ScotCHEM Computational Chemistry Symposium 2013

Advancing Computational Chemistry in Scotland

University of St Andrews, 13-14 June 2013

## Bringing together theoretically minded chemists

Sponsors of the 2013 Symposium:

Directions

St Andrews can be reached by car (free parking indicated on the map below) and by public transport via bus (www.stagecoachbus.com). There are frequent bus connections to Leuchars train station (10 min).

The Chemistry building is located on the North Haugh at the western entrance of the town. The lectures will take place in Lecture Theatres B or C on level 2 (main entrance level), coffee and lunch is served in the Common Rooms on level 1.

Map of the North Haugh Campus
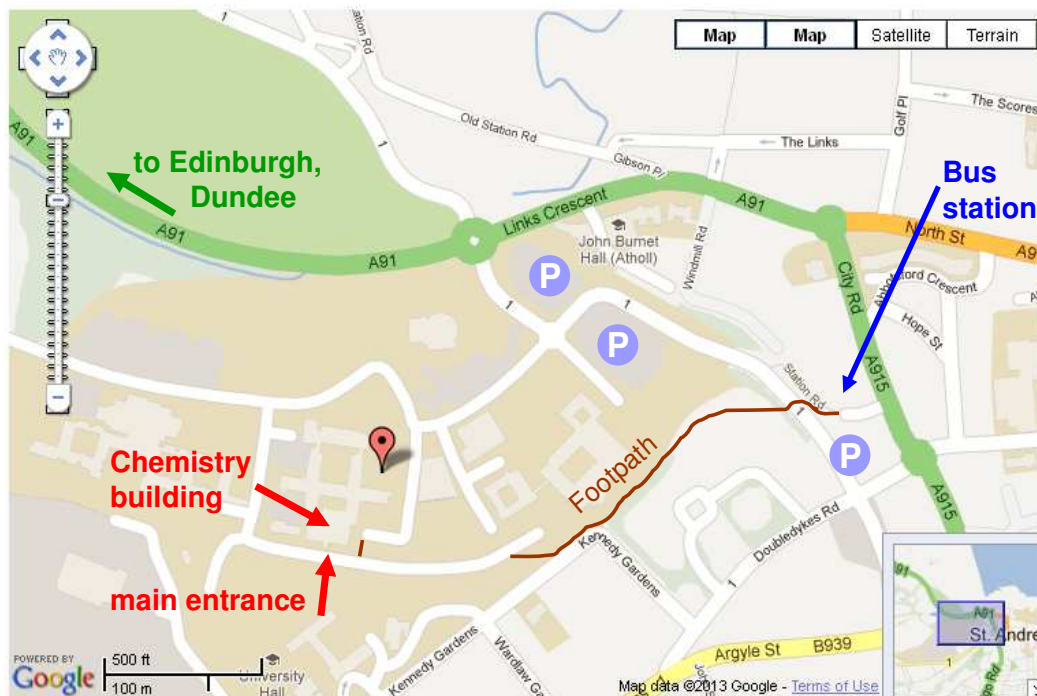
Symposium Programme

Thursday 13 June 2013, Lecture Theatre C

CCP5 Workshop: Modelling the Chemistry and Biochemistry of Condensed Phases

Session Chair: N.N.
  W1 **Prof. Marie-Pierre Gaigeot** (University of Evry, France)
  Cancelled.

14:00 Welcome and announcements

14:15 **Dr. Tanja van Mourik** (University of St. Andrews),
  The mutagenic action of 5-bromouracil.

14:45 *W2* **Dr. Carole Morrison** (University of Edinburgh)
  Modelling photochemical reactions in condensed matter. Applications in time-resolved diffraction.

15:15 *W3* **Prof. Christine Orengo** (University College London)
  Shifts in catalytic residues in enzyme families during evolution.

