Principle and Applications of
Electron Paramagnetic Resonance Spectroscopy

Overview

Electron Paramagnetic Resonance (EPR) also known as Electron spin resonance (ESR) is spectroscopic method of choice to study paramagnetic species. As EPR spectroscopy is very selective towards electron spin, it has the main advantage of providing insights into the nature of the paramagnetic center while also revealing detailed information on its environment and the dynamical processes. The rapid development of new methodologies in the past two decades such as time resolved EPR, Pulsed EPR, and High Field EPR have opened the door for scientists to apply EPR in a wide range of different fields spanning chemistry, biology, medicine, etc.

This short term course on EPR spectroscopy has been designed for students, scientists and faculty to provide sufficient exposure to the theory and applications of EPR spectroscopy and also the knowledge to choose appropriate EPR technique and to apply it properly to extract required information from the paramagnetic systems in the field of chemistry, biochemistry, medicine etc. Usually an introductory level EPR spectroscopy will be taught in the graduate level as a part of inorganic spectroscopy which is not sufficient to start research career with EPR spectroscopy as a primary tool to investigate chemical or biological problems. With more than three decades of teaching experience, the teaching experts of this course have carefully designed the syllabus with appropriate number of tutorial classes to ensure the proper understanding of the subject. This short term course covers both continuous wave and advanced time-domain EPR spectroscopy. The course starts with classical picture of resonance followed by quantum mechanical~~s~~ description in such a way that EPR will be easily understood by the audience having no strong quantum mechanics background. This course has been planned with a good number of examples for a detailed coverage of topics.

Successful completion of this course should result in (i) a clear understanding on theoretical aspects of CW and pulsed EPR spectroscopy, (ii) ability to record proper EPR spectrum for obtaining qualitative and quantitative information and to deriving EPR parameters from the CW EPR spectrum, (iii) Calculation of distance between spins in macromolecule/biomolecules and ability to analyse 1D and 2D hyperfine spectra, and (iv) importantly participants should be able to select proper EPR techniques to derive required information from chemical/biological systems.

Modules	Day	Course Details
	January 29, 2018	Classical picture of Electron Spin and orbital Angular momentum, magnetic moment and the Resonance phenomenon and the free electron g-factor
		CW EPR Spectrometer schematics, principles of operation – MW Klystron – wave guides – magnetic field regulation with Hall probe -Low frequency Modulation – phase sensitive detection – derivative spectra.
		Relaxation phenomena - Spin lattice and spin-spin relaxation – line width – Bloch equations - Saturation – CW methods of estimating T_1 and T_2.
		Instrument parameters (gain, modulation, scan time and filter time constant) optimization
	January 30, 2018	Isotropic and anisotropic EPR spectra. Orbital angular momentum and the deviation of the g-factor from 2.0023 – g-tensor.
		Electron-nuclear Hyperfine interaction – isotropic and anisotropic hyperfine interactions – spin density and the derivation of bond angles in simple inorganic radicals
		Organic radicals in solution – Hyperfine patterns from equivalent protons- organic radicals – McConnell's Q-values and polarization
		Deriving EPR parameters from isotropic and anisotropic spectra, Isotope effects on the EPR spectra – Identification of some organic radicals from their EPR Spectra
	January 31, 2018	EPR spectra in solids and single crystals. Powder spectra analysis. Derivation of g and hyperfine tensor from single crystals.
		EPR of transition metal compounds – Crystal and Ligand Field Theory and spin Hamiltonian of selected d^n systems. Derivation of bond covalency and MO

	coefficients from EPR data
	Methods of generation of free radicals – chemical redox reactions – electrochemical and photochemical; generation of radicals.
	Single crystal iso-frequency angular rotation spectra and derivation of principal g and hyperfine spectra from Cu(II) spectra.
February 1, 2018	Electron Nuclear Double Resonance (ENDOR) to resolve otherwise unresolved hyperfine coupling.
	EPR spectra of quadrupolar nuclei and 'forbidden' transitions.
	Some biological applications of EPR – spin labelling
February 2, 2018	Treatment of time-dependent phenomena: Time dependent Schrödinger-Equation, Density matrix, Spin Operators, Product operators
	Bloch equation revisited: Rotating frame, Larmor precession, Rabi nutation
	Relaxation, Homogeneous and inhomogeneous lines, excitation profiles of MW pulses
February 5, 2018	Free Induction decay and Hahn echo refocusing sequence
	Inversion recovery and stimulated echo pulse sequence
	Calculate time domain expectation values of spin ½ system without and with MW excitation
February 6, 2018	Magnetic dipole-dipole interaction between pair of spins
	Electron-Electron spin interaction, E-diagram
	Pulsed Electron-Electron Double Resonance (PELDOR) pulse sequence
February 7, 2018	4-pulse DEER sequence, DQ-EPR, SIFTER pulse sequences, Multi-spin effects
	Applications of dipolar spectroscopy to macromolecular complexes
	Calculate the distance between pair of spin labels, Calculate the number of coupled spins
February 8, 2018	Electron-Nuclear spin interaction, E-diagram
	Pulsed Davies ENDOR sequence, Pulsed Mims ENDOR sequence
	Electron spin echo envelope modulation (ESEEM), HYSCORE
February 9, 2018	Application of hyperfine spectroscopy to biological systems
	Orientation selection effects in hyperfine and dipolar spectroscopy, High-field pulsed EPR spectroscopy
	Analysis of 1D and 2D hyperfine spectra

