ScotCHEM 2018 Computational Chemistry Symposium

Bringing together theoretically minded chemists

Sponsors of the 2018 Symposium:

ScotCHEM | CCPBioSim | Royal Society of Chemistry Theoretical Chemistry Group | Atos

---

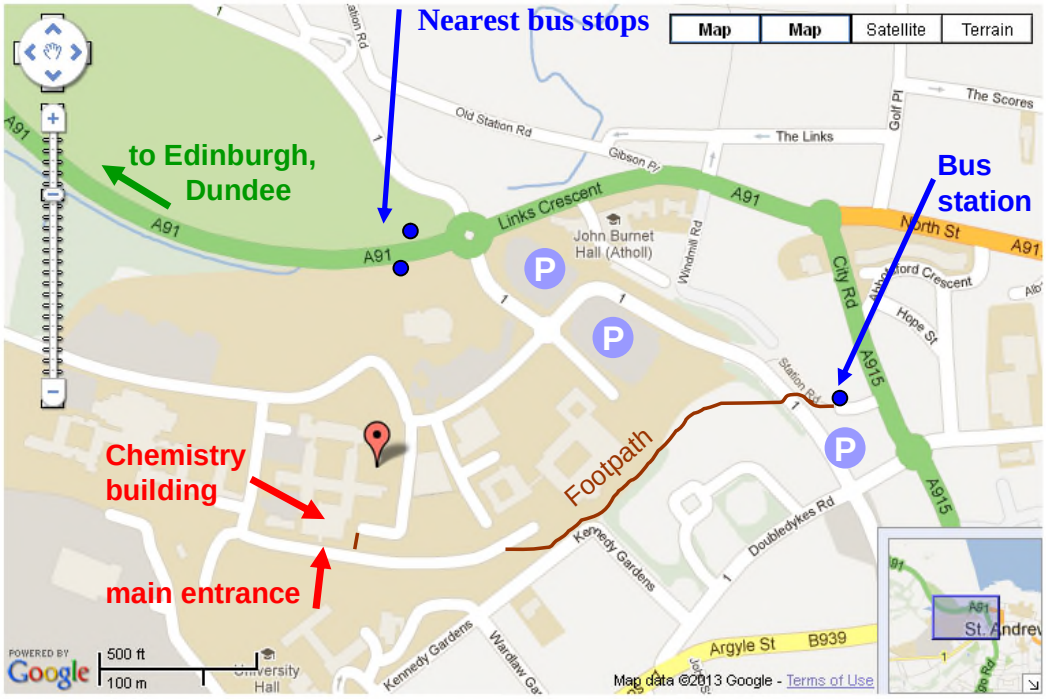
University of St Andrews

Directions

St Andrews can be reached by car (free parking indicated on the map below) and by public transport via bus (https://www.travelinescotland.com/). There are frequent bus connections to Leuchars railway station (journey approx. 10-12 minutes; buses 99, 99A, 99B, 99C, 99D, 92A, 92B, 92C, 92D, 94, 94A, 42).

The Chemistry building is located on the North Haugh at the western entrance to the town. Friday's lectures will take place in Lecture Theatre B (on level 2, the main entrance level; LT B exits also to level 1), coffee and lunch are served in the Common Room on level 1. Thursday's workshop will be in Lecture Theatre C on level 2.

Map of the North Haugh Campus



Symposium Programme

Thursday 14 June 2018, Lecture Theatre C

CCPBiosim Workshop: Biomolecular Modelling with QM/MM (Thomas Keal, Daresbury Laboratory)

10:00 Arrival/coffee

10:30 Lecture 1: Introduction to ChemShell

11:15 Hands-on tutorial session 1

12:30 Lunch

13:30: Lecture 2: Biomolecular modelling with QM/MM

14:15: Hands-on tutorial session 2

15:00 Coffee

15:30 Hands-on tutorial session (until 16:30)

Friday 15 June 2018, Lecture Theatre B

ScotCHEM Computational Chemistry Symposium

9:30 Registration

10:25 Welcome and announcements

Session I - Chair: M. Bühl

10:30 *PL1:* Plenary lecture: **Adrian Mulholland** (University of Bristol)
Multiscale modelling for chemical biology

11:10 *L2:* **Stefano Bosisio** (University of Edinburgh)
Towards high-throughput alchemical free energy calculations

11:35 *L3:* **Darren Belshaw** (University of Edinburgh)
Ab initio surface-hopping simulations of CS_2 photodissociation dynamics

12:00 *L4:* **Gregory S. Tschumper** (University of Mississippi, USA))
Big Electronic Structure Computations for Small Hydrated Anions

