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flStephenson Institute for Renewable Energy (SIRE)

is leading edge fundamental energy technology research. As a specialist energy technologies research institute, SIRE focuses on the physics and chemistry that will transform the future of energy generation and storage. We are bridging the gap between fundamental science and applied engineering by combining both academically, as well as industrially relevant questions. Prof Hardwick's research focus on 1) understand the chemistry of energy materials; 2) Establishment of surface sensitive spectroscopic techniques to probe interfaces; 3) Development of advanced materials for lithium & sodium batteries and supercapacitors. Selected publications: 1) Template-free Synthesis of Nitrogen doped Carbon Materials from an Organic Ionic Dye (Murexide) For Supercapacitor Application, Serwar M. et al **RSC Adv.** 2017, 7, 54626; 2) Batteries: Avoiding oxygen, Hardwick L. **Nature Commn.** 2016, 1, 16115; 3) Solvent-Mediated Control of the Electrochemical Discharge Products of Non-Aqueous Sodium-Oxygen Electrochemistry, Aldous I. et al **Angew. Chem. Int Ed.** 2016, 55, 8254; 4) Mechanistic Insight into the Superoxide Induced Ring Opening in Propylene Carbonate Based Electrolytes using In Situ Surface-Enhanced Infrared Spectroscopy Padmanabhan V. et al **JACS**, 2016, 138, 3745; 5) A Highly Active Nickel Electrocatalyst shows Excellent Selectivity for CO<sub>2</sub> Reduction in Acidic Media Gaia N. et al **Chem. Sci.** 2016, 7, 1521.

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Prof O'Neil's research interests include synthetic methodology including catalytic oxidation processes, fluorine substitution in bioorganic chemistry, drug metabolism and the medicinal chemistry of antimalarial and antimycobacterial drugs and novel drugs for the treatment of filariasis, pancreatitis and neuropathic pain. His group also has been involved in a project focused on the rationale redesign of resistance breaking vector control agents. He have published over 150 papers and reviews and fifteen patents. His research has led to a drug candidate (Isoquine) entering clinical trials in 2008 and they also have recently candidate selected three additional antimalarials (RKA 182, FAQ4, E209) for full preclinical testing on route to Phase 1 clinical trials in humans. More recently, they have also candidate selected a new potential drug, AWZ1066, for the treatment of the filarial diseases lymphatic filariasis (elephnatisais) and ochocerciasis (River blindness). They have also initiated research into superoxide dismutase (SOD-1) that are relevant to its involvement in motor neuron disease with Hasnain and Antonyuk. He currently run the Medicinal Chemistry Group at Liverpool which is one of Europe's leading academic groups focused on early stage drug discovery. Through the establishment of public private partnerships with major pharma and organisations such as the Medicines for Malaria Venture (MMV) and TB Alliance many of our early stage projects have been developed to the point of candidate selection and clinical trials in humans. His group works on a wide range of therapeutic areas focussed on antimalarial, antibacterial (Anti-Wolbachia), anti-tuberculous agents with more recent studies focused in the pain, pancreatitis and anti-fungal areas. There are four main research themes that include: (1) Drug Design of New Antimicrobial Agents; (2) Molecular Modelling and Cheminformatics; (3) Safe-Drug Design; (4) Semi-synthetic Natural Product Drug Design.<sup>1</sup> M. J. Capper, Gareth. S.A. Wright et al., The cysteine-reactive small molecule ebselen facilitates effective SOD1 maturation, *Nature Communications*, **2018**, 9, 1693 2 Johnston, K. L.; Cook, D. A. N.; Berry, N. G.; Hong, W. D.; Clare, R. H.; Goddard, M.; Ford, L.; Nixon, G. L.; O'Neill, P. M.; Ward, S. A.; Taylor, M. J., Identification and prioritization of novel anti-Wolbachia chemotypes from screening a 10,000-compound diversity library. *Science Advances* **2017**, 3 (9). 3 O'Neill, P. M.; Amewu, R. K. et al., A tetraoxane-based antimalarial drug candidate that overcomes PfK13-C580Y dependent artemisinin resistance. *Nature Communications*, **2017**, 8, 15159 4 Hong, W. D.; Gibbons, P. D. et al., Rational Design, Synthesis, and Biological Evaluation of Heterocyclic Quinolones Targeting the Respiratory Chain of Mycobacterium tuberculosis. *Journal of Medicinal Chemistry*, **2017**, 60, 3703-3726. 5 Ismail, H.M.; Barton, V.E.; Panchana, M.; Charoensutthivarakul, S. et al., A Click Chemistry-Based Proteomic Approach Reveals that 1,2,4-Trioxolane and Artemisinin Antimalarials Share a Common Protein Alkylation Profile, *Angewandte Chemie-International Edition* **2016**, 55, 6401-6405 6 Ismail, H. M.; Barton, V.; Phanchana, M.; Charoensutthivarakul, S.; Wong, M. H. L. et al., Artemisinin activity-based probes identify multiple molecular targets within the asexual stage of the malaria parasites Plasmodium falciparum 3D7. *Proc. Natl. Acad. Sci. U. S. A.*, **2016**, 113, 2080-2085 7 Wong, M.N.L.; Bryan, H.K.; Copple, I.M.; Jenkins, R.E. et al., Design and Synthesis of Irreversible Analogues of Bardoxolone Methyl for the Identification of Pharmacologically Relevant Targets and Interaction Sites, *J. Med. Chem.* **2016**, 59, 2396-2409