15:45 Coffee/tea

16:15 *W4* **Prof. Barbara Kirchner** (University of Bonn, Germany)
  Understanding ionic (and molecular) liquids from theoretical methods

17:00 *W5* **Dr. Barbara Holtz** (Materials Design S.A.R.L.)
  Industrial applications of computational materials science

17:20 Wine reception and network event to promote women in science

Friday 14 June 2013, Lecture Theatre B

ScotCHEM Computational Chemistry Symposium

 9:30 Registration

10:25 Welcome and announcements

Session I - Chair: M. Bühl
10:30 *L1:* Plenary lecture: **Tim Clark** (Universities of Portsmouth and Erlangen-
Nürnberg, Germany)
Anisotropic intermolecular interactions

11:20 *L2:* **Adam Kirrander** (University of Edinburgh)
New light sources and exotic quantum states

11:50 *L3:* **Linus Johannissen** (University of Manchester)
*How does flavin reduction drive domain motion in human cytochrome P450
reductase?*

12:10 *L4:* **Ling Ge** (NSCCS, Imperial College London)
EPSRC UK National Service for Computational Chemistry Software

12:30 Lunch (Common Room)

Session II - Chair: H. Früchtl
13:30 *L5:* **James McDonagh** (University of St Andrews)
Predictions of Intrinsic Aqueous Solubility of Crystalline Drug-like Molecules

14:00 *L6:* **Sven Tobisch** (Sasol/University of St Andrews)
Role of Lewis acids in the tungsten imido mediated dimerisation of olefins

14:30 *L7:* **David Cheung** (University of Strathclyde)
Simulation of complex molecules at interfaces

15:00 Coffee/tea

Session III - Chair: J. B. O. Mitchell
15:30 *L8:* **David McKay** (Heriot-Watt University)
*Computational Studies of Catalytic Hydrodefluorination at Ru(II) N-Heterocyclic
Carbene Complexes*

16:00 *L9:* **Jun Cheng** (University of Cambridge/University of Aberdeen)
Proton coupled electron transfer in water photo-oxidation at TiO_2 water interface

16:30 - 18:00 Poster session (Common Room)

ScotCHEM Lecture Abstracts

L1

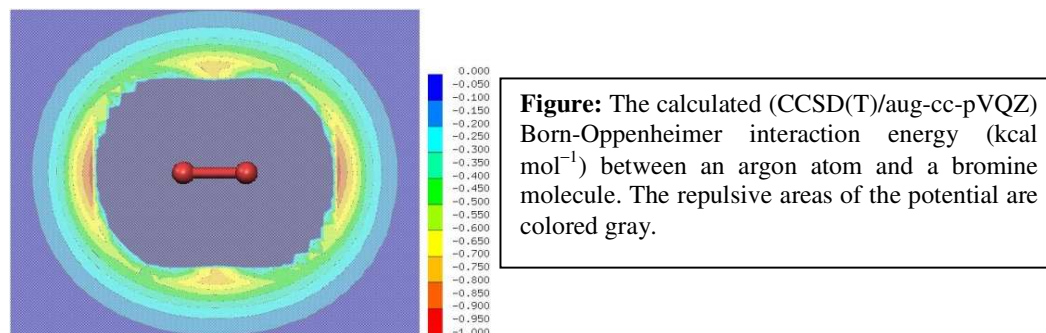### Anisotropic Interatomic Interactions

Tim Clark

Computer-Chemie-Centrum der Friedrich-Alexander-Universität Erlangen-Nürnberg, Nägelsbachstrasse 25, 91052 Erlangen, Germany.

Centre for Molecular Design, University of Portsmouth, King Henry Building, King Henry I Street, Portsmouth PO1 2DY UK.