12:25 *L5:* **April Cooper** (University of Stuttgart, Germany))
Potential Energy Surface Interpolation with Neural Networks for Instanton Rate Calculations

12:50 Lunch (Common Room)

Session II - Chair: T. van Mourik

14:00 *L6:* **Alexander Urban** (University of St Andrews)
Understanding Cation-Disordered Li-Ion Battery Cathodes by Computation

14:25 *L7:* **Jonathan G. Richardson** (University of Edinburgh)
Investigating CO_2 uptake in Sc_2BDC_3 using XRD, ab initio DFT and GCMC methods

14:50 *L8:* **Joan Clark-Nicolas** (University of Edinburgh)
From JEDI to SITH: A Journey to the Dark Side of Druggability

15:15 Coffee/tea

Session III - Chair: J. B. O. Mitchell

15:45 *L9:* **Bengt Tegner** (Heriot-Watt University)
Water Layers on Actinide Oxide Surfaces

16:10 *L10:* **Cesar Mendoza-Martinez** (University of Edinburgh)
Mechanisms of protein disorder-order transitions upon ligand binding: MDM2 as a case study

16:35 *PL2:* Plenary Lecture: **Sharon Ashbrook** (University of St Andrews)
Investigating Disorder in the Solid State: Multinuclear NMR Spectroscopy and First-Principles Calculations.

17:15-18:30 Poster session (Common Room)

ScotCHEM Lecture Abstracts

Plenary Lecture PL1

Multiscale modelling for chemical biology

Adrian Mulholland
Centre for Computational Chemistry, School of Chemistry, University of Bristol, Bristol BS8 1TS, UK

Biomolecular simulations have advanced to the stage where they can provide reliable predictions of enzyme mechanisms, selectivity, thermoadaptation and inhibition. Many 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 [1]. Simulations can identify mechanisms of catalysis in biosynthesis [2] and antibiotic resistance [3]. Simulations can identify and characterise catalytic interactions [4] and determinants of chemo-, regio- and stereospecificity [5] in biocatalysts. Increasingly, simulations are contributing to the design and engineering both of natural enzymes and of *de novo* biocatalysts [6]. 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 [7]. For modelling reactions within large systems such as proteins, multiscale combined quantum mechanics/molecular mechanics (QM/MM) methods are a good, practical approach, e.g. for modelling transition states and reaction intermediates, and to analyse structural and electronic determinants of reactivity. QM/MM methods treat the active site with a QM electronic structure method, while the effect of the enzyme environment is included by a simpler (MM) approach. Projector-based embedding techniques allow highly accurate correlated *ab initio* QM methods to be applied in QM/MM calculations [8].

1. *Multiscale methods in drug design bridge chemical and biological complexity in the search for cures* R.E. Amaro & A.J. Mulholland *Nature Reviews Chemistry* **2**, Article number: 0148 (2018)
2. *The Catalytic Mechanism of a Natural Diels-Alderase Revealed in Molecular Detail* M.J. Byrne *et al*. *JACS* **138**, 6095-8 (2016)
3. *Insights into the Mechanistic Basis of Plasmid-Mediated Colistin Resistance from Crystal Structures of the Catalytic Domain of MCR-1* P. Hinchliffe *et al*. *Scientific Reports* **7**, 39392 (2017)
4. *A catalytic role for methionine revealed by a combination of computation and experiments on phosphite dehydrogenase* K.E. Ranaghan *et al*. *Chemical Science* **5** 2191-2199 (2014)
5. *Construction and in vivo assembly of a catalytically proficient and hyperthermostable de novo enzyme* J.R. Anderson *et al*., *Nature Communications* **8** Article number: 358 (2017)
6. *Structural Basis of Catalysis in the Bacterial Monoterpene Synthases Linalool Synthase and 1,8-Cineole Synthase* Vijaykumar Karuppiah *et al*. *ACS Catalysis* **7** 6268–6282 (2017)
7. *Dynamical origins of heat capacity changes in enzyme-catalysed reactions* M.W. van der Kamp *et al. Nature Communications* **9**, Article number: 1177 (2018)
8. *A Projector-Embedding Approach for Multiscale Coupled-Cluster Calculations Applied to Citrate Synthase* S.J. Bennie *et al*. *J. Chem. Theory Comput*. **12** 2689–2697 (2016)

L2

Towards high-throughput alchemical free energy calculations

Stefano Bosisio[1], Antonia S J S Mey,[1] Julien Michel[1]

[1] *EaStCHEM School Of Chemistry, University of Edinburgh, D. Brewster Road EH9 3FJ, UK*

There is a strong interest in use of alchemical free energy calculations to support early-stage drug discovery in academia and in the pharmaceutical industry. However significant efforts are still needed to translate the 'free energy science' into a robust engineering tool that may be used routinely. In particular, free energy simulation protocols show a lack of reproducibility of results among different simulation packages, even starting from the same initial conditions.

