

## News from the UK cwEPR National Service at Manchester

- *cw EPR Service renewed (2006-2010), W-band operational*
- *Funding for the EPSRC cwEPR National Service has been renewed from March 2006 until February 2010.*

Applications can be made to the Service by any academics eligible for EPSRC funding. The Service is free at the point of use and access is guaranteed to EPSRC grant-holders. All other applicants must supply a justification for use of the Service (no more than half a page), which will be reviewed by two members of the MAP under the direction of the Chair of MAP (Professor C.D. Garner, FRS). Any applications that are not awarded Service time will receive feedback from the MAP. Users should discuss their requirements with Service personnel before making an application. Full training on the spectrometers is available to all users.

The cw W-band spectrometer is now fully operational (5 – 300 K), and is highly sensitive, requiring tiny samples, and is already proving valuable for problems involving: (i) resolution of weakly anisotropic g-values, (ii) measurement of large zero-field splittings, (iii) detection of integer spin systems, (iv) suppression of second order effects, (v) detection of EPR signals when sample size is limited.

### Facilities available at the EPR Centre:

Bruker ESP 300E, EMX-hybrid, Elexsys E600 EPR spectrometers

L-band 1 GHz S-band 4 GHz X-band 9 GHz (|| and  $\perp$  mode)

K-band 24 GHz Q-band 34 GHz W-band 94 GHz

Magnetic fields up to 2 Tesla (up to 6 T at W-band)

Temperature range 4-300 K (up to 600 K at X-band)

Simulation software for  $S = \frac{1}{2}$  and  $S > \frac{1}{2}$  systems

*In situ* electrochemical EPR spectroscopy

*In situ* optical excitation

Information about application procedures, forms, membership of the Management Advisory Panel (MAP) and their terms of reference and Service Benchmarks are on the new Service website at [www.epr.chemistry.manchester.ac.uk](http://www.epr.chemistry.manchester.ac.uk).

The new Service grant will allow upgrades and extensions of the EPR equipment, and there will be further refurbishment of the Service Laboratories. The W-band spectrometer is housed in the newly refurbished Lewis Magnetism Laboratory, which was opened by the Lord Lewis of Newnham in Autumn 2005. Dr Joanna Wolowska has become Service Manager and Mr Dan Sells is a full time technician supporting the Service. Projects awarded time on the EPR Service can also have access to the National Service for Computational Chemistry Software (NSCCS), subject to agreement of the NSCCS Service.

Training and extending the user base are important elements of the Service and the centre encourages suppliers of samples to visit the laboratories in order to gain hands-on experience in EPR.

To discuss applications for time on the Service contact: [eric.mcinnnes@manchester.ac.uk](mailto:eric.mcinnnes@manchester.ac.uk), tel: 0161-275-4469, [david.collison@manchester.ac.uk](mailto:david.collison@manchester.ac.uk), tel: 0161-275-4660 or [Joanna.wolowska@manchester.ac.uk](mailto:Joanna.wolowska@manchester.ac.uk), tel: 0161-275-4580/2.

Contact Carmine Ruggiero at [carmine.ruggiero@epsr.ac.uk](mailto:carmine.ruggiero@epsr.ac.uk) for information about other EPSRC services.

**Membership** of the ESR Group currently stands at about 100. All scientists who are members of the Royal Society of Chemistry, and have an interest in ESR/EPR spectroscopy, are invited to join by ticking the ESR Group box on their RSC membership renewal forms. The cost is only £2 per annum! Membership carries entitlement to reduced registration fees at the ESR Group annual conference.

**Website:** <http://www.esr-group.org.uk> **Web Editor:** Dr John Maher

**Newsletter Editor:** Dr Shirley Fairhurst

# ELECTRON SPIN RESONANCE GROUP

## Newsletter June 2006

# RSC

ROYAL SOCIETY OF CHEMISTRY

The 39<sup>th</sup> Annual ESR Conference took place from Sunday 2nd – Wednesday 5th April 2006 at the University of Edinburgh and included a joint session with COST P15 action: ‘Advanced Paramagnetic Resonance Methods in Molecular Biophysics’ led by Sabine Van Doorslaer. This was a lively conference with over 100 delegates and an unprecedented number of talks and posters.