We are conditioned to believe that non-covalent interactions (e.g. Coulomb or dispersion) cannot result in directional preferences. The best known example is that a "covalent component" (aka "donor-acceptor interaction") is assumed to be important in hydrogen bonding because the preferred angle at the donor hydrogen is 180°. In fact, a purely electrostatic model reproduces the angle preference quite well.[1] Our use of isotropic atom-based models for non-covalent interactions (e.g. net atomic charges with Coulomb's law or Lennard-Jones potentials for repulsion/dispersion) leads us to assume that any directional preference must be due to covalent interactions, even though 27 years ago Price called the *"assumption that the charge distribution around each atom is spherical"* a *"travesty of bonding theory"*.[2]

Just how good (or how bad) are isotropic atom-atom models? The question is especially important today because many density-functional theory (DFT) techniques are supplemented by isotropic atom-atom potentials to compensate for the missing dispersion interaction in DFT. Like electrostatics, dispersion is generally assumed to be isotropic, but Stone has shown that both repulsion[3] and dispersion[4] are significantly anisotropic. Can DFT, for instance, reproduce the energy contour diagram for the interaction of an argon atom with a bromine molecule shown below?[5]

Figure: The calculated (CCSD(T)/aug-cc-pVQZ) Born-Oppenheimer interaction energy (kcal mol^{-1}) between an argon atom and a bromine molecule. The repulsive areas of the potential are colored gray.

The lecture will discuss some historical examples of how the spherical atom assumption has led to false conclusions and describe new attempts to analyze intermolecular interactions uniquely and rationally.

[1] *Directional Weak Interactions: σ-Hole Bonding,* J. S. Murray, K. E. Riley, P. Politzer and T. Clark, *Aus. J. Chem.,* **2010**, *63*, 1598-1607.

[2] *Applications of realistic electrostatic modelling to molecules in complexes, solids and proteins*, S. L. Price, *J. Chem. Soc. Faraday Trans*, **1996**, *92*, 2997-3008.

[3] *Anisotropy of Atom-Atom Repulsions*, A. J. Stone and C.-S. Tong, *J. Comput. Chem.*, **1994**, *15*, 1377-1392.

[4] *Distributed dispersion: A new approach*, G. J. Williams and A. J. Stone, *J. Chem. Phys.*, **2003**, *119*, 4620-4628.

[5] *Directional Non-covalent Interactions: Repulsion and Dispersion*, A. El Kerdawy, J. S. Murray, P. Politzer, P. Bleiziffer, A. Hesselmann, A. Görling and T. Clark, *J. Chem. Theor. Comput.,* **2013**, *9*, 2264–2275 (DOI: 10.1021/ct400185f).

L2

New light sources and Exotic quantum states
Adam Kirrander, School of Chemistry, University of Edinburgh

New light sources produce ever-shorter pulses of light over an increasing range of energies and intensities, and many new experiments follow. Our research focuses on the intersection of quantum dynamics, photochemistry and AMO physics, trying to provide the tools to interpret experiments, as well as to anticipate and stimulate new experiments yet to be tried. I will discuss some of our recent predictions for time-resolved x-ray diffraction imaging of electron motion in highly excited atoms.

If time permits, I will also touch briefly on our work relating to exotic states known as heavy Rydbergs, extremely long-range vibrational states observed in recent experiments. These states exhibit distinct interferometric lifetime modulations, which are manifestations of the matter-wave properties of molecular vibrations.

L3

How does flavin reduction drive domain motion in human cytochrome P450 reductase?

Linus O. Johannissen

Cytochrome P450 reductase (CPR) mediates uni-directional electron transfer along the chain NADPH -> FAD -> FMN -> heme. This involves large-scale domain motion from a "closed" conformation optimal for the interflavin electron transfer (FAD -> FMN) to an "open" conformation required for interaction with cytochrome P450s. A recent study has employed time-resolved Förster resonance energy transfer (FRET) measurements to study the time-dependence and magnitude of conformational changes associated with hydride and electron transfer in human CPR. These experiments revealed that the switch from closed to open conformation is driven by the change in flavin redox state. Nevertheless, the precise mechanism for this domain motion remains unknown. Here we present a molecular dynamics study into the mechanism of conformational change in CPR. We have identified the "drivers" for these large-scale motions and resolved uncertainties in the mechanism, such as which specific intermediate in the electron transfer chain undergoes conformational change.