Thus, we have pursued a collaborative effort to systematically compare the reproducibility of computed hydration free energies between our in-house free energy code SOMD, GROMACS (Mobley group, UCI) and AMBER (Hannes Loeffler, STFC). This work has shown that reasonable reproducibility can be achieved for small organic neutral molecules, but code-specific details in the implementation of the free energy algorithm currently prevents the use of a generic simulation protocol. This work suggests steps the field could consider to facilitate wider use of free energy methods for molecular design.

A more challenging situation arises when molecules carry a net charge. In this case reproducibility and accuracy of free energy predictions are affected by finite size artefacts. Therefore, we took part in the SAMPL5 competition (Statistical Assessment of the Modelling of Proteins and Ligands) and submitted blinded predictions using multiple protocols. Specifically, binding free energies for 22 host-guest systems and distribution coefficients of 53 drug-like molecules were computed with alchemical free energy calculations, featuring cutoffs and standard state corrections. We achieved a significant correlation with experimental data for host-guest binding energies, but encountered major difficulties in estimating distribution coefficients of ionisable species.

L3

Ab initio surface-hopping simulations of CS2 photodissociation dynamics

Darren Bellshaw and Adam Kirrander

We simulate the nonadiabatic photodissociation dynamics of CS_2 molecules excited by UV light [1] using surface-hopping as implemented in the SHARC code [2]. A benchmark system in ultrafast small molecule dynamics, the photochemistry of CS_2 is dictated by complex interplay between a dense manifold of electronic excited states, complicated further by the presence of strong spin-orbit coupling between the singlet and triplet states due to the sulfur atoms. The propensity for intersystem crossing gives rise to multiple accessible reaction channels whose branching ratios are typically difficult to measure accurately.

Here we compare two simulations of this system carried out at different levels of electronic structure theory, discuss the differences in predicted reactivity in the system in terms of the behaviour of the vibrational wavepacket and population changes between the singlet and triplet manifolds, and comment on our ongoing work to improve the description of the photodynamics of this key system [1].

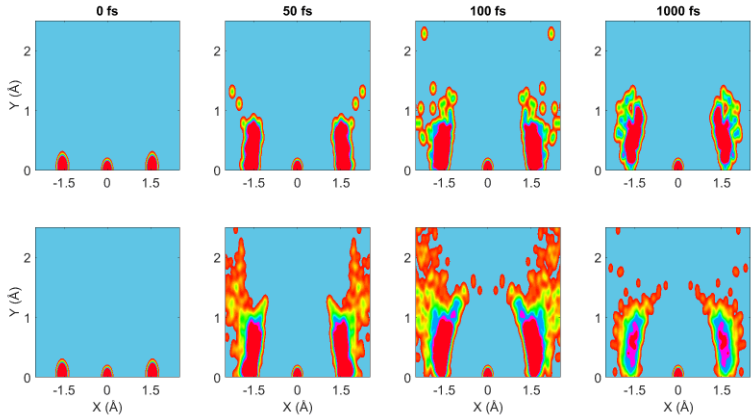


*Figure 1: Snapshots of the nuclear probability density at selected time points in two simulations of CS_2 photodissociation carried out at different levels of theory (simulation **1**, top row; simulation **2**, bottom row). The carbon atom is kept fixed at the origin.*

[1] A. D. Smith, E.M. Warne, D. Bellshaw, D. Horke, M. Tudorovskya, E. Springate, ... & R.S. Minns. (2018). Mapping the complete reaction path of a complex photochemical reaction. *Physical Review Letters*. Accepted 23 March 2018**.**

[2] M. Richter, P. Marquetand, J. González-Vázquez, I. Sola, and L. González. SHARC: *ab initio* molecular dynamics with surface hopping in the adiabatic representation including arbitrary couplings. *J. Chem. Theory Comp*., 7(5):1253-1258, 2011.

