

## Full program

### Sunday 14 July 2019 – location Building G Middelheim Campus

→ **MODULE 1**

16.00 – 17.00 h Registration to the school 17.00 – 17.15h Welcome – Mario Chiesa

17.15 – 18.00h Small history of Electron Paramagnetic Resonance – Sabine Van Doorslaer/Andreas Pöpl

**Abstract.** *Magnetic resonance techniques were introduced at the end of World War II. This timing is not random. Because of the war, research in radar technology involving radio and microwaves was intensified and furthermore, many of the key discoveries in physics, crucial for the development of magnetic resonance, were in place. This talk will highlight some of the main discoveries and the scientists that have led to the success of magnetic resonance techniques, and more specifically EPR. While the lectures of the following days will focus on the physical principles behind these discoveries, this lecture aims at highlighting the interaction between different EPR scientists (and society) and the cross-fertilization between different disciplines within magnetic resonance.*

18.00 - 20.00h Reception

### Monday 15 July 2019 – location Building G Middelheim Campus

→ **MODULE 2**

9.00 – 9.30 h Science and ethics. What is at stake? - Patrick Loobuyck

9.30 – 10.30 h Research integrity – Sabine Van Doorslaer

**Content.** *Starting from the ALLEA code, the topic of scientific integrity and scientific ethics will be introduced. Some examples will be given of scientific misconduct cases involving 'FFP' (fabrication, falsification and plagiarism), but also those that can be categorized in the 'grey zone' of sloppy science. The participants will be asked to reflect on some of these cases and will be asked to reflect on how they would react under these circumstances. Some of the reasons why scientists shift to unethical behavior and scientific misconduct will also be discussed. Finally, a number of the measures that are taken on national and European levels will be pointed out.*

10.30 – 10.45 h coffee break

10.45 – 11.45 h Research integrity - continued – S. Van Doorslaer

11.45 – 12.45 h Towards open science (+ Q&A) – Frederick Verbruggen

**Abstract.** *In the last couple of years, there have been calls from governments, research funders, publishers, as well as grassroots activists, for science to be more open. To some extent, this has to do with recent cases of scientific misconduct or bad research practice that have troubled many disciplines. However, a much more positive case can be made for Open Science as well. In this presentation, I will discuss why Open Science is important and why we should embrace it (even though it undeniably comes with certain challenges).*

12.45 – 13.30 h Lunch + discussion

13.30 – 15.00 h Dilemma game scientific integrity – P. Loobuyck

**Abstract.** *An adapted version of the Dilemma Game on Scientific Integrity developed at the Erasmus University of Rotterdam will be used to confront the participants with common dilemmas in science.*

15.00 – 15.15 h Coffee break

15.15 – 16.30 h The Overproduction of truth. Passion, competition, and integrity in modern science (+ Q&A) - Gianfranco Pacchioni

**Abstract.** *The way science is done has changed radically in recent years. Scientific research and institutions, which have long been characterized by passion, dedication and reliability, have increasingly less capacity for more ethical pursuits, and are pressed by hard market laws. From the vocation of a few, science has become the profession of many – possibly too many. These trends come with consequences and risks, such as the rise in fraud, plagiarism, and in particular the sheer volume of scientific publications, often of little relevance. We will critically review and assess the present-day policies and behaviors in scientific production and publication. We will touch on the tumultuous growth of scientific journals, in parallel with the growth of self-declared scientists over the world. We will investigate the loopholes and hoaxes of pretend journals and nonexistent congresses, so common today in the scientific arena, and discuss problems connected to the incorrect use of bibliometric indices, which have resulted in large part from the above distortions of scientific life. The solution? A slow approach with more emphasis on quality rather than quantity that will help us to rediscover the essential role of the responsible scientist.*

16.30 – 18.00 h Interactive session – all PIs

**Goal.** *In this session the participants will exchange experiences, good/bad practices and discuss about how to improve research integrity. The participants present and discuss their **preparatory work** and findings. To facilitate these discussions, the group will be split in small subgroups.*