L4

EPSRC UK National Service for Computational Chemistry Software

Ling Ge

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The EPSRC UK National Service for Computational Chemistry Software (NSCCS) at Imperial College London provides UK academics with free access to computing resources, software, specialist consultation and software training.

The NSCCS high performance computer is based and managed by our partner at the Rutherford Appleton Laboratory (RAL) of the Science and Technology Facilities Council (STFC).

The supercomputer hosts a wide range of up-to-date modelling software packages such as Gaussian, CP2K, ADF, Amber and Jaguar.

Training is an important part of the service. We organise computational workshops catered for users with different levels of modelling experience ranging from experimentalists to advanced theoreticians. We also provide one-to-one training and group training sessions on our software packages.

In addition to these, Specialist consultation and support are available where users can receive advice on how to tackle specific scientific problems and appropriate software to use.

Predictions of Intrinsic Aqueous Solubility of Crystalline Drug-like Molecules

James L. McDonagh[1], David S. Palmer[2], Tanja van Mourik[1], John B. O. Mitchell[1] Maxim V. Fedorov[2]

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Accurate predictions of solubility could save time and money in the drug development process by providing early stage viability screening of drug candidates. Whilst noting the success of QSAR models in this area, such models can lack physical insight. As such, a purely theoretical method, capable of achieving similar levels of accuracy at an appropriate computational cost, would be a powerful research and development tool. We have recently shown that it is possible to estimate with reasonable accuracy the solubility of drug-like molecules, from a set of 25 diverse drug-like compounds using a thermodynamic cycle.[1]
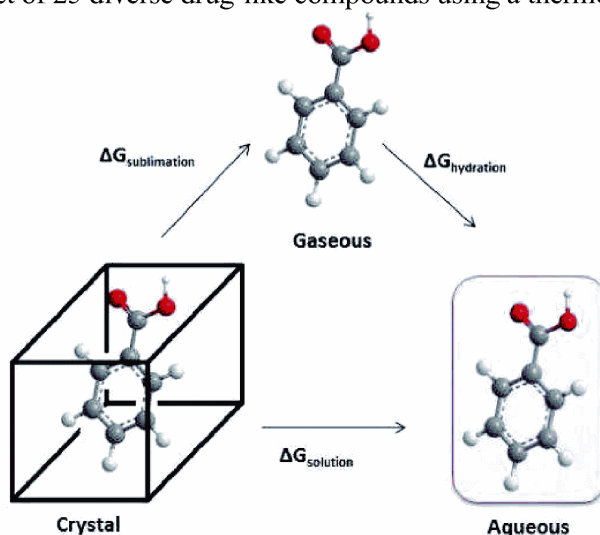
We predicted the free energy of sublimation, via lattice simulation in DMACRYS and the free energy of hydration, via the 3D reference interaction site model with the universal correction[2] (3D-RISM-KH-UC). The method produces a correlation coefficient R=0.85 and RMSE=1.45 $\log_{10}S$ units when compared to experiment. These results show a significant improvement compared to the use of continuum solvent methods, in a corresponding model, for solution free energy prediction. The method is not directly parameterised against experimental solubility data and allows for a full charaterisation of the thermodynamics of solvation of crystalline organic molecules.

Following from this work, we have created a hybrid QSAR methodology that uses traditional descriptors and energies, calculated by computational chemistry methods, in order to make a prediction of solubility. We are also currently exploring more accurate methodologies for sublimation free energy prediction.

[1]   Palmer, D.S., McDonagh, J.L., Mitchell, J.B.O., van Mourik, T., Fedorov M.V., Journal of Chemical Theory and Computation, 8, 3322, (2012).
[2]   Palmer, D.S., Frolov, A.I., Ratkova, E.L., Fedorov M. V., Journal of Physics: Condensed Matter, 22, 492101, (2010).

