

## News from the UK cwEPR National Service at Manchester

The cwEPR National Service is now located on a single site, and as well as the unique range of microwave frequencies (L, S, X, K and Q-bands), the W-band (94 GHz) spectrometer has been installed and is proving to be sensitive, responsive and relatively robust. The magnetic field is supplied by a 6 T Oxford horizontal magnet, allowing wide field sweeps routinely. Resolution of very small *g*-value anisotropies, measurement of tiny samples, determination of large zero-field splittings and power saturation studies (even at room temperature) will extend the range of experiments for users of the Service. Recent developments with the microwave frequencies include routine *in situ* electrochemical generation and also optical excitation. Interpretation by spectrum simulation of data collected in users' own laboratories is also provided in some cases. Recently, pilot studies in collaboration with the EPSRC National Service for Computational Chemistry Software have been initiated, whereby in the future a project being studied by one Service could have access to the other. It is hoped to implement this inter-Service arrangement if both Services are renewed this year, and subject to the approval of EPSRC. EPR spectra at higher frequencies (180/270 GHz) remain available through collaborations with St Andrews (Dr Graham Smith), as do ENDOR measurements (X and Q-bands) with Cardiff (Dr Damien Murphy).

The process for the renewal of the cwEPR National Service from March 2006 is underway, although the provision of pulse spectroscopy is specifically excluded in the call made by EPSRC. However, they are encouraging collaborative applications to obtain pulse equipment through responsive mode funding. Users or potential users are welcome to contact the co-Directors, David Collison or Eric McInnes, for discussions about this possibility.

Training and extending the user base are important elements of the Service and the centre encourages suppliers of samples to visit the centre in order to gain hands-on experience in EPR. The 4<sup>th</sup> annual training workshop, with lectures, hands-on practicals and problem classes will be held in September 2005 in Manchester; contact the Service for details.

For more information about the EPR Service or to discuss applications for time on the Service contact: [eric.mcinnnes@manchester.ac.uk](mailto:eric.mcinnnes@manchester.ac.uk), tel: 0161-275-4469 or [david.collison@manchester.ac.uk](mailto:david.collison@manchester.ac.uk), tel: 0161-275-4660; whilst the University website remains under development contact through that route is unreliable. Contact Carmine Ruggiero at [carmine.ruggiero@epsrc.ac.uk](mailto:carmine.ruggiero@epsrc.ac.uk) for information about other EPSRC services.

David Collison

## ESR GROUP COMMITTEE.

The ESR Group committee was elected at the AGM held in Bath on the 23rd March 2005 and has the following members:

*Chair:* Dr. Shirley A. Fairhurst 2004-2007 [Chair@esr-group.org.uk](mailto:Chair@esr-group.org.uk)  
*Secretary:* Dr. Victor Chechik 2005-2006 [Secretary@esr-group.org.uk](mailto:Secretary@esr-group.org.uk)  
*Treasurer:* Dr. Victor Chechik 2005-2010 [Treasurer@esr-group.org.uk](mailto:Treasurer@esr-group.org.uk)

### Ordinary Members

Dr. Eric McInnes 2005-2008 [eric.mcinnnes@man.ac.uk](mailto:eric.mcinnnes@man.ac.uk)  
Dr. David Keeble 2005-2008 [d.j.keeble@dundee.ac.uk](mailto:d.j.keeble@dundee.ac.uk)  
Dr. David Lurie 2005-2008 [d.lurie@abdn.ac.uk](mailto:d.lurie@abdn.ac.uk)  
Prof. Brian Hoffman 2004-2007 [bmh@northwestern.edu](mailto:bmh@northwestern.edu)  
Dr. Philip James 2004-2007 [Jamespp@cardiff.ac.uk](mailto:Jamespp@cardiff.ac.uk)  
Dr. Graham Smith 2004-2007 [gms@st-andrews.ac.uk](mailto:gms@st-andrews.ac.uk)  
Dr. Christiane Timmel 2004-2007 [timmel@physchem.ox.ac.uk](mailto:timmel@physchem.ox.ac.uk)  
Dr. Fraser Macmillan 2003-2006 [macmillan@chemie.uni-frankfurt.de](mailto:macmillan@chemie.uni-frankfurt.de)  
Dr. Tim Smith 2004-2006 [tim.smith@bruker.co.uk](mailto:tim.smith@bruker.co.uk)  
Dr. John Maher 2005-2006 [esr@argonet.co.uk](mailto:esr@argonet.co.uk)  
Dr. Damien M. Murphy 2005-2006 [murphydm@cardiff.ac.uk](mailto:murphydm@cardiff.ac.uk)

