherence than both Surface Hopping and Ehrenfest [2]. However, in its initial implementation calculation of the electronic structure at each electronic time-step relied on expensive TD-DFT calculations. This has resulted in simulations carried out on systems no larger than a single oxirane molecule [3]. In this work I propose a new fragment-orbital based CTMQC scheme that combines CTMQC with an efficient analytical overlap method in order to simulate hundreds of molecules [4]. This relies on an ultra-fast estimation of the Hamiltonian from the overlap between optimised Slater p-orbitals.

[1] Oberhofer, H., Reuter, K. & Blumberger, J. Chem. Rev. 117, 10319-10357 (2017). [2] Agostini, F., Min, S. K., Abedi, A. & Gross, E. K. U. Journal of Chemical Theory and Computation 12, 2127-2143 (2016). [3] Min, S. K., Agostini, F., Tavernelli, I. & Gross, E. K. U. The Journal of Physical Chemistry Letters 8, 3048-3055 (2017). [4] Spencer, J., Gajdos, F. & Blumberger, J. The Journal of Chemical Physics 145, 064102 (2016).

Poster n. 81 - Wei Fang
ETH Zurich
wei.fang@phys.chem.ethz.ch

Development of a nonadiabatic quantum transition-state theory for electron transfer reactions

Wei Fang, Manish J. Thapa, Rhiannon Zarotiadis, and Jeremy O. Richardson

Despite the tremendous success of the Marcus theory of electron transfer rates, it is not always accurate due to the absence of nuclear quantum effects and anharmonicity. In recent year, interest in understanding nuclear quantum effects in nonadiabatic reactions have been blooming. Different from the idea of extending heuristic methods (i.e. ring-polymer molecular dynamics) to treat these reactions, we propose a new quantum transition-state theory that accounts for quantum delocalization, zero-point energy, and tunnelling in electron-transfer reactions. The method utilise a natural constraint based on energy conservation, and we have proven that it tends to the correct classical limit and is exact for linear crossings. It can be computed by ring-polymer optimisations or by path-integral molecular dynamics, thus applicable to molecular systems as well as to treat reactions in solution. We showed that it has good performance on a difficult model system with multiple transition states, avoiding the problems of the Wolynes method. We also demonstrate its application to molecular systems.

Poster n. 82 - Shalini Awasthi
University of Warwick
shalini.awasthi@warwick.ac.uk

Understand fundamental chemistry behind rechargeable Lithium ion batteries : An ab initio study

Dr Shalini Awasthi, Dr Dhammika Widanalage
Warwick Manufacturing Group, University of Warwick, Gibbet Hill Road, Coventry, CV47AL, UK

In recent years, due to increase in global energy demand, developing energy storage systems with higher energy densities are an urgent need. Rechargeable Li-ion batteries (LIBs) emerge as an important power sources for energy storage device for portable electronics and are being continuously investigated and developed for use in automobile electric vehicles (EV). However, during the cycling of LIBs, due to the decomposition of electrolyte, a passivation layer called solid electrolyte interphase (SEI) is formed on electrode surface. Although, SEI formation is vital in LIBs for long term performance, it leads to irreversible loss of lithium and thus, storage capacity of battery. While several studies have been performed in the past few decades on SEI, it is difficult to control its formation and growth, as the chemical composition, and stability of SEI depend on a list of factors. These factors include the electrode material, electrolyte composition, electrochemical conditions, and cell temperature. The perfect SEI would be a fast forming, flexible, stable, and contains insoluble species with low electronic and high ionic conductivity. Thus, the formation of SEI and the electrochemical stability of SEI components should be a primary topic of investigation in future development of LIBs. To understand the stability and chemistry of SEI layer, density function theory based molecular dynamics simulations were performed. We use metadynamics to understand various degradation pathways of electrolyte decomposition in LIBs in various reaction conditions.

Poster n. 83 - Thomas Fay
University of Oxford
thomas.fay@chem.ox.ac.uk

Do spin selective radical pair reactions act as quantum measurements?

Thomas P. Fay, Lachlan P. Lindoy, David E. Manolopoulos
*Department of Chemistry, University of Oxford, Physical and Theoretical Chemistry
Laboratory, South Parks Road, OX1 3QZ*

Radical pair reactions are often electron spin state spin selective; singlet and triplet radical pairs react to form different products at different rates.[1] Furthermore, small energy differences between radical pair spin states allow quantum coherences between the radical pair spin states to be long lived. This means that very weak magnetic interactions between electron and nuclear spins in the radical pair and applied magnetic fields lead to coherent interconversion of spin states, which in turn controls the chemical reactivity of the radical pair.[1] The radical pair dynamics are described using a quantum master equation for the reduced density operator for the radical pair spins. In recent years there has been some debate as to what the correct quantum master equation is, in particular it has been argued that the spin selective chemical reactions may act as quantum measurements on the radical pair spins.[2-4] We have applied reaction rate theory to the problem in order to derive the general exact quantum master equation for radical pair reactions, as well as several useful approximations to this.[5] Our theoretical results may have implications for the interpretation of experiments on radical pairs and models of biologically relevant radical pair reactions, such as those proposed as forming the basis of the magnetic compass sense of birds and other animals.