L6

Role of Lewis Acids in the Tungsten-Imido-Catalysed Dimerisation of alpha-Olefins

Sven Tobisch

Abstract: The complete catalytic cycle for dimerisation of ethylene chosen as a prototypical alpha-olefin by a tungsten-imido compound has been explored computationally. This study was conducted by using a reliable DFT method for the experimentally employed catalyst compound and the Lewis acid cocatalyst, as well as by taking bulk solvent effects into explicit consideration. The aptitude for Lewis adduct formation in catalytically relevant tungsten-imido species has been scrutinised. Specific catalyst-cocatalyst interactions through Lewis acid association at the W=NR functionality are identified, with four-membered chelates identified as being most favourable. The chelate formation is seen to have a pronounced influence on the catalytic ability of tungsten-imido compounds. The identified specific catalyst-cocatalyst associations are the key for the understanding of the observed dimerisation activity, thereby demonstrating what crucial role the Lewis acid is playing in achieving an efficient catalysis.

L7

Simulation of complex molecules at liquid interfaces

David Cheung

The behaviour of complex molecules, such as nanoparticles, polymers, and proteins at liquid interfaces is of increasing importance in a number of areas of science and technology. It has long been recognised that solid particles adhere to liquid interfaces, which provides a convenient method for the preparation of nanoparticle structures or to modify interfacial properties. The adhesion of proteins at liquid interfaces is important in many biological processes and in a number of materials applications of biomolecules. As the reduced dimensions of these particles makes experimental investigation challenging, molecular simulations provide a natural means for the study of these systems.

In this talk I will describe some of my recent research on the study nanoparticles [1,2], proteins [3], and polymers [4] at liquid interfaces using molecular simulation. In particular I will discuss the role of microscopic effects such as capillary waves in the effective interaction between a nanoparticle and a fluid interface, how the stablity of nanoparticles and proteins at liquid interfaces depends on their surface structure and conformation and stability of functionalised dendrimers at liquid interfaces.

[1] DL Cheung and SAF Bon, Phys. Rev. Lett., 102, 066103 (2009)
[1] DL Cheung and SAF Bon, Soft Matter, 5, 3969 (2009)
[3] DL Cheung, Langmuir, 28, 8730 (2012)
[4] DL Cheung and P Carbone, Soft Matter, in press

Computational Studies of Catalytic Hydrodefluorination at Ru(II) N-Heterocyclic Carbene Complexes

David McKay,[1] Stuart A. Macgregor,[1] Julien A. Panetier[1] and Michael K. Whittlesey[2]

[1] Institute of Chemical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK
[2] Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, UK

Ru(II) N-heterocyclic carbene complexes of the type $[Ru(NHC)(PPh_3)_2(CO)(H)_2]$ (NHC = IMes, SIMes, IPr, SIPr) catalyse the hydrodefluorination (HDF) of C_6F_5H with an unusual *ortho*-selectivity to give $1,2,3,4$-$C_6F_4H_2$.[1] Density functional theory (DFT) was used to locate two mechanisms based on a novel nucleophilic attack of a hydride ligand at the fluoroarene substrate (Scheme 1). Pathway I sees a concerted Ru–H/C–F exchange process while Pathway II features a stepwise process in which the rate-determining transition state (TS) involves formation of HF and a Ru-σ-fluoroaryl complex. Pathway II accounts for the unusual ortho-selectivity of this HDF process in the full experimental system (NHC = IMes).[2]