*Local Organiser (Edinburgh)* Dr. Paul Murray

## ELECTRON SPIN RESONANCE GROUP

### Newsletter April 2005

# RS•C

ROYAL SOCIETY OF CHEMISTRY

The 38<sup>th</sup> Annual ESR Conference took place from 20<sup>th</sup> – 24th March 2005 at the University of Bath. This meeting was on the theme of Advanced Techniques and Applications of EPR. Plenary lectures were presented by: John Davies (University of Bath) who described some optical methods for the detection of ESR in semiconductors. Yuri Tsvetkov (Institute of Chemical Kinetics, Novosibirsk) described the application of Pulsed Double Electron-Electron Resonance (PELDOR). Edgar Groenen (Huygens Laboratory, Leiden) describing recent advances using pulsed EPR and ENDOR at 95 and 275 GHz. Motiji Ikeya (Osaka University) studies of interdisciplinary ESR from Earth to planetary science: dating and radiation dosimetry. Zbigniew Sojka (Jagellonian University, Poland) described a computational approach combining a hybrid genetic algorithm for optimization of EPR spectra with DFT calculations of magnetic parameters. Joshua Telsor (Roosevelt University) took us on a journey across the first row transition metals with high field/frequency EPR. Jack Peisach (Albert Einstein College of Medicine) brought us up to date with his long interest in EPR spectroscopy of transition metal proteins, from his early studies on copper and iron, up to the present with his on-going work on prion proteins.



Jack and Estelle Peisach at the Conference Dinner

Heinz-Jurgen Steinhoff (University of Osnabruck) showed how multifrequency EPR spectroscopy and site directed spin labelling reveal the structure and conformational dynamics of membrane bound proteins complexes. Sabine Van Doorslaer (University of Antwerp) described The Echo of Life - Pulse EPR analyses of paramagnetic metalloproteins and related macrocyclic metal complexes, concentrating on globin proteins. The 2005 Bruker Lecture was presented by Professor Klaus-Peter Dinse of Darmstadt University of Technology who posed the question: *EPR- an interesting topic?* In an elegant and amusing lecture we were able persuaded that the subject has not only an interesting past and present but that a bright future awaits.



**Klaus-Peter Dinse received his Bruker Lecture certificate from Shirley Fairhurst (ESR Group Chair) and Dieter Schmalbein (Bruker BioSpin)**

Neil Connelly (Bristol University) introduced the session dedicated to the memory of the late Phil Rieger (Brown University, Providence USA). Phil's interest in EPR spectra from systems with non-coincident **g** and **A** tensors and his long-standing ties with the group were elaborated. His wife and collaborator Anne Rieger was able to join us.

The JEOL prize for the best oral presentation by a young scientist saw Malika Bouterfas (Ecole Polytechnique Federale de Lausanne) received the JEOL Prize Medal for her talk entitled: Longitudinally detected ESR (LODESR) using miniaturized Hall sensors. Joint runners-up were Katerina Pirker (ARC Seibersdorf Research GmbH) and Evi Vinck (University of Antwerp). All three student talks were of a very high calibre but sadly there was only one medal to be won. All three received cheques for £100 from JEOL.

**THANKS** The ESR Group thanks Dr John Maher and Dr Damien Murphy as retiring Secretary and Treasurer respectively for their endeavours. The organisation of our conferences in Warwick and Bath have been due to their efforts. The work involved in organising the meetings and coordinating the work of the ESR Group is huge and it is our intention that in future other committee members will take on extra duties. Thanks go to Professor John Walton our past Chairman who leaves the committee and also to retiring committee members Drs David Collison, Mark Newton and Lesley Yellowlees.