**Tuesday 16 July 2019 – location Building G Middelheim Campus**

**→ MODULE 1**

9.00 – 10.00 h Theory of magnetic impurities in oxides. Complex problem, pragmatic solution – G. Pacchioni

**Abstract.** *Dopants in insulating and semiconducting oxides are of fundamental importance for the design of new materials and often result in the presence of holes or electrons trapped at particular sites. The proper identification of these paramagnetic centres is crucial for the understanding of the optical, magnetic, photocatalytic and transport properties of oxides. The nature of magnetic impurities can be studied by comparing DFT calculations using hybrid functionals electron paramagnetic resonance, EPR, measurements. We will provide some historical perspective on the description of holes in the O 2p valence band of SiO<sub>2</sub> as a paradigmatic example of interaction between theory and experiment. Then we will discuss N-dopants in TiO<sub>2</sub>, ZnO, SnO<sub>2</sub>, ZrO<sub>2</sub> and MgO. Here nitrogen can enter as interstitial or can replace an anion in the material leading to isolated magnetic defect centres. Also in this case a comparison with EPR data allows one to assess the accuracy of the DFT calculations. At high N-dopant concentrations the occurrence of a magnetic ordering has been suggested in some of these materials, which implies the existence of magnetic interactions between the isolated defects. While the use of hybrid functionals allows one to properly describe the nature of isolated magnetic defects in oxides, no magnetic ordering is predicted at this level of theory and for the dopant concentrations used in experiments. The problems related to the theoretical treatment within DFT of magnetic impurities in insulating and semiconducting oxides are discussed.*

10.00 – 10.45 h General tools from mathematics and physics needed to understand Magnetic Resonance – Andreas Pöppel

**Main topics:** Introduction into some basics of radio frequencies, microwaves, simple concept of spin (magnetic moment equivalence), Zeeman effect (just principle for free electron spin and magnetic nucleus, not  $g$  tensor), Bloch equations,  $T_1$ ,  $T_2$  [Note: participants will have to do preparatory work for this part]

10.45 – 11.00 h coffee break

11.00 – 11.45 h – CW EPR – Damien Murphy

**Main topics:** The concept of resonance, basic principle of CW-EPR (based on just two-level scheme), Basic outline of set-up and hardware, effect of modulation amplitude and microwave power

11.45 – 12.30 h –  $g$  tensor – George Mitrikas

**Main topics:** Spin Hamiltonian (with introduction into some basic quantum mechanics), What info is in a  $g$  tensor?, Effect on CW-EPR in solution (rapid motion limit) and solid state.

12.30 – 13.30 h Lunch

13.30 – 14.15 h – The hyperfine tensor and nuclear quadrupole tensor – Mario Chiesa

**Main topics:** Fermi contact + dipolar part, Effect on CW-EPR at room and low temperature, quadrupole tensor

14.15 – 15.00 h Spin trapping and spin probing – Damien Murphy

**Main topics:** what is spin trapping? What is spin probing? Typical spin traps and spin probes. How to interpret the spectra? Typical applications.

15.00 – 15.30 h Coffee break

15.30 – 18.00 h Interactive session – all PIs

**Goal.** Students present about the general background of their PhD (or Master thesis or research) topic (overview of problem setting and most relevant literature) and PIs discuss with them what they think would be something they can learn from EPR – depending on number of students, we split them up into different groups.