[1] U.E. Steiner and T. Ulrich, *Chem. Rev.* 89, 51 (1989). [2] K.L. Ivanov, M. V. Petrova, N.N. Lukzen, and K. Maeda, *J. Phys. Chem. A* 114, 9447 (2010). [3] J.A. Jones and P.J. Hore, *Chem. Phys. Lett.* 488, 90 (2010). [4] I.K. Kominis, *Phys. Rev. E - Stat. Nonlinear, Soft Matter Phys.* 80, 056115 (2009). [5] T.P. Fay, L.P. Lindoy, and D.E. Manolopoulos, *J. Chem. Phys.* 149, 064107 (2018).

Poster n. 84 - Khaled Abdel-Maksoud
University of Southampton
K.Abdel-Maksoud@soton.ac.uk

Accelerated sampling of secondary structure formation pathways using digital filtering

Khaled Abdel-Maksoud, Jonathan W. Essex
School of Chemistry, University of Southampton, Highfield Campus, SO17 1BJ

The dynamics of proteins involve the evolution of slow degrees of freedom (DoF) over timescales that cannot be feasibly simulated within conventional all-atom molecular dynamics (MD) [1,2]. Enhanced sampling methods accelerate the system dynamics such that it can be modelled on a computationally feasible timescale. Many of the commonly used procedures for enhanced sampling, including metadynamics [3] and umbrella sampling [4], involve the modification of the system potential energy by adding bias potential defined with respect to a set of collective variables (CVs) over which the system dynamics are projected. The selection of appropriate CVs is problematic for many applications of enhanced sampling. Prior knowledge of the system dynamics is required to propose good CVs. Furthermore, any chosen CVs will not directly target the desired degrees of freedom. Digital filtering can be applied in molecular dynamics simulations [5,6] (DFMD, RDFMD) to enhance the velocity components attributed to the targeted DoF. As the targeted DoF is identified by its vibrational frequency range, the only prior information required for filtering is a molecular vibrational spectrum. Presented here is the implementation of digital filtering to Hamiltonian Monte Carlo simulations – DFHMC. As a principal benchmark, DFHMC, DFMD and RDFMD folding simulations are tested against secondary structure formation in a range of traditional enhanced sampling simulations.

[1] Duan, Y., Kollman, P. A. *Science*. 1999, 282, 740-744. [2] Snow, C. D., Qui, L., Du, D., Gai, F., Hagen, S. J., Pande, V. S. *Proc. Natl. Acad. Sci. U.S.A.* 2004, 101, 4077-4082. [3] Laio, A. Parrinelo, M. *Proc. Natl. Acad. Sci. USA.* 2002, 99, 12562-12566. [4] Torrie, G. M., Valleau, J. P. *J. Comp. Phys.* 1977, 23, 2, 187-199. [5] Philips, S. C., Essex, J. C. *J. Chem. Phys.* 2000, 112, 2586-2597 [6] Philips, S. C., Swain, M. T., Wiley, A. P., Essex, J. W. *J. Phys. Chem. B.* 2003, 107, 9, 2098-2110.