A very special thanks goes to Bath local organisers Professor John Davies and Dr Steve Bingham.

#### **CALL FOR NOMINATIONS**

The ESR Group invites nominations for the Bruker Lecturer 2006. All nominations should be accompanied with a 100-150 word citation plus website details and affiliation and should be sent in confidence to [Shirley.Fairhurst@bbsrc.ac.uk](mailto:Shirley.Fairhurst@bbsrc.ac.uk) or [Chair@esr-group.org.uk](mailto:Chair@esr-group.org.uk). Please do not inform the nominee of any nomination.

This year there were 33 posters and as usual one was selected to win the poster prize with the traditional bottle of whisky going to Stephan Stoll (ETH Zurich) for his poster on *A Suppression Effect in ESEEM spectra of multinuclear spin systems.*



**Stephan Stoll receives his poster prize**

*Full abstracts of the Plenary lectures, short talks and posters are on the website*



**JEOL Prize: Evi Vinck, Katerina Pirker, John Gibson (JEOL UK) and Malika Bouterfas (Medal Winner)**

#### **CONGRATULATIONS**

Professor Klaus Peter Dinse on the award of the 2005 Bruker Lectureship.  
JEOL Prize 2005 Malika Bouterfas  
Poster Prize 2005 Stephan Stoll  
Lesley Yellowlees MBE (Services to Science) 2005 New Years Honours List

#### **IES Awards 2005**

**Gold Medal:** Wolfgang Lubitz (MPI for Bioinorganic Chemistry, Mulheim)

**Silver Medal for Instrumentation:** Jos Disselhorst (Leiden)

**IES Young Investigator Medal:** Eric McInnes (Manchester)

#### **IES Fellows 2005**

Keith McLauchlan

Harold M Swartz

George D Watkins

Harvey Buckmaster

Further information in the International EPR Society (IES) 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 from: <http://www.epr-newsletter.ethz.ch/>

#### **FORTHCOMING EVENTS**

**29 June - 1 July 2005** [Specialized Colloque AMPERE, EPR and ENDOR Spectroscopy of Metal Proteins and Spin-labelled Proteins](#) Leiden, The Netherlands

**3 - 8 July 2005** ["Magnetic resonance for the Future", EUROMAR Conference](#) Veldhoven, The Netherlands

**17 - 24 July 2005** [3rd EPR Summer School of EFEPR](#) Wiesbaden, Germany

**31 July - 4 Aug 2005** [28th International EPR Symposium](#) University of Denver, Denver, Colorado, USA (email: [seaton@du.edu](mailto:seaton@du.edu))

**4-8 Sept 2005** [Joint Conference of the 11th In Vivo EPR Spectroscopy and Imaging and the 8th International EPR Spin Trapping](#) Ohio State University, Columbus, Ohio, USA (email: [epr2005@medctr.osu.edu](mailto:epr2005@medctr.osu.edu))

**7- 9 Sept 2005** Metals: Centre of Biological Activity. University of Nottingham, UK  
[www.rsc.org/DD8](http://www.rsc.org/DD8)

**20-24 Sept 2005** [4th International Conference on Nitroxide Radicals: Synthesis, Properties and Implications of Nitroxides \(SPIN-2005\)](#) Akademgorodok, Novosibirsk, Russia (email: [spin2005@nioch.nsc.ru](mailto:spin2005@nioch.nsc.ru))

**5-6 Jan 2006** Joint meeting of ESR Group & IBDG: Metals and Radicals, QMC London  
[www.le.ac.uk/chemistry/el10/ibdg/](http://www.le.ac.uk/chemistry/el10/ibdg/)

**2-6 April 2006** 39<sup>th</sup> International Meeting of ESR Group. Edinburgh [www.esr-group.org.uk](http://www.esr-group.org.uk)

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

**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 and urged to tick the ESR Group box on their membership renewal forms. The cost is only £5 per annum! Membership carries entitlement to reduced registration fees at ESR Group annual conferences.

#### **Website:**

<http://www.esr-group.org.uk>  
Webmaster Dr John Maher

#### **Newsletter Editor:**

Dr Shirley Fairhurst