L4

Big Electronic Structure Computations for Small Hydrated Anions

Gregory S. Tschumper
Department of Chemistry and Biochemistry, University of Mississippi

The structures, energetics and harmonic vibrational frequencies of explicitly solvated halide ions (X^- $(H_2O)_n$ where n = 1 - 4 and X = H, F, Cl, Br, I) have been probed with the MP2 and CCSD(T) quantum mechanical electronic structure techniques and large correlation consistent basis. The N-body:Many-body QM:QM method has been used to extend the demanding large basis set CCSD(T) computations, particularly the analytic Hessians, to the larger solvated ion clusters. Some of the smaller clusters exhibit exceptionally large deviations between the MP2 and CCSD(T) harmonic vibrational frequencies (>100 cm^{-1}). CCSDT, CCSDT(Q) and CCSDTQ computations are being performed to examine higher-order correlation effects on the structures, energetics and vibrational frequencies on these challenging systems.

L5

Potential Energy Surface Interpolation with Neural Networks for Instanton Rate Calculations

April Cooper[1], Johannes Kästner[1]

[1]*Institute for Theoretical Chemistry, University of Stuttgart, Germany*

For the calculation of reaction rate constants with instanton theory an accurate description of the sector of the potential energy surface (PES) containing the transition state and the reactant state of the reaction of interest is needed. However, obtaining information on the PES on the fly during the rate constant calculation is computationally very demanding. Therefore, we interpolate the PES with artificial neural networks (NNs) and calculate the reaction rate constants with the instanton method using this NNPES. In instanton theory it is assumed that the energy, but also the gradient and the Hessian of the energy with respect to the input coordinates, is a continuous function of the input coordinates. Therefore, we incorporate not only information on the energy, but include also information on the gradient and Hessian in the NN training to ensure their continuity and accuracy.

To demonstrate the capabilities of this approach we calculated reaction rate constants with the instanton method for the reaction $CH_3OH + H \rightarrow CH_2OH + H_2$ on an average NNPES fitted to CCSD(T)-F12/VTZ-F12 data. We demonstrate that these rate constants are in excellent agreement with rate constants that were calculated on the same level of theory performing energy, gradient and Hessian calculations on the fly, while the computational effort of the rate constant calculation is significantly lower if a NNPES is used instead of on the fly calculations.

L6

Understanding Cation-Disordered Li-Ion Battery Cathodes by Computation

Alexander Urban[1], Aziz Abdellahi[2], Stephen Dacek[2], Nongnuch Artrith[3,4], Gerbrand Ceder[3,4]
[1]*University of St Andrews, Scotland, UK.*
[2]*Massachusetts Institute of Technology, Cambridge, USA.*
[3]*University of California, Berkeley, USA;* [4]*Lawrence Berkeley National Laboratory, Berkeley, USA.*

Cation-disordered oxides have recently emerged as a promising new class of high-energy-density cathode materials for Li-ion batteries. Theory and computation have played a fundamental role in the discovery and exploration of this new materials class. Compared to conventional ordered cathodes, disordered oxides offer the prospect of improved structural stability, extraordinary reversible Li storage capacities, and a rich chemistry that holds the promise of yet undiscovered superior materials. Using tailored computational models including electronic structure calculations, lattice-model simulations, and percolation theory, we have developed a comprehensive understanding of the effects of cation disorder on the performance: (i) We identified the factors that determine the practical capacity of disordered cathodes, (ii) established how the voltage profile and the redox mechanism are affected by cation disorder, and (iii) devised guidelines for the prediction of novel disordered compositions. Many of our theoretical results have since been confirmed experimentally, stimulating entirely new research directions within the battery community.

L7

Investigating CO_2 uptake in Sc_2BDC_3 using XRD, *ab initio* DFT and GCMC methods

J. G. Richardson[a], J. Sotelo[a], S. A. Moggach[a], J. McHardy[a], C. A. Morrison[a], T. Düren[b], P. A. Wright[c]

[a] School of Chemistry, University of Edinburgh, UK

[b] Centre for Advanced Separations Engineering, University of Bath, UK

[c] School of Chemistry, St Andrews, UK

Despite the large number of MOFs that have been synthesised, a large proportion have not been studied for their gas adsorption and mechanical properties using in-situ diffraction techniques.[1,2] Most investigations concerning the former are based upon adsorption isotherms and hence there is a lack of understanding concerning the location of adsorbed guest molecules within the pores and the nature of specific interactions between the guest molecules and the framework.