Course Exam will be conducted on February 9, 2018 for the participants interested to earn credit

You Should Attend If…

- Students at all levels, MSc/M.Tech/PhD and Faculties from academic and technical institutions.

Fees

The participation fees for taking the course is as follows:

Participants from abroad: US $300

Participants from India
Faculty: Rs. 4,000/-
Students: Rs. 1,500/ (For SC/ST students 50% fee is waived)

The above fee includes all instructional materials, computer use for tutorials and assignments,

How to register for the course

Step-1: *First register in GIAN portal, http://www.gian.iitkgp.ac.in/GREGN/, get application Number.*

Step-2: *Fill in the registration from downloaded from http://www.nitgoa.ac.in/gian/proposals.html. Take a print out of it. Get is signed by corresponding authority.*

Step-3: *Draw DD (amount specified in brochure) in favor of* **"Director NIT Goa"** *payable at Goa and send the hard copy of the registration form along with DD to***: Dr. Velavan Kathirvelu, Department of Humanities and Sciences, National Institute of Technology Goa, Farmagudi, Ponda, Goa 403 401**.

Step-4: *Send a scanned copy of registration form and DD to velavan@nitgoa.ac.in as an advance copy.*

The Faculty

Prof. Thomas Prisner

Prof. Thomas Prisner is a senior professor at Institute of Physical and Theoretical Chemistry, Goethe University, Germany. He studied physics at University of Heidelberg, and Max Planck Institute for Medical Research, Germany and received his Ph.D from Physics Department, University Dortmund, Germany. After his post-doctoral research at MIT, USA, he served at the Free University, Berlin between 1990 and 1996. Later, he moved to Goethe University and became professor of Physical Chemistry.

Prof. Thomas Prisner's main research interests revolve around the methodological development of magnetic resonance spectroscopy, especially Electron Paramagnetic Resonance (EPR) and Dynamic Nuclear Polarization (DNP) with the main focus on structural and biological applications. He has made significant impact on the development of high field EPR spectroscopy (eg., He has developed 180 GHz EPR spectrometer, and pulsed EPR instrument for PELDOR spectroscopy in his laboratory with the worldwide highest magnetic field strength and microwave frequency). His current research focus is application of PELDOR spectroscopy on RNA and DNA molecules. In the last few years, he has developed the Dynamic Nuclear Polarization (DNP) spectroscopy at high field (9.2 T, 400 MHz, 260 GHz) with liquid/ solution samples. He has also demonstrated that an unexpected high increase of the NMR polarization is possible at this high field.

Prof. Sankaran Subramanian

Prof. Sankaran Subramanian received his PhD degree at the University of Leicester. Subsequently, he finished his post-doctoral research at University of Leicester and Michigan State University. After returning to India, he was Assistant Professor of Chemistry and became Professor at Department of chemistry, IIT Madras. He was working as Scientist at National Institute of Health, Bethesda between 1998 and 2014.

Prof. Sankaran Subramanian had been part of research group in United States developing time-domain and CW EPR imaging for last 16 years, and published many mile-stone paper in cutting edge area of EPR spectroscopy applied to biology and medicine. Along with his colleagues in USA, he is developing imaging techniques based on electron paramagnetic resonance (EPR) to obtain physiological information such as oxygen or tissue redox stats in pathological situations such as solid tumors or ischemic/hypoxic tissue, quantitatively. He is involved in instrumentation development to detect and image the free radical for medical noninvasive imaging applications using FT EPR, Continuous wave EPR and Overhauser enhanced MRI (OMRI). After his retirement from NIH, Maryland, USA, he has been working as Adjunct Professor, Department of chemistry, IIT Madras

Location:

National Institute of Technology Goa
Farmagudi, Ponda, Goa 403401, India

Course Duration:

Two Week: Jan 29 - Feb 09, 2018

Course Coordinators:

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Course Registration Link:

http://www.gian.iitkgp.ac.in/GREGN
http://www.nitgoa.ac.in/gian/