Scheme 1

Scheme 2
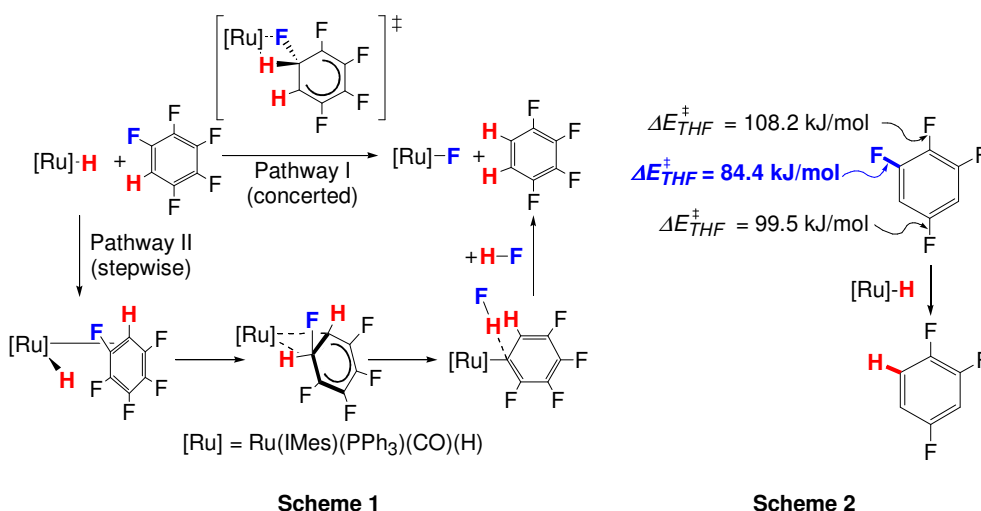
Here we report further DFT calculations on the extension of this HDF reaction to lower fluorinated $C_6F_{6-n}H_n$ (n = 2-5) species and the selectivity of such processes. Computed C–F bond dissociation energies (BDEs) for $C_6F_{6-n}H_n$ substrates are weakest for small n and particularly so when *ortho*-F substituents are present. Formulae are parameterised from multiple regression analysis of computed relative BDEs, providing a tool to guide experimental co-workers.[3] For Pathway II the presence of bulky N-aryl NHC ligand directs reactivity to sites with only one ortho-F substituent. In contrast, the TS in Pathway I experiences a constant steric effect and is therefore correlated with the C–F BDE. Pathways I and II thus have complementary selectivities and present the possibility of exerting control over regioselectivity as a function of the choice of auxiliary ligand. Calculations predict $1,2,3,5$-$C_6F_4H_2$ (Scheme 2) and $1,2,3,4$-$C_6F_4H_2$ are viable candidates for selective HDF at $[Ru(IMes)(PPh_3)_2(CO)(H)_2]$ giving $1,2,4$-$C_6F_3H_3$ and $1,2,3$-$C_6F_3H_3$ respectively.[3]

[1] S. P. Reade, M. F. Mahon and M. K. Whittlesey, *J. Am. Chem. Soc.*, 2009, **131**, 1847–1861.
[2] J. A. Panetier, S. A. Macgregor and M. K. Whittlesey, *Angew. Chem. Int. Ed.*, 2011, **50**, 2783–2786.
[3] S. A. Macgregor, D. McKay, J. A. Panetier and M. K. Whittlesey, *Dalton Trans.*, 2013, 7386–7395.

L9

Proton coupled electron transfer in water photo-oxidation at TiO$_2$water interface

Jun Cheng

Four-electron transfer reactions in water photo-oxidation on TiO2 have been studied using a newly developed method. This method combines ab intio molecular dynamics simulations and free energy perturbation theory to compute thermochemistry of proton coupled electron transfer (PCET).[1] Decomposition of dehydrogenation into deprotonation and oxidation allows us to scrutinize the PCET steps at the interface and better understand the activity/inactivity of catalysts. On the other hand, such a separation is crucial to understand the error in the calculations using standard GGA density functionals.[2] The inaccuracy in GGAs, namely delocalization error, has profound consequence in calculation of defects in semiconductors, and has been widely studied and relatively well understood in solid state community.[3] In this respect, there is a close parallel between semiconductor photoelectrocatalysis and defect physics.[4] Inclusion of a fraction of exact exchange in density functionals can alleviate this error, giving rise to correct localization of electronic holes on reaction intermediates at the interface. On the basis of understanding of delocalization error, we will present the energetics of reaction intermediates calculated by using a screened hybrid functional (HSE06[5]), and also some discussions on reaction mechanism and activity of materials.