The 2006 Bruker Prize Lecture by Professor Yuri Tsvetkov of the Institute of Chemical Kinetics and Combustion, Novosibirsk was introduced by Michael Bowman (Pacific Northwest National Laboratory, USA) who recounted meeting Yuri for the first time and the early days of pulsed EPR. Professor Tsvetkov then presented his lecture on *Pulsed Dipolar ESR Spectroscopy and Its Applications*. We heard how early work on two pulse ESE spectroscopy led to the development of Pulse Double Electron Electron Resonance (PELDOR/ DEER) for distance measurements by EPR. This was followed by a wine reception sponsored by Bruker. Plenary lectures were presented by: Lesley Yellowlees (University of Edinburgh) who described the *EPR spectroelectrochemical study of reduced species*. Louis Claude Brunel (Florida State University) in his talk *Novel approach to EMR: Fundamentals and applications* told us about the efforts to develop CW and pulse instruments in the 200 GHz to 1 THz range at the National High Magnetic Field Laboratory. Daniella Goldfarb (Weizmann Institute of Science) described the *High field EPR/ENDOR studies of Mn (II) sites in protein single crystals*. Georg Gescheidt (University of Graz) described his *Time-resolved studies of radical reactions*



**Michael Bowman (PNL), Dieter Schmalbein (Bruker BioSpin), Yuri Tsvetkov (2006 Bruker Prize) and Shirley Fairhurst (ESR Group)**

using CW EPR and CIDNP. Chris Kay (University College London), newly moved from the Free University Berlin began the COST P15 session with his talk entitled ‘*From alcohol oxidation to liver regeneration: Applications of EPR to biology*’. Gunnar Jeschke (MPI for Polymer Research, Mainz) told us about the latest developments in *Pulsed ELDOR: measuring more than a single distance*.

As well as the Plenary lectures we had a series of excellent short talks, a poster session and a student talk session.

**Full abstracts of the Plenary lectures, short talks and posters are on the website** [www.esr-group.org.uk](http://www.esr-group.org.uk)

### Late News

**We are delighted to announce that Professor Daniella Goldfarb will present the 2007 Bruker Prize Lecture**

The JEOL prize Medal for the best oral presentation by a young scientist, was presented to Janet Banham (Oxford University) for her talk entitled: *Testing the limits of the DEER method for distance measurements in proteins*. Joint runners-up were Riccardo Garzelli (University of York) and Alexey Silakov (MPI Mülheim). All three student talks were of a very high calibre but sadly there was only one medal to be won. All three were presented with cheques by Peter Meadows (JEOL).



**JEOL Prize: Peter Meadows (JEOL) with Riccardo Garzelli, Janet Banham (Medal Winner) and Alexey Silakov**

Vasily Oganessian (UEA, Norwich) the winner of the IBDG Young Investigator Award 2006 presented a talk on *Advanced spectroscopic methods in bioinorganic chemistry: A theoretical insight* before being presented with a certificate and cheque by the Inorganic Biochemistry Discussion Group.

This year there were 70 posters and as usual one was selected to win the poster prize with the traditional bottle of whisky going to Stefan Stoll (ETH, Zurich) for his poster on *Simulating Pulse EPR Spectra*.

### **Professor Arthur Schweiger: 1946-2006**

We dedicated the first session on Tuesday to the life and scientific contributions of Arthur Schweiger (ETH, Zurich) who died suddenly in January. The scientific community has lost an outstanding researcher and a leading scientist in the field of advanced methodology and applications of EPR spectroscopy.

His friend and colleague Gunnar Jeschke gave a short appreciation of Arthur the man and scientist. This was followed by lectures by Daniella Goldfarb, Sabine Van Doorslaer (University of Antwerp) and Jeffrey Harmer (ETH, Zurich).

Although this was a very busy meeting we managed to find time for a whisky tasting, sponsored by JEOL, on the Sunday evening. After a short talk by Paul Murray on whisky production, we all enjoyed a 'wee dram'.



**Stefan Stoll, Marilena Di Valentin, Chris Kay, Riccardo Garzelli and Katherina Pirker watch the sun rise over Edinburgh**

The view of Arthur's Seat from the Conference Venue proved inviting, and many of the participants enjoyed the walk to the top, including some (above) who watched the sun rise over Edinburgh.