In a previous study, the small-pore MOF Sc_2BDC_3 (where BDC = benzenedicarboxylate) was initially observed to undergo an orthorhombic-to-monoclinic phase transition, via rotation of one pair of BDC linkers, under 1 bar of CO_2 and at 235 K.[3,4] Here, we have used in-situ X-ray diffraction alongside *ab initio* DFT and grand canonical Monte Carlo computational methods to show that the framework also undergoes the same phase transition, gradually, at 298 K at higher CO_2 pressures (complete at 3 bar). A third adsorption site, which was not observed in the original investigation at 235 K, was experimentally observed in the monoclinic phase, which verified the expected maximum uptake of CO_2 in Sc_2BDC_3.

Ab initio DFT calculations determined that the monoclinic form of Sc_2BDC_3 is the lower energy geometry-optimised structure (by 13.3 kJ mol^{-1}). GCMC simulations, utilising experimental framework structures to model CO_2 uptake at room temperature, highlighted stronger CO_2-framework interactions in the monoclinic phase, and hence show that these interactions counteract the energy barrier to linker rotation. Additionally, there was good agreement between the binding site energies observed by the two independent computational methods, and the experimental binding site hierarchy was verified. Sc_2BDC_3 was also shown, by all three methods, to have selective uptake for CO_2 over CH_4, as a result of weaker CH_4-framework interactions and the strongest CO_2 adsorption site being uninhibited when CO_2/CH_4 mixtures were studied.

References

[1] Moghadam, P. Z. *et al*. (2017). *Chem. Mater.* **29**, 2618-2635
[2] Carrington, E. J., Vitórica-Yrezábal, I. J., Brammer, L. (2014). *Acta.Cryst.* **B70**, 404-422
[3] Miller, S. R. *et al*. (2009). *Langmuir*. **25**, 3618-3626
[4] Mowat, J. P. S. *et al*. (2011). Inorg. Chem. **50**, 10844-10858

L8

From JEDI to SITH:

A Journey to the Dark Side of Druggability

Joan Clark-Nicolas[1], and *Julien Michel*[1]
[1]*EaStCHEM School of Chemistry, The University of Edinburgh, EH9 3FJ, Scotland*

j.clark-nicolas@ed.ac.uk

Although proteins represent the vast majority of targets of pharmaceutical interest, only a small portion of the human proteome is known to be able to bind drug-like molecules. Proteins, however, are flexible and they often undergo conformational rearrangements that may reveal pockets that could potentially be druggable (*i.e.* able to bind a drug-like molecule). The study of these pockets, known as cryptic pockets, could potentially lead to the development of new drugs that target proteins that *a priori* would be considered undruggable. Cryptic pockets exist for very short times and they usually cannot be detected at experimental time scales, which makes the use of computational methods such as molecular dynamics necessary to characterise them. However, their transient nature implies that very long simulation times may be be necessary in order to detect them, a difficulty that can be overcome by using enhanced sampling methods such as those based in collective variables.

Using human Phenylethanolamine N-Methyl Transferase (hPNMT) as a case study, the present work makes use of the JEDI druggability function [1] to limit the sampling of the conformational space to states with a high druggability, and combines it with the SITH taboo search protocol in order to iteratively bias the simulations away from previously visited states. Using a structure that binds an inhibitor at micromolar concentrations as a starting point, the results of the taboo search have been compared to a structure that presents a cryptic pocket that binds a larger inhibitor at nanomolar range concentrations [2].

References

1. Cuchillo, R. *et al*, *J. Chem. Theor. Comput*, 11, 1292-1307, **2015**
2. Grunewald, G.L. *et al, J. Med. Chem*, 46, 5424-5433, **2006**

L9

Water Layers on Actinide Oxide Surfaces

Dr. Bengt Tegner
Macgregor group
Institute for Chemical Sciences
Heriot-Watt University

My contribution is concerned with the medium term storage of the UK's civilian stocks of plutonium. Presently, this is stored as PuO_2 powder in stainless steel containers at Sellafield, while the government decides its long term fate. Some of these containers have buckled, leading to the suggestion that gas build-up is causing pressurisation. Several different mechanisms have been proposed for this gas build-up, including (i) steam produced by H_2O desorption from hygroscopic PuO_2 due to self-heating (ii) radiolysis of adsorbed water and (iii) generation of H_2 by chemical reaction of PuO_2 with H_2O, producing a postulated PuO_{2+x} phase. These hypotheses, along with a desire to better understand the chemistry of these systems, have lead me to investigate water interactions with actinide oxide surfaces using plane-wave density functional theory at the PBE+*U* level.

The initial focus of this work was the geometries and energetics of up to a single monolayer of water on the stoichiometric {111}, {110} and {100} surfaces. This study has now been published [1] and I have since been studying sub-stoichiometric surfaces (oxygen vacancy formation geometries and energies) and water adsorption on them [2], as well as multiple water layers. Initial results from the multiple water layer study suggest that the second layer is quite strongly bonded to the first, and that with additional layers, the average binding energy rapidly approaches a constant value of about 0.54 eV/water molecule independent of the surface or mode of binding of the first two monolayers.