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(ribonucleic acid), represent one of the greatest ever triumphs for chemistry and biology. It is not surprising that most of the licensed antiviral drugs (e.g. Zovirax and AZT) and many anticancer drugs are nucleoside analogues which are able to interfere with nucleic acid biosynthesis in a selective manner. Additionally, much of the recent information on the structure/function relationship of nucleic acids has come from using DNA/RNA probes that contain a subtle chemical modification. Present work within the group is concerned with studies on the synthesis of novel nucleic acids analogues as both potential therapeutic agents and as probes for understanding the precise mechanism by which nucleic acids fulfill their biological functions

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Prof. Dmitry Shchukin, works on controlled delivery of active agents

and energy (electric, bio, thermal) by Layer-by-Layer planar and encapsulation approaches (>250 publications, H-factor 60, >10000 citations). He has been awarded by ERC Consolidator grant (2015), ERC Proof-of-concept grant (2017), and RSC Brian Mercer (UK) awards, Nanofutur and ForMat (Germany) prizes.

Research activities include the study of the non-equilibrated interfaces, development of composite hollow nanocontainers with controlled shell permeability for encapsulation of the energy-enriched materials, phase change materials, drugs, corrosion inhibitors; development of nanocontainer-based feedback active surfaces for further application in active self-healing materials, catalysis, biochemistry and medicine; synthesis of nanomaterials with new properties in the ultrasonic cavitation zone, synthesis of amorphous nanocomposites with enhanced catalytic performance in non-equilibrated conditions at the cavitation interface; ultrasonic surface modification of metals for catalytic and biomedical (implants) applications.

Applications from students with the background in materials chemistry, polymer chemistry, ultrasound, physical chemistry, self-healing materials, energy harvesting, storage and controlled delivery and other related fields.

Potential research topics are 1 new nanomaterials for energy applications; 2 self-healing materials (also including materials for wood and historical heritage preservation); 3 antifouling coatings; 4 application of ultrasound in photocatalysis and photovoltaics

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Christophe Aïssa obtained his PhD under the

supervision of Professor Malacria (University Paris 6, France) in 2001, focussing on the study of the factors influencing the outcome of transannular radical cyclisations cascades directed toward the synthesis of natural sesquiterpenes. He then joined Professor Fürstner group (MPI for coal research, Mülheim/Ruhr, Germany) as postdoctoral research assistant, working on the total synthesis of biologically active marine secondary metabolites. In 2003, he was appointed senior scientist within the same group, working further on total syntheses, but also on transition-metal catalysed reactions. In July 2007, he was appointed Lecturer at The University of Liverpool with a RCUK fellowship.

His group works on organic synthesis through transition-metal-catalysed activation of otherwise inert bonds, in particular C–H and C–C bonds, with the long-term aim to develop sustainable synthetic chemistry. Here is a selection of papers that illustrate their work : Barday, M.; Janot, C.; Halcovitch, N. R.; Muir, J.; Aïssa, C. Cross-Coupling of  $\alpha$ -Carbonyl Sulfoxonium Ylides with C–H Bonds. *Angew. Chem. Int. Ed.* 2017, 56, 13117–13121. 2) Yip, S. Y. Y.; Aïssa, C. Isomerization of Olefins Triggered by Rhodium-Catalyzed C–H Bond Activation: Control of Endocyclic  $\beta$ -Hydrogen Elimination. *Angew. Chem. Int. Ed.* 2015, 54, 6870–6873. 3) Aïssa, C.; Ho, K. Y. T.; Tetlow, D. J.; Pin-No, M. Diastereoselective Carbocyclization of 1,6-Heptadienes Triggered by Rhodium-Catalyzed Activation of an Olefinic C–H Bond. *Angew. Chem. Int. Ed.* 2014, 53, 4209–4212. 4) Ho, K. Y. T. H.; Aïssa, C. Regioselective Cycloaddition of 3-Azetidinones and 3-Oxetanones with Alkynes through Nickel-Catalysed Carbon-Carbon Bond Activation. *Chem. Eur. J.* 2012, 18, 3486–3489. 5) Crépin, D.; Dawick, J.; Aïssa, C. Combined Rhodium-Catalyzed Carbon-Hydrogen Activation and  $\beta$ -Carbon Elimination to access Eight-Membered Rings. *Angew. Chem. Int. Ed.* 2010, 49, 620–623.

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Porous materials are permeable, high

surface area materials with applications in gas storage, catalysis, and filtration. There has been considerable interest in porous materials over the last ten years, and metal-organic frameworks and porous polymers with incredible properties have been reported. However, many of these new materials are limited in application due to the high cost of production. We are developing new porous materials from inorganic waste and other low cost or renewable resources. The target is to produce materials with superior properties, but at a cost that makes them useful for widespread practical applications, especially filtration of toxic pollutants from water and air flows. A good example is sulphur-polymers. Sulfur is an industrial by-product of oil refining. We recently showed that when polymers made from elemental sulfur are made porous, they can be used to filter mercury from

water.

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Dr Alex Cowan (AC) is a Reader in Chemistry and EPSRC Research Fellow (2013-21) in the Department of Chemistry and the Stephenson Institute for Renewable Energy at the University of Liverpool (UoL). Prior to this role AC held the independent positions of Senior Lecturer (2015-2017) and Lecturer (2012-2015) at UoL and Lecturer in Renewable Fuel Synthesis at Imperial College London (2011-12). AC is a former associate edit

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