**Stefan Stoll receives his poster prize**

**THANKS** The organisation of our conference in Edinburgh have been due in large part to the efforts of Dr Victor Chechik who has served as both Secretary and Treasurer for the last year. At the AGM Victor relinquished the Secretary's role to Dr Chris Kay, but he continues as Treasurer. Thanks go to retiring committee members Drs Damien Murphy, Graham Smith and Fraser Macmillan who left the committee at the AGM.

Very special thanks go to Edinburgh local organisers Professor Lesley Yellowlees and Dr Paul Murray.

### **CONGRATULATIONS**

**Professor Brian Hoffman** (Northwestern University) on being elected to the US National Academy of Science. Election to the Academy is considered one of the highest honours that can be accorded a U.S. scientist or engineer.

### **IES AWARDS 2006**

**Silver Medal for Chemistry: Professor Kálmán Hideg, (Pécs University, Hungary)**

**Silver Medal for Biology and Medicine:** jointly awarded to **Professor Periannan Kuppusamy and Professor Jay Zweier (Ohio State University, USA)**

**IES Fellow: Professor John Pilbrow (Monash University, Australia)**

Further information in the International EPR Society (IES), including how to make Award nominations, can be found on their website: [www.IEPRS.org](http://www.IEPRS.org). Each year one issue of the Society's Newsletter is a public issue which can be downloaded free from: <http://www.epr-newsletter.ethz.ch/>

### **FORTHCOMING EVENTS**

**16-21 July 2006:** EUROMAR York <http://www.euromar.org/york/>

**5-8 September 2006:** EFEPR 06 Madrid <http://efepr-2006.unicongress.com/>

**25-29 March 2007:** ESR Group 40<sup>th</sup> International Meeting Oxford [www.esr-group.org.uk](http://www.esr-group.org.uk)

### **ESR GROUP COMMITTEE.**

The ESR Group's AGM was held in Edinburgh on the 4th April 2006 and has the following committee members:

<i>Chair</i>	Dr Shirley Fairhurst	2004-2007	<a href="mailto:shirley.fairhurst@bbsrc.ac.uk">shirley.fairhurst@bbsrc.ac.uk</a>
<i>Secretary</i>	Dr Chris Kay	2006-2011	<a href="mailto:c.kay@ucl.ac.uk">c.kay@ucl.ac.uk</a>
<i>Treasurer:</i>	Dr Victor Chechik	2005-2010	<a href="mailto:vc4@york.ac.uk">vc4@york.ac.uk</a>
<i>Web Editor</i>	Dr John Maher	2006-2007	<a href="mailto:ct04@esr-group.org.uk">ct04@esr-group.org.uk</a>
<i>Ordinary Members</i>			
Prof Brian Hoffman		2004-2007	<a href="mailto:bmh@northwestern.edu">bmh@northwestern.edu</a>
Dr Philip James		2004-2008	<a href="mailto:jamespp@cardiff.ac.uk">jamespp@cardiff.ac.uk</a>
Dr David Keeble		2005-2008	<a href="mailto:d.j.keeble@dundee.ac.uk">d.j.keeble@dundee.ac.uk</a>
Prof David Lurie		2005-2008	<a href="mailto:lurie@abdn.ac.uk">lurie@abdn.ac.uk</a>
Dr Eric McInnes		2005-2008	<a href="mailto:eric.mcinnes@manchester.ac.uk">eric.mcinnes@manchester.ac.uk</a>
Mr Peter Meadows		2006-2008	<a href="mailto:peterm@jeoleuro.com">peterm@jeoleuro.com</a>
Dr Mark Newton		2006-2009	<a href="mailto:mark.newton@warwick.ac.uk">mark.newton@warwick.ac.uk</a>
Dr Christiane Timmel		2004-2008	<a href="mailto:timmel@physchem.ox.ac.uk">timmel@physchem.ox.ac.uk</a>
Mrs Helen Williams		2006-2009	<a href="mailto:helen.williams@astrazeneca.com">helen.williams@astrazeneca.com</a>
Dr Jonny Woodward		2006-2009	<a href="mailto:jrw16@le.ac.uk">jrw16@le.ac.uk</a>