

# The 45th Annual International Meeting of the ESR Spectroscopy Group: 25<sup>th</sup> – 29<sup>th</sup> March 2012: Conference Programme

| Sunday 25 <sup>th</sup> March            |                                 |                                                                                                                                                                                                               |
|------------------------------------------|---------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 16.00 – 18.30                            | Registration                    | Chancellors Reception                                                                                                                                                                                         |
| 18.30 – 20.00                            | Dinner                          | Chancellors Carriage Restaurant                                                                                                                                                                               |
| 20.00 – 22.30                            | RSC Wine Reception and free bar | Chancellors Conservatory and bar                                                                                                                                                                              |
| Monday 26 <sup>th</sup> March            |                                 |                                                                                                                                                                                                               |
| 07.30 – 08.55                            | Breakfast                       | Chancellors or Luther King House or Willowbank Hotel                                                                                                                                                          |
| <b>Session 1 Chair: David Collison</b>   |                                 |                                                                                                                                                                                                               |
| 08.55 – 09.00                            | Mark Newton                     | Conference opening and welcome note                                                                                                                                                                           |
| 09.00 – 09.30                            | Richard Winpenny                | <b>Keynote Lecture:</b> EPR Studies of Rings and Dimers of Rings                                                                                                                                              |
| 09.35 – 09.50                            | Irina Drozdyuk                  | Intercluster exchange interactions and spin state switching in copper nitroxide based molecular magnets Cu(hfac) <sub>2</sub> LR studied by EPR                                                               |
| 09.55 – 10.10                            | Shigeaki Nakazawa               | Quantum operations by pulsed ESR spectroscopy: Molecular design for biradical and triradical qubits                                                                                                           |
| 10.15 – 10.30                            | Petra Lüders                    | Relaxation Enhancement in Orthogonal Spin Pairs – Precision and Short Distance Limitation –                                                                                                                   |
| 10.35 – 11.05                            | Tea & Coffee                    | Chancellors Conservatory                                                                                                                                                                                      |
| <b>Session 2 Chair: Ilya Kuprov</b>      |                                 |                                                                                                                                                                                                               |
| 11.05 – 11.25                            | Gavin Morley                    | <b>Invited Lecture:</b> Quantum control of hybrid nuclear-electronic qubits                                                                                                                                   |
| 11.30 – 11.45                            | David Keeble                    | EPR of Fe <sup>3+</sup> centres in SrTiO <sub>3</sub> : Monodomain crystals to thin films                                                                                                                     |
| 11.50 – 12.05                            | Vasile Nistor                   | Spying with Mn <sup>2+</sup> ions the structure changes during the thermal decomposition of Zn <sub>5</sub> (CO <sub>3</sub> ) <sub>2</sub> (OH) <sub>6</sub> and Zn(OH) <sub>2</sub> into nanostructured ZnO |
| 12.10 – 12.25                            | Mario Chiesa                    | Elucidating the Nature and Reactivity of Metal Ions Incorporated in the Framework of Aluminophosphate Molecular Sieves. New Evidences from HYSCORE and Pulse-ENDOR Spectroscopy                               |
| 12.30 – 14.00                            | Lunch                           | Chancellors Conservatory                                                                                                                                                                                      |
| <b>Session 3 Chair: Fraser MacMillan</b> |                                 |                                                                                                                                                                                                               |
| 14.00 – 4.15                             | Alice Bowen                     | <b>Jeol Student Prize Talk:</b> Utilizing the TWT linear region: Double Electron-Electron Resonance (DEER) with multiple excitation pulses and dead-time free three-pulse DEER                                |
| 14.20 – 14.35                            | Ilia Kaminker                   | <b>Jeol Student Prize Talk:</b> A novel triple resonance correlation sequence for Resolving and Assigning Signals in ELDOR-Detected NMR Spectra                                                               |
| 14.40 – 14.55                            | Tomasz Mazur                    | <b>Jeol Student Prize Talk:</b> EPR/HYSCORE and DFT study of nickel adducts with O <sub>2</sub> , CO and NO molecules encaged in zeolites                                                                     |
| 15:00 – 15:15                            | Christoph Meier                 | <b>Jeol Student Prize Talk:</b> Microcrystalline Silicon: Orientation dependence of light induced EDMR signals                                                                                                |
| 15:20 – 15:35                            | Gunnar W. Reginsson             | <b>Jeol Student Prize Talk:</b> Trityl: A new spin label for nanometer distance measurements                                                                                                                  |