References

1. J. Cheng, M. Sprik, Phys. Chem. Chem. Phys. 2012, 14, 11245.
2. J. Cheng, M. Sulpizi, J. VandeVondele, M. Sprik, ChemCatChem, 2012, 4, 636.
3. C. G. Van de Walle, A. Janotti, Phys. Status Solidi B 2011, 248, 19.
4. C. Adriaanse, J. Cheng, M. Sulpizi, J. VandeVondele, M. Sprik, J. Phys. Chem. Lett. 2012, 3, 3411.
5. A. V. Krukau, O. A. Vydrov, A. F. Izmaylov, G. E. Scuseria, J. Chem. Phys. 2006, 125, 224106.

ScotCHEM Posters

P1. **Investigation of Non-Additivity in Protein-Ligand Binding**, <u>Gaetano Calabro</u>, Julien Michel.

P2. *Withdrawn*.

P3. **Excited potential curves and vertical excitations using state-averaged Monte Carlo configuration interaction**, <u>J. P. Coe</u> and M. J. Paterson.

P4. **New DFT Insights Into Methyl Propanoate Formation at a Palladium Catalyst**, <u>Luke Crawford</u> & Michael Bühl.

P5. **Modelling Isotope Effects on Nuclear Shielding in Rh(III) and Pt(IV) Complexes**, <u>John Davis</u>, Klaus R. Koch & Michael Bühl.

P6. **Predicting NMR Parameters from the Structures of Aluminophosphates**, <u>Daniel M. Dawson</u> & Sharon E. Ashbrook.

P7. *Withdrawn.*

P8. *Withdrawn.*

P9. **A theoretical investigation of azophenine: A remarkable molecular switch for nano-electronics**, Tanja van Mourik, <u>Herbert Früchtl</u>, Simon Hogan, Grant Simpson and Renald Schaub.

P10. **Rational design of isoform specific ligands**, <u>Charis Georgiou</u>, Malcolm Walkinshaw & Julien Michel.

P11. **Hydration thermodynamics: from small molecules to proteins**, <u>Georgios Gerogiokas</u>, Richard Henchman, Michelle Southey, Richard Law & Julien Michel.

P12. **Theoretical Insights into the Nature of Halogen Bonding**, <u>J. Grant Hill</u> & Xiaojun Hu.

P13. **On the mechanism of CO_2 absorption in 1,3-dialkylimidazolium acetate ionic liquids**, <u>Oldamur Holloczki</u> & Barbara Kirchner.

P14. **Advances in The Theoretical Determination of Molecular Structure with Application to Photoelectron Spectroscopy**, <u>Zibo Keolopile.</u>

P15. **Exotic states of molecules**, <u>Adam Kirrander</u>.

P16. **Gas-phase structures of carboranes**, <u>Paul D. Lane</u>, Drahomír Hnyk & Derek A. Wann.

P17. **Haem Ring Conformation as a Mediator of Biological Function - Modelling of Redox Control in the B. viridis Reaction Center Cytochrome**, <u>Stuart A. MacGowan</u> & Mathias O. Senge

P18. **Understanding selectivity in the extraction of chloridometallates by computational methods**, <u>Kirstian J MacRuary</u>, Richard A Grant, Ross J Gordon, Carole Morrison, Jason B Love & Peter A Tasker.

P19. **A conformational conundrum**, Christopher O. Burn & <u>Sarah L. Masters</u>.

P20. **Predicting the protein targets for athletic performance-enhancing substances**, <u>Lazaros Mavridis</u> & John BO Mitchell

P21. **Computing Intrinsic Aqueous Solubility of Crystalline Drug-like Molecules**, James L. McDonagh, David S. Palmer, Tanja van Mourik, John B. O. Mitchell & Maxim V. Fedorov.