Participants list

Aaron Kelly	aaron.kelly@dal.ca	Elizaveta Suturina	e.suturina@bath.ac.uk
Abdel Maksoud K.	K.Abdel-Maksoud@soton.ac.uk	Ellie Louise Field	ellie.Field@warwick.ac.uk
Abhishek Khedkar	abhishek.khedkar@rub.de	Emiliano Poli	epoli@ictp.it
Adam McSloy	adam.mcsloy@warwick.ac.uk	Eszter Szekely	es732@cam.ac.uk
Adrian Mullholland	adrian.mullholland@bristol.ac.uk	Eva Pluharova	eva.pluharova@jh-inst.cas.cz
Alessandro Troisi	A.Troisi@liverpool.ac.uk	Fabian Thiemann	ucapflt@ucl.ac.uk
Alex Jamieson-Binnie	alexander.jamieson-binnie@bristol.ac.uk	Fabienne Bachtiger	f.bachtiger@warwick.ac.uk
Alexander Duthie	alexander.duthie@chch.ox.ac.uk	Felix Plasser	F.Plasser@lboro.ac.uk
Alexandre Tkatchenko	alexandre.tkatchenko@uni.lu	Fernanda Duarte	fernanda.duarte@chem.ox.ac.uk
Alexandru Moldovan	pmaam@leeds.ac.uk	Filip Szczypinski	f.szczypinski@imperial.ac.uk
Anatole von Lilienfeld	anatole.vonlilienfeld@unibas.ch	Frank Neese	frank.neese@cec.mpg.de
Andela Saric	a.saric@ucl.ac.uk	Fred Manby	fred.Manby@bristol.ac.uk
Aron Walsh	a.walsh@imperial.ac.uk	Gabriele Sosso	gabriele.sosso@warwick.ac.uk
Barbara Montanari	barbara.montanari@stfc.ac.uk	Gareth Richings	gareth.richings@warwick.ac.uk
Ben Atkinson	benjamin.atkinson@manchester.ac.uk	George Booth	george.booth@kcl.ac.uk
Ben Hourahine	benjamin.hourahine@strath.ac.uk	Gergely Juhasz	juhasz@chem.titech.ac.jp
Benjamin Sutherland	benjamin.sutherland@bnc.ox.ac.uk	Germain Clavier	germain.clavier@uca.fr
Berk Onat	B.Onat@warwick.ac.uk	Giullia Galli	gagalli@uchicago.edu
Bethan Cornell	bethan.cornell@kcl.ac.uk	Haiyuan Wang	hwang@fhi-berlin.mpg.de
Billal Sohail	billal.sohail@warwick.ac.uk	Hannah Fowler	hannah.fowler@queens.ox.ac.uk
Bora Karasulu	bk393@cam.ac.uk	Harry Jenkins	JenkinsHJ1@Cardiff.ac.uk
Chi Yang Cheng	c.y.cheng@soton.ac.uk	Harry Morgan	harry.morgan@univ.ox.ac.uk
Chris Skylaris	C.Skylaris@soton.ac.uk	Harry Tunstall	h.tunstall@warwick.ac.uk
Christian Ahart	ucapca1@ucl.ac.uk	Henrik Mortensen	henriklundmortensen@gmail.com
Christine Peter	christine.peter@uni-konstanz.de	Hui Yang	hui.yang@imperial.ac.uk
Christopher Miles	c.miles.1@warwick.ac.uk	Idil Ismail	idil.Ismail@warwick.ac.uk
Christopher Penschke	c.penschke@ucl.ac.uk	Irene Bechis	i.bechis18@imperial.ac.uk
Christopher Robertson	christopher.robertson@warwick.ac.uk	Isabel Gonzalez	isabel.gonzalez@bnc.ox.ac.uk
Christopher Taylor	C.R.Taylor@soton.ac.uk	Isabelle Apostolopoulos	isabelle.hapostolopoulos@gmail.com
Connor Box	connor.box@warwick.ac.uk	Ivan Scivetti	ivan.scivetti@stfc.ac.uk
Craig Devonport	craig.devonport@warwick.ac.uk	Jakub Janowiak	pm11j@leeds.ac.uk
Daniel Corken	daniel.corken@warwick.ac.uk	James Brixey	james.Brixey@warwick.ac.uk
Daniele Fazzi	dfazzi@uni-koeln.de	James Kermode	james.kermode@warwick.ac.uk
David Furman	df398@cam.ac.uk	James William Whipham	j.whipham@soton.ac.uk
David Glowacki	glowacki@bristol.ac.uk	Joao Dos Santos Morado	J.Morado@soton.ac.uk
David McDonagh	dm1m15@soton.ac.uk	Joly Aarons	J.Aarons@warwick.ac.uk
David O'Regan	david.o.regan@tcd.ie	Jonathan Jenkins	jonnie@interactivescientific.com
David Quigley	david.quigley@warwick.ac.uk	Jyoti Gupta	vyotikg@liverpool.ac.uk
Dawn Geatches	dawn.geatches@stfc.ac.uk	Kakali Sen	kakali.sen@stfc.ac.uk
Eleanor Jayawant	E.Jayawant@warwick.ac.uk	Kieron Burke	kieron@uci.edu
Elena Besley	elena.Besley@nottingham.ac.uk	Kimberly Bowal	kib83@cam.ac.uk
Elizabeth Decolvenaere	decolven@DEShawResearch.com		