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| 15.40 – 17.00                          | Tea & Coffee:<br><b>Posters (EVEN)</b> | Chancellors Conservatory                                                                           |
| <b>Session 4 Chair: Victor Chechik</b> |                                        |                                                                                                    |
| 17.00 – 17.25                          | Arzhang Ardavan                        | <b>Invited Lecture:</b> Quantum information processing with molecular nanomagnets                  |
| 17.30 – 17.45                          | Simon Bennie                           | Electronic and Magnetic Properties of a Tris( hydroxo) bridged Chromium dimer, A challenge for DFT |
| 17.50 – 18.05                          | Johannes McKay                         | New techniques in determining the spin label orientation using high power W-Band PELDOR            |
| 19.00 – 20.30                          | Dinner                                 | Chancellors Carriage Restaurant                                                                    |
| 20.30 – 24.00                          | JEOL Reception and free bar            | Chancellors Conservatory and Bar                                                                   |

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| <b>Tuesday 27<sup>th</sup> March</b>      |                                                                                                                                                                        |                                                                                                                                                                                                                                                                              |
| 07.30 – 09.00                             | Breakfast                                                                                                                                                              | Chancellors or Luther King House or Willowbank Hotel                                                                                                                                                                                                                         |
| <b>Session 5 Chair: Christiane Timmel</b> |                                                                                                                                                                        |                                                                                                                                                                                                                                                                              |
| 09.00 – 09.30                             | Walter Kockenberger                                                                                                                                                    | <b>Keynote Lecture:</b> From electron-nuclear spin pairs to the electron spin interaction with the bulk nuclei: A closer look at dynamic nuclear polarisation                                                                                                                |
| 09.35 – 09.50                             | Graham Smith                                                                                                                                                           | Techniques to improve sensitivity and capability in high field pulsed EMR experiments                                                                                                                                                                                        |
| 09.55 – 10.10                             | Wei Wu                                                                                                                                                                 | Theoretical modelling of orientation-dependent EPR spectra in organic solar cells                                                                                                                                                                                            |
| 10.15 – 10.30                             | Ilya Kuprov                                                                                                                                                            | Closing the simulation loop: direct fitting of atomic coordinates of radicals to experimental ESR data                                                                                                                                                                       |
| 10.35 – 11.05                             | Tea & Coffee                                                                                                                                                           | Chancellors Conservatory<br>Group photograph of delegates                                                                                                                                                                                                                    |
| <b>Session 6 Chair: Damien Murphy</b>     |                                                                                                                                                                        |                                                                                                                                                                                                                                                                              |
| 11.05 – 11.25                             | Georg Gescheidt                                                                                                                                                        | <b>Invited Lecture:</b> Probing (Anti)-oxidative effects with time-resolved EPR and CIDNP                                                                                                                                                                                    |
| 11.30 – 11.45                             | René Boéré                                                                                                                                                             | ESR and Electrochemistry Studies on Sterically Congested R <sub>3</sub> E (E=As,P) and R <sub>2</sub> PPR <sub>2</sub>                                                                                                                                                       |
| 11.50 – 12.05                             | Goetz Bucher                                                                                                                                                           | Naphthoxanthenyl: An Unusually Stable Carbon-Centered Free Radical                                                                                                                                                                                                           |
| 12.10 – 12.25                             | Jeffrey Harmer                                                                                                                                                         | Electron delocalization in multi-porphyrin systems probed by EPR                                                                                                                                                                                                             |
| 12.30 – 12.45                             | Dimitri Svistunenko                                                                                                                                                    | Dehaloperoxidase – a Tyrosine Radical Juggler                                                                                                                                                                                                                                |
| 12.50 – 14.00                             | Lunch                                                                                                                                                                  | Chancellors Conservatory                                                                                                                                                                                                                                                     |
| 14.00 – 18.00                             | Free afternoon: opportunity to visit Manchester attractions, <i>e.g.</i> Museum of Science and Industry or other cultural assets – see info leaflets in delegate pack. | Frequent buses into Manchester city centre from Wilmslow Road. See separate map in folder for details of bus routes and location of attractions. To get to Museum of Science and Industry or the Imperial War Museum North, it may be easier to share a Taxi there and back. |
| 18.00 – 19.30                             | Dinner                                                                                                                                                                 | Chancellors Carriage Restaurant                                                                                                                                                                                                                                              |