P22. **Uniting Cheminformatics and Chemical Theory to Predict the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules**, James L. McDonagh, Neetika Nath, Luna De Ferrari, Tanja van Mourik & John B. O. Mitchell.

P23. **DFT Computation of ^{103}Rh NMR Chemical Shifts of Cationic Rhodium-Bis(Phosphine) Complexes**, Manuel Ortuno, Ludovic Castro & Michael Bühl.

P24. **Computational Chemistry for Time-Resolved Gas Electron Diffraction**, Matthew S. Robinson, Lennart Ramakers, Paul D. Lane & Derek A. Wann.

P25. **Docking and Dynamics of Native and Non-Native Substrates of the Non-Heme Fe (II) Halogenase SyrB2**, Graham Rugg & Hans-Martin Senn.

P26. **Combined Solid-State NMR and DFT Study of Hydrated AlPO-34**, V. R. Seymour, E. C. Pearson, R. E. Morris & S. E. Ashbrook.

P27. **Liquid Methanol from DFT and DFT/MM Molecular Dynamics Simulations**, Sieffert, N.; Bühl, M.; Gaigeot M.-P. & Morrison C. A.

P28. **Exploiting the ^{31}P Chemical Shift Anisotropy of Aluminophosphates**, Scott Sneddon, Daniel M. Dawson & Sharon E. Ashbrook

P29. **Isotherms of Fluids in Native and Defective Zeolite and Alumino-Phosphate Crystals: Monte-Carlo Simulations with 'On-the-Fly' Ab Initio Electrostatic Potential**, Xavier Rozanska, Gregor N. Stipicic, Barbara Holtz, Marianna Yiannourakou, Benoit Leblanc & Philippe Ungerer.

P30. **HECToR: The UK National Supercomputing Service**, Andy Turner.

P31. **Bridging structures and isomerism in silicon-silicon and silicon-germanium hydrides**, Tanja van Mourik, William Kew, Lukasz Serafin & Mark Law.

P32. **Design, synthesis and testing of ligands for high-value mineral collection**, C.N. Waterson, C.A. Morrison & P.A. Tasker.

P33. **Combining calculations and gas electron diffraction; structural determination of weakly associated species**, Stuart Young, Matthew Robinson, Paul Lane & Derek Wann.

P34. **Molecular Dynamics Simulations for Peptide Self-Assembly**, Pim W.J.M. Frederix, Rein V. Ulijn, Neil T. Hunt & Tell Tuttle.

P35. **Stabilization of metastable hydrogen trioxides (HOOOH and HOOO•) by complexation with sulfuric acid,** Daniel Cannon, Tell Tuttle, Joze Koller & Bozo Plesnicar.

P36. **Calculations of One-Electron Redox Potentials of Oxoiron(IV) Porphyrin π-Cation Radical Complexes,** Ludovic Castro & Michael Bühl.

P37. **Conformational analysis study of Ac-gly-NHMe, CF$_3$-C(O)-gly-NHMe and Ac-gly-NH(Me)$_2$ through theoretical calculations and NMR spectroscopy,** Rodrigo A. Cormanich, Luke Crawford, Michael Bühl, Claudio F. Tormena & Roberto Rittner

P38. **Theoretical and Experimental Study of the Amide I Vibrational Mode as a Structural Diagnostic Method for Short Peptides Bound to Aromatic Groups**, Ivan Ramos Sasselli, Scott Fleming, Pim W. J. M. Frederix, Rein V. Ulijn, Tell Tuttle & Neil T. Hunt

P39. **Challenges for wavefunction and density functional response methods in benchmarking the electronic excited states of 1st row transition metal complexes**, <u>Nuno M.S. Almeida</u>, Russell McKinlay & Martin J. Paterson.

P40. **Superelectrophilic Amidine Dications: A synthetic and computational investigation**, <u>Greg Anderson</u>, Tell Tuttle & John Murphy.

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