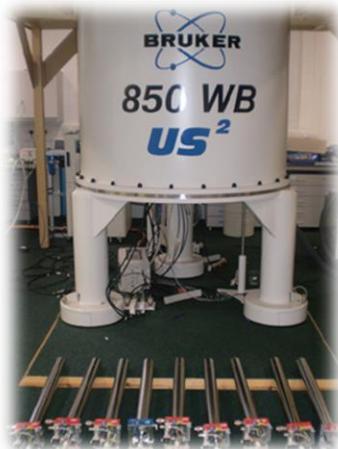




## 11<sup>th</sup> Annual NMR Discussion Group Postgraduate Meeting

The Royal Society of Chemistry NMR Discussion Group held its 11<sup>th</sup> annual Postgraduate Meeting on 21<sup>st</sup> June 2018, at the Department of Physics, University of Warwick. With a strong legacy of NMR-based research in conjunction with ongoing high levels of investment in NMR, the University of Warwick provided an excellent venue. Again, this event was extremely popular and enjoyable, with the modern on-campus facilities providing the perfect informal setting for early career researchers to showcase their work, either by oral or poster presentations. A representative cross section of academic UK NMR research-based groups attended the meeting, with presentations covering a wide range of related disciplines, including small molecule characterisation, molecular biology, solid-state characterisation, materials science and imaging. Poster sessions were vibrant allowing open and informal discussion between all meeting participants, including established researchers. The programme incorporated eight oral presentations from early career researchers, again in a relaxed environment, covering a range of subjects:



**Sarah Mann**, *Department of Physics, University of Warwick*

**Probing structure and dynamics in ionic liquid pharmaceuticals by NMR Spectroscopy**

**Thomas Deo**, *School of Physics and Astronomy,  
University of Nottingham*

**Structural studies of amyloid-beta interacting with  
cell membranes using magic angle spinning DNP**



**Andrew Hall**, *Centre for Sustainable  
Chemical Technologies, University of Bath*

**Insights into homogenous catalysis using  
multi-nuclear high resolution FlowNMR  
spectroscopy**

**Abby Haworth**, *Department of Chemistry, University of  
Durham*

**Probing ion mobility in Li-stuffed garnets using multi-  
nuclear solid-state NMR**



**Ashlea Hughes**, *School of Chemistry, University of  
Liverpool*

**Ultra-fast molecular rotors within porous organic  
cages**

**Ariana Jones, Department of Chemistry,  
University of Edinburgh**

**Developments in reaction monitoring by NMR**



**Suzi Pugh, Department of  
Chemistry, University of St  
Andrews**

**Solid-state NMR study of  
flexibility in zeolite frameworks**

**Nikita Harvey, MRC-NIHR National  
Phenome Centre, Imperial College, London**

**Diffusion-ordered NMR spectroscopy  
method optimisation for metabolic profiling  
of human biofluids**



In each case, the presentations represented cutting-edge research and were very well-received by meeting participants. The quality of the oral and poster presentations was such that judging was an impossible task and, in addition to winners, a series of runner-up prizes were awarded. The judging panel comprised **Prof Simon Duckett** (University of York, NMR DG Chairperson), **Dr Stephen Byard** (Arcinova) and **Dr Matthew Wallace** (University of East Anglia). Both prize winners will be invited to give presentations at the **2018 NMR DG Christmas meeting, which will be held at The Institute of Structural and Molecular Biology, University College London, on Thursday 13<sup>th</sup> December.**



A prize was awarded to **Sarah Mann** (University of Warwick) for the best oral presentation, and this was presented by **Prof Simon Duckett**, the Chairperson of the NMR DG (shown left). The prize was sponsored by the Royal Society of Chemistry Journal, Physical Chemistry Chemical physics (PCCP). Two runner-up prizes for the best oral

presentation were awarded to Ashlea Hughes (University of Liverpool) and Abby Haworth (University of Durham).

**Emily Corlett** (Department of Physics, University of Warwick) was awarded a prize for the best poster presentation, and this was presented by **Dr Mark Dunham**, of Jeol UK, who sponsored the event. Emily's research involved the evaluation of a NMR crystallography-based approach for the characterisation of Lutidine Fumarate compounds.



A runner-up prize for best poster presentation was awarded to **Callum Wallace (University of Lancaster)** for his work on determination of half-lives and exposure time to attain photostationary states for novel materials capable of storing solar energy.