| <b>Session 7 Chair: Mark Newton</b> |                               |                                                                                                         |
|-------------------------------------|-------------------------------|---------------------------------------------------------------------------------------------------------|
| 19.30 – 21.00                       | Kev Salikhov                  | <b>Bruker Lecture:</b> Quantum computing on electron spins using the pulse EPR spectroscopy methodology |
| 21.00 – 24.00                       | Bruker Reception and free bar | Chancellors Conservatory and Bar                                                                        |

| <b>Wednesday 28<sup>th</sup> March</b>    |                                |                                                                                                                                                       |
|-------------------------------------------|--------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
| 07.30 – 09.00                             | Breakfast                      | Chancellors or Luther King House or Willowbank Hotel                                                                                                  |
| <b>Session 8 Chair: David Norman</b>      |                                |                                                                                                                                                       |
| 09.00 – 09.30                             | Heinz-Juergen Steinhoff        | <b>Keynote Lecture:</b> Structure and Conformational Dynamics of Nucleic Acids and Membrane Protein Complexes Studied by Site-Directed Spin Labeling  |
| 09.35 – 09.50                             | Chris Kay                      | Investigation of IKK Structure and Activation by site-directed spin labeling and EPR Spectroscopy                                                     |
| 09.55 – 10.10                             | Elena Gabriela Ionita          | Investigating cyclodextrin/ PEG hydrogels properties with spin probes                                                                                 |
| 10.15 – 10.30                             | Alistair Fielding              | Multifrequency Electron Paramagnetic Resonance Characterization of PpoA, a CYP450 Fusion Protein that Catalyses Fatty Acid Dioxygenation              |
| 10.35 – 11.05                             | Tea & Coffee                   | Chancellors Conservatory                                                                                                                              |
| <b>Session 9 Chair: Chris Kay</b>         |                                |                                                                                                                                                       |
| 11.05 – 11.25                             | Christiane Timmel              | <b>Invited Lecture:</b> A multifrequency approach: using RF and microwave fields to unravel the recombination kinetics of a photoinduced radical pair |
| 11.30 – 11.45                             | Marilena Di Valentin           | Insight into the Electronic Structure of the Carotenoid Triplet state in Photosynthetic Proteins revealed by ESEEM and Pulse ENDOR                    |
| 11.50 – 12.05                             | Fraser MacMillan               | EPR accessibility measurements of P-glycoprotein show topography of TM6/TM12 region in different conformational states                                |
| 12.10 – 12.25                             | Johann Klare                   | Structure and Function of the Sodium/Proline Transporter PutP studied by EPR Spectroscopy                                                             |
| 12.30 – 14.00                             | Lunch                          | Chancellors Conservatory                                                                                                                              |
| <b>Session 10 Chair: Dima Svistunenko</b> |                                |                                                                                                                                                       |
| 14.00 – 14.15                             | David Norman                   | Using very long distance and orientation measurement to elucidate the structure of the histone Chaperone Vps75                                        |
| 14.20 – 14.35                             | Katharina Pirker               | Investigation of the intermediate state of the chaperone usher pathway in Type 1 <i>E. coli</i> using SDSL-EPR                                        |
| 14.40 – 14.55                             | Dennis Kurzbach                | Assessing the Solution Shape and Size of Charged Dendronized Polymers Using Double Electron Electron Resonance                                        |
| 15.00 – 15.15                             | Claire Motion                  | Composite Pulses in W-band PELDOR experiments                                                                                                         |
| 15.20 – 16.40                             | Tea & Coffee: Posters (ODDS)   | Chancellors Conservatory                                                                                                                              |
| <b>Session 11 Chair: Graham Smith</b>     |                                |                                                                                                                                                       |
| 16.40 – 17.00                             | Steffen Glaser                 | <b>Invited Lecture:</b> Optimal Control of Spin Dynamics in Magnetic Resonance                                                                        |
| 17.05 – 17.20                             | Gunnar Jeschke                 | Characterization of protein conformational changes with sparse spin label distance constraints                                                        |
| 17.25 – 17.40                             | Bela Bode                      | PELDOR in membrane proteins: potential pitfalls and loopholes                                                                                         |
| 17.20 – 17.35                             | Janet Lovett                   | DEERS – combining the sensitivity of 3p-DEER with the versatility of 4p-DEER                                                                          |
| 17.40 – 18.10                             | AGM RSC ESR Spectroscopy Group | Flowers Lecture Theatre (all welcome to attend)                                                                                                       |
| 19.30 – 22.30                             | Banquet                        | Woolton Hall (short walk from Chancellors)                                                                                                            |