[1] B. E. Tegner, M. Molinari, A. Kerridge, S. C. Parker, and N. Kaltsoyannis,
J. Phys. Chem. C, 2017, 121, 1675-1682, DOI: 10.1021/acs.jpcc.6b10986

[2] J. P. W. Wellington, B. E. Tegner, J. Collard, A. Kerridge and N. Kaltsoyannis
J. Phys. Chem. C, 2018, 122, 7149-7165, DOI: 10.1021/acs.jpcc.7b11512

L10

Mechanisms of protein disorder-order transitions upon ligand binding: MDM2 as a case study

Cesar Mendoza-Martinez, Antonia S J S Mey, Stefano Bosisio, Kirsten Ritchie, Julien Michel

EASTCHEM, University of Edinburgh, Joseph Black Building, David Brewster Road, Edinburgh, Scotland EH9 3FJ

A major frontier for current drug discovery is that about a third of all proteins present in living organisms are considered 'intrinsically disordered'. Unlike conventional drug targets, these proteins constantly change shape and are considered 'undruggable' because we do not currently understand how to target disordered proteins with man-made small molecules. We seek to understand how such molecular recognition principles may be mimicked using small molecules.
Our efforts have focused specifically on the protein MDM2 that contains a 'disordered' lid region at the interface of a 'well structured' region. MDM2 is a major anti-cancer drug target and there are currently several different classes of small molecules that are MDM2 ligands in clinical trials worldwide. Some MDM2 ligands have been shown to induce ordering of the MDM2 'disordered' lid. We have implemented a multidisciplinary research program that combines molecular simulation and biophysical experiments to rationalize the mechanisms that underpin this unique example of a small molecule induced protein disorder-order transition. Our results pave the way for broader targeting of protein disordered regions in drug discovery.

References:
1. Michelsen K., Jordan J. B., Lewis J., Long A. M., Yang E., Rew Y., Zhou J., Yakowec P., Schnier P. D., Huang X., Poppe L. *J. Am. Chem. Soc*. 2012, 134: 17059−17067.
2. Bueren-Calabuig J. A., Michel J. *PLoS Comput. Biol.* 2015. Jun 5;11(6):e1004282.
3. Loeffler H., Michel J., Woods C. J. *J Chem Inf Model.* 2015, 28;55(12):2485-90.

Plenary Lecture PL2

Investigating Disorder in the Solid State: Multinuclear NMR Spectroscopy and First-Principles Calculations

Sharon E. Ashbrook, EaStCHEM School of Chemistry and Centre of Magnetic Resonance, University of St Andrews, UK.

NMR spectroscopy provides an element-specific, sensitive probe of the local environment, enabling detailed information to be extracted. However, in the solid state the vast majority of this information remains unexploited, owing to the challenges associated with obtaining high-resolution spectra and the ease with which these can be interpreted. For inorganic solids, this problem is amplified by the large range of nuclides studied, the lack of information available in the literature and the practical challenges of experimental implementation.

Recent advances enabling accurate and efficient calculation of NMR parameters in periodic systems have revolutionized the application of such approaches in solid-state NMR spectroscopy, particularly among experimentalists. The use of first-principles calculations aids in the interpretation and assignment of the complex spectral lineshapes observed for solids. Furthermore, for materials with poorly characterized structures calculations provide a method for evaluating potential structural models against experimental measurements. As NMR is sensitive to the atomic-scale environment, it provides a particularly useful tool for studying disordered materials, and the combination of experiment with first-principles calculations offers a particularly attractive approach. This will be illustrated using examples from recent work investigating ceramic wasteforms proposed for the encapsulation of nuclear waste, and the hydration of wadsleyite, a high-pressure silicate phase found in the inner layers of the Earth.

ScotCHEM Posters

P1. **Probing the local structure of copper complexes through DFT calculations of paramagnetic NMR parameters**, Zhipeng Ke, Daniel M. Dawson, Freddie Mack, Sharon E. Ashbrook, Michael Bühl.