### **Wednesday 17 July 2019 – location Building G Campus Middelheim**

**→ MODULE 1**

9.00 – 09.45 h EPR to detect molecular motion – Sabine Van Doorslaer

**Main topics:** Basic ideas about detecting motional behavior with magnetic resonance, physics behind slow and fast motions, isotropic and anisotropic motion, common examples

09.45 – 10.30 h CW-ENDOR – George Mitrikas

**Main topics:** Introduction into CW-ENDOR techniques

10.30 – 11.00 h Coffee break

11.00 – 12.00 h Zero field splitting and exchange coupling – Etienne Goovaerts

**Main topics:** Introduction in zero-field splitting/ $J$  coupling with the emphasis on examples

12.00 – 13.00 h Lunch

13.00 – 18.00 h EasySpin simulation module Inés García-Rubio (+ assistance from UAntwerp PhD/postdocs)

**Main content:** *Theoretical lecture on EasySpin (How to start up EasySpin, How to define a spin system, How to set up a simulation of a room temperature EPR spectrum and of a low-temperature EPR spectrum); Exercises: Some examples to be worked out in group + specific individual exercises to be completed by the participants (to be uploaded in portfolio)*

*NOTE: the time will also be used to provide students the opportunity to ask feedback and questions on the theory of the different lectures so far.*

### **Thursday 18 July 2019 – location Building N Campus Drie Eiken**

→ **MODULE 1**

**Day of hands-on practicals** on standard and high-field EPR instrumentation (see

9.00 – 10.00 h Introduction to the experiments – Vincent Ching+ Sabine Van Doorslaer

10.00 – 10.15 h Coffee break

10.15 – 13.00 h Experiments in groups

13.00 – 13.30 h Lunch

13.30 – 18.00 h continuation experiments

#### **Experiments include:**

- Room-temperature X-band EPR
- W-band EPR (solid state experiment)
- All EPR spectra will need to be simulated using EasySpin and an analysis report of the data will need to be made -> upload on portfolio.

18.00 – 18.30 h (Only for PARACAT PhD) – Feedback Personal Career Development Plan

### **Friday 19 July 2019– location Building G Campus Middelheim**

→ **MODULE 1**

9.00 – 9.45 h Dipolar interactions: CW-EPR for distance determination - Vincent Ching

**Main topics:** *Dipolar interactions in magnetic resonance, How to measure distances with CW-EPR, effect of relaxation properties of the two spins*

9.45 – 10.45 h CW-EPR examples in homogeneous catalysis (including examples from industry) – Mario Chiesa

**Abstract.** *The students will be introduced into typical examples of the use of CW-EPR in elucidating mechanistic aspects in homogeneous catalysis.*

10.45 – 11.00 h Coffee break

11.00 – 11.45 h CW-EPR examples in heterogeneous catalysis (including examples from industry) – Mario Chiesa

**Abstract.** *The students will be given typical examples of the use of CW-EPR in elucidating mechanistic aspects in heterogeneous catalysis, including the use of EPR in material characterization.*

11.45 – 12.30 h CW-EPR examples in biocatalysis and biochemistry (including examples from industry) – Inés García-Rubio

**Abstract.** *The students will be given typical examples of the use of CW-EPR in elucidating mechanistic aspects in biocatalysis and biochemistry. Special attention will be given to examples from metallo-enzyme research.*

12.30 – 13.30 h Lunch

13.30 – 18.00 h Exercise on applications (coffee available) – all PIs

**Goal.** *The students will be divided in small groups. Starting from their preparatory work and using the knowledge obtained on continuous-wave EPR during the school, each group will have to discuss their assigned papers, fully understand the EPR part and relate the information of the papers within one group. Each group should make a final presentation from this and present it to the full group at the end of the session. The PIs will then ask questions to assess to what degree the students have understood the EPR concepts used in the different papers .*

Group dinner

**Saturday 20 July 2019– location Building N Campus Drie Eiken**

**→ MODULE 1**

9.00-10.30 Short introduction to pulsed EPR – George Mitrikas

**Content.** *In a final lecture, the students will be given a first insight into pulsed EPR as an outlook to the advanced course on this topic that will be organized by the European Federation of EPR groups in November. The lecture will involve the following : What is a microwave/rf pulse?, FID and pulse echo and a brief introduction into the different classes of pulsed EPR techniques (ESEEM, ENDOR, ELDOR) and what to expect from them.*

10.30 – 10.45 h coffee break

10.45-11.30 h Proclamation + final remarks

11.45 h-12.15 h lunch + departure to Ghent