| Thursday 29 <sup>th</sup> March       |                  |                                                                                                                                                          |
|---------------------------------------|------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------|
| 07.30 – 09.00                         | Breakfast        | Chancellors or Luther King House or Willowbank Hotel                                                                                                     |
| <b>Session 12 Chair: Eric McInnes</b> |                  |                                                                                                                                                          |
| 09.00 – 09.30                         | Takeji Takui     | <b>Keynote Lecture:</b> New aspects of nitroxides and open-shell graphene fragments chemistry: From quantum computers to energy conversion elements      |
| 09.35 – 9.50                          | Alena Nishchenko | EPR study of the mobility of nitroxide radicals confined in MIL-53(Al) nanochannel system                                                                |
| 9.55 – 10.10                          | Mariana Stefan   | Multifrequency EPR of Mn <sup>2+</sup> in II-VI semiconductor nanocrystals                                                                               |
| 10.15 – 10.45                         | Tea & Coffee     | Chancellors Conservatory                                                                                                                                 |
| <b>Session 13 Chair: Mark Newton</b>  |                  |                                                                                                                                                          |
| 10.45 – 11.05                         | Robert Bittl     | <b>Invited Lecture:</b> EPR in bioenergetics and photovoltaic research                                                                                   |
| 11.10 – 11.25                         | Maxie Roessler   | Nature of the Fe-N bond in the reversibly superoxidized proximal [4Fe-3S] cluster of O <sub>2</sub> -tolerant [NiFe]-hydrogenases as revealed by HYSCORE |
| 11.30 – 11.45                         | Till Biskup      | Cryptochromes: Potential compass molecules with an unexpected variety of electron transfer pathways                                                      |
| 11.50 – 14.00                         | Lunch            | Chancellors Conservatory                                                                                                                                 |
| <b>CONFERENCE END - DEPARTURE</b>     |                  |                                                                                                                                                          |

## Information for delegates

### Getting there:

#### By Train

Most Intercity trains call or terminate at Manchester Piccadilly Station. Either take a taxi (approx. 15 minutes) or take a five minute walk to Piccadilly Gardens Bus Station. More local rail services also stop at Manchester Oxford Road Station and Manchester Victoria Station.

#### From Manchester International Airport

Manchester International Airport is approximately 5 miles from Chancellors (about 20 minutes by taxi, which costs about £15-20 and is the most convenient route). If you wish to take the train from the airport there is a 24-hour service which runs 7 days a week, every 15 minutes during peak times and goes direct to Piccadilly Train Station. From the station either take a taxi or take the short walk to Piccadilly Gardens Bus Station and catch one of the many buses that follow the route to Wilmslow Road, Fallowfield.

#### By Bus from the City Centre

Take a bus numbered 41, 42, 42A, 43, 44, 48, 142, 143, 157, X57 from Piccadilly Gardens Bus Station to Wilmslow Road, Fallowfield. Walk to the junction with Moseley Road and turn left. At the next set of traffic lights turn left into Chancellors Way and the hotel is on your left, opposite the Armitage Sports Centre.