Kjell Jorner kjell.jorner@astrazeneca.com
Laura Zoppi laura.zoppi@nature.com
Lee Steinberg ls2m15@soton.ac.uk
Letitia-Ioana Birnoschi letitia.birnoschi@postgrad.manchester.ac.uk
Liam Wilbraham l.wilbraham@ucl.ac.uk
Liljana Stojanovic l.stojanovic@qmul.ac.uk
Livia Bartok-Partay l.bartokpartay@reading.ac.uk
Mads-Peter Christiansen machri@phys.au.dk
Matthe Kjaer Bisbo mkb@phys.au.dk
Mariana Rossi rossi@fhi-berlin.mpg.de
Mark Driver mdd31@cam.ac.uk
Martin Lea martin.lea@warwick.ac.uk
Martina Stella m.stella@imperial.ac.uk
Mathias Jørgensen mj@inano.au.dk
Matt Turner M.Turner.1@warwick.ac.uk
Matthew Addicoat matthew.addicoat@ntu.ac.uk
Matthias Golomb mjg3518@ic.ac.uk
Max Veit max.veit@epfl.ch
Maximilian Saller maximilian.saller@phys.chem.ethz.ch
Micaela Matta matta.micaela@gmail.com
Michael Davies michael.davies.14@ucl.ac.uk
Michael Luya michael.luya@warwick.ac.uk
Michele Vendruscolo mv245@cam.ac.uk
Miguel Rivera m.rivera@qmul.ac.uk
Mike O'Connor m.oconnor@bristol.ac.uk
Mirko Vanzan mirko.vanzan@studenti.unipd.it
Miroslav Suruzhon m.suruzhon@soton.ac.uk
Mohamed Ali Al-Badri mohamed.al-badri@kcl.ac.uk
Narjes Ansari nansari@ictp.it
Nathan Fitzpatrick nfitzpatrickchem@gmail.com
Nicholas Hine N.D.M.Hine@warwick.ac.uk
Olexander Isayev olexandr@olexandrisayev.com
Orestis George Ziogos o.ziogos@ucl.ac.uk
Pablo Sanchez-Palencia p.sanchez-palencia@upm.es
Peter Spackman p.r.spackman@soton.ac.uk
Priya Gupta priya.gupta1931@gmail.com
Raphael Chantreau R.Chantreau-Majerus@warwick.ac.uk
Rebecca Notman r.notman@warwick.ac.uk
Rebecca Twidale rebecca.twidale@bristol.ac.uk
Reinhard Maurer reinhard.maurer@warwick.ac.uk
Sam Hall s.hall.4@warwick.ac.uk
Samantha Hood s.hood@imperial.ac.uk
Samuele Giannini samuele.giannini.16@ucl.ac.uk

Scott Habershon scott.habershon@warwick.ac.uk
Shalini Awasthi shalini.awasthi@warwick.ac.uk
Shiyue Yang sy1u17@soton.ac.uk
Siva Chiriki chsiva.chem@gmail.com
Soeren Ager Meldgaard sm@phys.au.dk
Sophie Cooper sophie.cooper-4@postgrad.manchester.ac.uk
Stefano A. Serapian stefano.serapian@bristol.ac.uk
Stela Makri stela.Makri@warwick.ac.uk
Steven Bennett s.bennett18@imperial.ac.uk
Sunghyun Kim sunghyun.kim@imperial.ac.uk
Syma Khalid S.Khalid@soton.ac.uk
Tahereh Nematiamram tahereh.nematiamram@liverpool.ac.uk
Thomas Corry thomas.Corry@postgrad.manchester.ac.uk
Thomas Fay thomas.fay@worc.ox.ac.uk
Tom Hardcastle cp14tej@leeds.ac.uk
Tom Young tom.young@balliol.ox.ac.uk
Venkat Kapil venkat.kapil@epfl.ch
Victor Do Nascimento vdn1m17@soton.ac.uk
Wei Fang wei.fang@phys.chem.ethz.ch
Wilke Dononelli wd@phys.au.dk
Will Gerrard will.gerrard@bristol.ac.uk
Yasir Altaf yasir.altaf@vuw.ac.nz
Yasmine S. Al-Hamdani yas.alhamdani@gmail.com
Ya-Wen Hsiao ya-wen.hsiao@stfc.ac.uk
Ying-Chih Chiang Y-C.Chiang@soton.ac.uk
Yu Che Y.Che@liverpool.ac.uk
Yu Che ichen@liverpool.ac.uk
Zack Williams zack.williams@bristol.ac.uk
Zdenek Futera z.futera@ucl.ac.uk



Sponsored by

We are grateful for the support of:

- **CCP5: Collaborative Computational Project for Simulations of Condensed Phases** (<https://www.ccp5.ac.uk>)
- **CCP9: Computational Electronic Structure of Condensed Matter** (<https://www.ccp9.ac.uk>)
- **The Royal Society of Chemistry** (<http://www.rsc.org>), and particularly **the Faraday Division** (<http://www.rsc.org/Membership/Networking/InterestGroups/FaradayDivision/>)
- **Physical Chemistry Chemical Physics** (<http://www.rsc.org/journals-books-databases/about-journals/PCCP/>)
- **Warwick Global Research Priorities Materials** (<https://warwick.ac.uk/research/priorities/materials/>)
- **Warwick Global Research Priorities Energy** (<https://warwick.ac.uk/research/priorities/energy/>)



WARWICK
GLOBAL RESEARCH PRIORITIES
MATERIALS

Warwick
ENERGY
GRP

PCCP

Editorial Board Chair
David Rueda