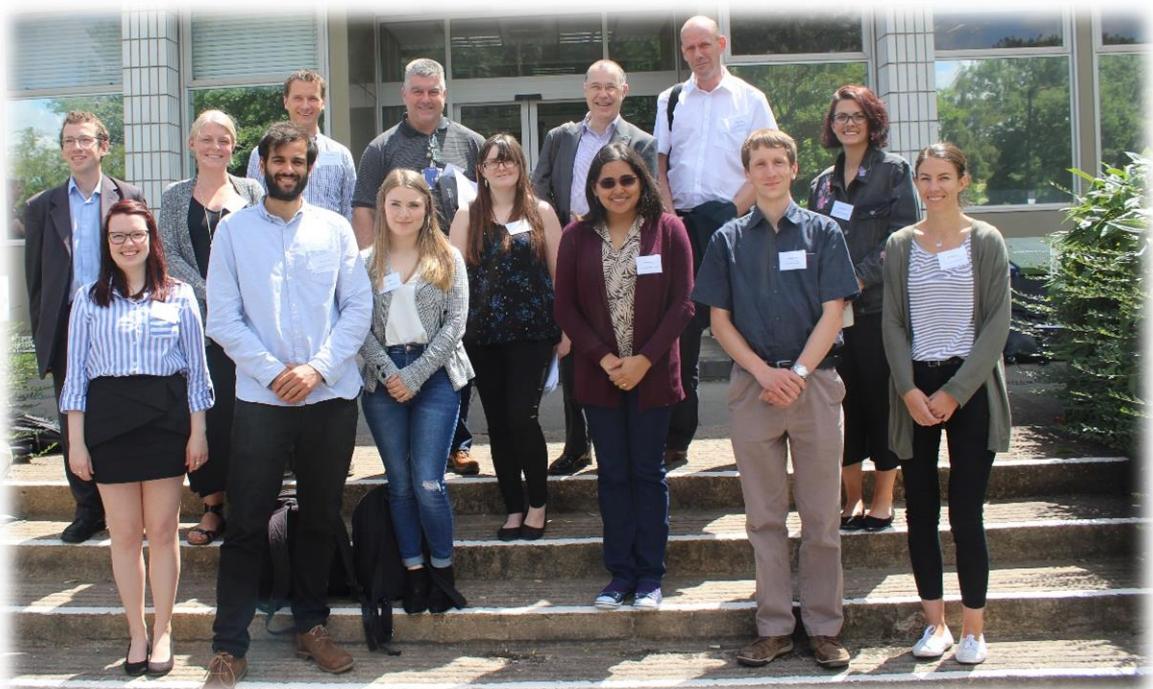


solid-state NMR techniques and instrumentation have evolved. As a University Vice Chancellor, Mark was able to conclude his presentation with some reflections on his own career, combining scientific and non-scientific roles in academia.

In recent meetings, ‘overview presentations’ given by established researchers have been introduced into the programme. On this occasion, **Prof Mark Smith** (Vice Chancellor, University of Lancaster) opened the meeting with a presentation titled ‘Some recent observations of low-gamma quadrupolar nuclei with solid-state NMR and thoughts on career paths for NMR spectroscopists’. Mark gave a presentation outlining some of his early scientific contributions but, importantly, he presented some of his more recently acquired data indicating how

**Ann Dixon** (University of Warwick) opened the afternoon session with an overview presentation titled ‘Application of NMR to Characterisation of Membrane Proteins: Highlights and Challenges’. In particular, Ann gave an insight into the complexities associated with analysis of proteins associated with virally-induced cancers. The value of NMR in conjunction with computational techniques in molecular biology is evident, to permit the elucidation of membrane protein mediated mechanisms of cellular transformation in diseased states. Again, Ann was able to provide an interesting overview of her career, and some of the rewards of working with NMR in this discipline.





*Some organisers, speakers and session chairs - From left to right: Matthew Wallace (University of East Anglia), Abby Haworth (University of Durham), Ann Dixon (University of Warwick), Thomas Deo (University of Nottingham), Suzi Pugh (University of St Andrews), John Hanna (University of Warwick), Ashlea Hughes (University of Liverpool), Mark Smith (University of Lancaster), Nikita Harvey (Imperial College, London), Simon Duckett (NMR DG Chairperson), Andrew Hall (University of Bath), Ariana Jones (University of Edinburgh) and Sarah Mann (University of Warwick).*



*2018 NMR Discussion Group Postgraduate Meeting participants*

In particular, the NMR DG would like to acknowledge **Steven Brown** (University of Warwick), **Dinu Iuga** (University of Warwick) and **Matthew Wallace** (University of East

Anglia) for their contributions towards the organisation of the meeting, and also Jeol UK for generous sponsorship and attendance at the meeting.

**Steve Byard – NMR DG Secretary, July 2018**