#### By Car Using GPS

Chancellors Hotel and Conference Centre has free on site car parking for hotel and conference guests. SatNav users should use the following postcode: M14 6ZT. This will lead you to Moseley Road, from Moseley Road turn onto Chancellors Way and Chancellors Hotel and Conference Centre is signposted on the left hand side across from the Armitage Sports Centre.

#### By Car from the North

Leave the M6 at Junction 20a (Lymm Interchange), onto the M56, following signs for Manchester Airport/City Centre. Take the right hand lanes at the end of the motorway where it becomes the A5103 - signposted Manchester City Centre. At the 5th set of traffic lights turn right onto Wilbraham Road (A6010 signposted Sheffield). At the 4th set of traffic lights turn left onto Chancellors Way. Chancellors Hotel and Conference Centre is situated on the left hand side opposite the Armitage Sports Centre.

#### By Car from the East

From the M62, leave at J18 (Simister Island) and follow the M60 S&E (Stockport). From the end of the M67 turn left/south onto the M60 S&E (Stockport). Leave the M60 at Junction 5 and join the A5103 - signposted Manchester City Centre. At the 5th set of lights turn right onto Wilbraham Road (A6010 signposted Sheffield). At the 4th set of traffic lights turn left onto Chancellors Way. Chancellors Hotel and Conference Centre is situated on the left hand side opposite the Armitage Sports Centre.

#### By Car from the South

From the M6, leave at J19 (Knutsford) and follow the A556 to Manchester. From the end of the A556 turn right onto the M56 following signs for Manchester Airport/City Centre. Take the right hand lanes at the end of the motorway where it becomes the A5103 - signposted Manchester City Centre. At the 5th set of traffic lights turn right onto Wilbraham Road (A6010 signposted Sheffield). At the 4th set of traffic lights turn left onto Chancellors Way. Chancellors Hotel and Conference Centre is situated on the left hand side opposite the Armitage Sports Centre.

#### Going to the Willowbank Hotel

The hotel is at 340 Wilmslow Road, which is to the south of Chancellors and on the opposite side of the road. From Wilbraham Rd turn right at the 3<sup>rd</sup> set of traffic lights onto Wilmslow Rd. The Willowbank Hotel is approx ¼ mile on the right. Postcode is: M14 6AF.

#### Going to Luther King House

Luther King House is on Brighton Grove, which is off Wilmslow Road to the north of Chancellors and on the same side of the road. From Wilbraham Rd turn left at the 3<sup>rd</sup> set of traffic lights onto Wilmslow Rd. Brighton Grove is approx ⅓ mile on the right. Postcode is: M14 5JP.

## How to find:

- **Registration**

Registration will be in **the Reception area at Chancellors** from 16.00 to 18.30 on Sunday 25<sup>th</sup> March (see map below). When you arrive, either go to registration, or if your accommodation is in the Willowbank Hotel or Luther King House you should check in there first (accommodation check-in available from 14:00 at all 3 locations). Please wear your conference badge **at all times** (including lunches/dinners).

- **Accommodation**

Delegates staying at Luther King House or the Willowbank Hotel are within 10-15 minutes walking distance of Chancellors (see map for footpaths).

Chancellors Hotel and Conference Centre

Chancellors Way

Off Moseley Road

Fallowfield

Manchester M14 6ZT

Tel: +44 (0)161 907 7414

Email: [chancellors@manchester.ac.uk](mailto:chancellors@manchester.ac.uk)

<http://www.chancellorshotel.co.uk/>

Luther King House

Brighton Grove

off Wilmslow Road

Manchester M14 5JP

Tel:

+44 (0)161 224 6404

Email: [reception@lkh.co.uk](mailto:reception@lkh.co.uk)

<http://www.lutherkinghouse.co.uk/>

BEST WESTERN Willow Bank Hotel

340 Wilmslow Road

Manchester M14 6AF

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+44 (0)161 224 0461

Email: [willowbank@bestwestern.co.uk](mailto:willowbank@bestwestern.co.uk)

<http://www.feathers.uk.com/willow-bank-hotel/>

Map of Conference venue