P2. **Searching For Insulin-boosting Drugs: A Theoretical Study**, Xiaotong Zhang, Tanja van Mourik, Michael Bühl

P3: **Complete dehydrogenation of alcohols catalysed by [$RuH_2(PPh_3)_3(CO)$]**, Shahbaz Ahmad, David Cole-Hamilton, Patrizia Larusso, Nicolas Sieffert, Michael Bühl

P4: **DFT studies of the mechanism of iron-catalysed transfer hydrogenation using amines and boranes**, Samuel E. Neale, Nathan T. Coles, Maialen Espinal-Viguri, Ruth L. Webster, and Stuart A. Macgregor

P5: **Modelling heme peroxidases with QM/MM**, Jonathan Colburn, Michael Bühl

P6: **Optimising activity and selectivity in biomimetic capsules through computational design**, Sofia Bariami

P7: **Quantifying and visualising NMR J-coupling interactions in the solid state**, Oliver J. R. Gilford, David McKay, Jonathan R. Yates, Sharon E. Ashbrook

P8: **Novel statistical approaches to gain insight into protein allostery**, Lisa Patrick, Ben Cossins, Julien Michel

P9: **BioSimSpace - an interoperable collaborative bimolecular simulation environment**, Antonia Mey, Lester Hedges, Julien Michel, Christopher Woods

P10: **Changes in ns time scale motions are sufficient to explain allosteric effects in a catalytically impaired variant of cyclophilin A**, Pattama Wapeesittipan, Antonia Mey, Malcolm D Walkinshaw, Julien Michel

P11: **Structure-Based Prediction of Solid-State NMR Parameters in Zeolites and Zeotypes**, Daniel M. Dawson, Robert F. Moran, Scott Sneddon, Valerie R. Semour and Sharon E. Ashbrook

P12: **Potential Energy Surface Interpolation by Neural Networks**, April Cooper, Johannes Kästner

P13: **Excited states of squaraines via linear and non-linear electronic absorption**, Freda Mwasha, Martin Paterson

P14: **Molecular Motions in a Fluxional (h6-Indenyl)Tricarbonylchromium Hemichelate: a DFT Molecular Dynamics Study**, Nicolas Sieffert

P15: **GAsol: a new tool for predicting water sites in protein cavities**, Lucia Fusani, Ian Wall, David Palmer, Alvaro Cortes

P16: **Electrochemical metal deposition controlled by surface-based molecular self-assemblies**, Zhen Yao, Michael Bühl, Manfred Buck

P17: **The Big Bang Theory: a Pathway to the Athermal Impact Initiation of Energetic Materials**, Adam Michalchuk, Peter Finchamn, Peter Portius, Colin Pulham and Carole Morrison

P18: **Post Synthetic ^{17}O Enrichment and Solid-State NMR Characterisation of Niobates**, Ingo Gert, Daniel Dawson, Arantxa Frenandes, Nasima Kanwal, David McKay, Robert Moran, Sharon Ashbrook

P19: **Investigating Disorder and Dynamics in a Novel Gallophosphate**, Joseph E. Hooper, Daniel M. Dawson, Lucy Broom, Mahrez Amri, Nathalie Guillou, Sharon E. Ashbrook, Richard I. Walton.

P20: **DFT Study of Heterobimetallic Complexes Derived from the e-deficient Ru–H Complex, [Ru(IPr)$_2$(CO)H]$^+$**, Nasir A. Rajabi, Ian M. Riddlestone, John P. Lowe, Mary F. Mahon, Stuart A. Macgregor, Michael K. Whittlesey

P21: **Disorder to order transitions of MDM2 lid upon ligand binding**, Salome Llabres, Cesar Mendoza, Arun Gupta, Julien Michel

P22: **Approaching Full CI limits by Systematic Truncations in the Configuration Space**, Andrew W. Prentice, Jeremy Coe and Martin J. Paterson

P23: *retracted*

P24: **Valence Bond and Molecular Orbital Methods to Probe Boradioxazole Chemistry: A Dynamic Test Case for Complex Chemical Systems**, T. Malcomson, M. Paterson, G. Lloyd, C. Shepherd

P25: **Computing NMR Chemical Shifts of Paramagnetic Compounds**, Ben Griffiths, Michael Bühl

P26: **Electron Transfer Reactions: KOtBu Photoreduces Benzophenone, under activation by Visible light,** Allan Young, Giuseppe Nocera, Fabrizio Palumbo, Thomas McGuire, Tell Tuttle, John A. Murphy

List of CCP5Biosim (*Q*) and ScotCHEM Participants

Shahbaz	**Ahmad**	sa223@st-andrews.ac.uk	*Q*, P3
Sofia	**Bariami**	sofia.bariami@ed.ac.uk	*Q*, P6
Darren	**Bellshaw**	Darren.Bellshaw@ed.ac.uk	L3
Stefano	**Bossi**	stefanobosisio1@gmail.com	L2
Michael	**Bühl**	buehl@st-andrews.ac.uk	*Q*, P1, P2, P3, P5,P16, P25
Philip	**Camp**	philip.camp@ed.ac.uk	
Sonia	**Chabbra**	sc262@st-andrews.ac.uk	*Q*
Joan	**Clark-Nicolas**	j.clark-nicolas@ed.ac.uk	L8
Jonathan	**Colburn**	jdc6@st-andrews.ac.uk	*Q*, P5
April	**Cooper**	ac361@st-andrews.ac.uk	*Q*, L5
Daniel	**Dawson**	dmd7@st-andrews.ac.uk	P11
Herbert	**Früchtl**	hf63@st-andrews.ac.uk	*Q*
Licia	**Fusani**	lucia.x.fusani@gsk.com	P15
Ingo	**Gert**	ig55@st-andrews.ac.uk	*Q*, P18
Ben	**Griffiths**	bg29@st-andrews.ac.uk	P25
Joseph	**Hooper**	jeh22@st-andrews.ac.uk	P19
Jack	**Hemingway**	jackhemingway96@gmail.com	
Zhipeng	**Ke**	zk25@st-andrews.ac.uk	*Q*, P1
Thomas	**Keal**	thomas.keal@stfc.ac.uk	
Tobias	**Kraemer**	tobias.kraemer@mu.ie	*Q*
Philip	**Lane**	b2014038@my.shu.ac.uk	*Q*
Salome	**Llabres**	s.llabres@ed.ac.uk	*Q*, P21
Thomas	**Malcomson**	thomasmalcomson2761@gmail.com	P24
Alexandra	**Mayo**	amayo@princeton.edu	
David	**McKay**	dm228@st-andrews.ac.uk	P7
Cesar	**Mendoza-Martinez**	Cesar.Mendoza@ed.ac.uk	*Q*, L10
Antonia	**Mey**	antonia.mey@gmail.com	*Q*, P9
Adam	**Michalchuk**	adam.michalchuk@ed.ac.uk	*Q*, P17
John	**Mitchell**	jbom@st-andrews.ac.uk	
Carole	**Morrison**	c.morrison@ed.ac.uk	L7, P17
Adrian	**Mulholland**	Adrian.Mulholland@bristol.ac.uk	PL1
Freda	**Mwasha**	fjm1@hw.ac.uk	*Q*, P13
Sam	**Neale**	sen1@hw.ac.uk	*Q*, P4
Anna	**Olszewska**	anna.olszewska.2014@uni.strath.ac.uk	
David	**Palmer**	david.palmer@strath.ac.uk	
Michail	**Papadourakis**	s1771676@ed.ac.uk	*Q*
Kyle	**Paterson**	s1679948@sms.ed.ac.uk	*Q*
Lisa	**Patrick**	lisa.patrick@ed.ac.uk	*Q*, P8
Andrew	**Prentice**	awp2@hw.ac.uk	*Q*, P22
Iain	**Prentice**	iain.prentice@ed.ac.uk	
Nasir	**Rajabi**	nr9@hw.acuk	P20
Jonathan	**Richardson**	J.G.Richardson@ed.ac.uk	L7
Simon	**Rohrbach**	simon.rohrbach@strath.ac.uk	

Hans	**Senn**	hans.senn@glasgow.ac.uk	
Ashbrook	**Sharon**	sema@st-andrews.ac.uk	PL2
Nicolas	**Sieffert**	nicolas.sieffert@univ-grenoble-alpes.fr	*Q*, P3, P14
Gulia	**Tamburrino**	gtamburrino@dundee.ac.uk	*Q*
Bengt	**Tegner**	b.tegner@hw.ac.uk	*Q*, L9
Georgia	**Tsagaropoulou**	georgiatsagaropoulou@gmail.com	*Q*
Gregory	**Tschumper**	tschumpr@olemiss.edu	L4
Tell	**Tuttle**	tell.tuttle@strath.ac.uk	P26
Alexander	**Urban**	au25@st-andrews.ac.uk	*Q*, L6
Tanja	**van Mourik**	tvm22@st-andrews.ac.uk	*Q*, P2
Pattama	**Wapeesittipan**	s1467112@sms.ed.ac.uk	*Q*, P10
Zhen	**Yao**	zy9@st-andrews.ac.uk	P16
Allan	**Young**	a.young@strath.ac.uk	*Q*, P26
Xiaotong	**Zhang**	xz41@st-andrews.ac.uk	*Q*, P2