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Technical Workshops Series - 2014

One-Day Intensive, Hands-on Workshop on Fundamentals of X-ray Diffraction (XRD)

- Organized by SPIRIT, NCL & Venture Center -

Learn	X-ray Diffraction (XRD): Operational principles and essential concepts. Theory of x-ray diffraction. Understanding the instrumentation including hardware configurations and their functions, detectors; Set-up of measurement programs, Set-up of analysis routines, Automation of data collection and data analysis, Pattern treatment and phase identification; Customized reporting; Practical applications of XRD in the Industry. Best practices in acquisition of reliable experimental data and qualitative phase identification using both manual and automated search techniques. Live demonstration of experiments; Simple group practical/hands-on session ; Mini-workshop on data interpretation with real data; Quick update on latest techniques/developments; Workshop is intended to be basic but shall include a few special applications illustrated with real case studies . Learn from faculty with extensive practical experience with industrial applications.
Organized by	<ul style="list-style-type: none">• Venture Center – a Technology Business Incubator
Anchor Faculty	<ul style="list-style-type: none">• Dr. Rahul Banerjee, Scientist, National Chemical Laboratory
VC Organization team	Sujaya Ingale, Edna Joseph, Pratima Jagtap
For whom	<ul style="list-style-type: none">• Industry professionals wishing to expand their skill sets (Industries – Pharma; Environmental; Forensic ; Food, Petrochemicals etc)• Students and staff of polymer/ materials sciences/ engineering/ analytical/physical chemistry wishing to equip themselves for industry jobs• Maximum 20 seats; First-come-first-serve.
When	Saturday, 20th September 2014 , 8:30 am – 5:00 pm
Where	Training Room, Venture Center, 100 NCL Innovation Park, Dr. Homi Bhabha (Pashan) Road, Pune-411008
Contact	Ms. Lipika Biswas Venture Center, 100, NCL Innovation Park, Dr. Homi Bhabha Road, Pune – 411008; Phone: +91-20-25865877 Email: eventsdesk@venturecenter.co.in
Cost	<ul style="list-style-type: none">• Students with valid ID card: Rs. 900/-• Micro and small enterprises/ individuals: Rs. 2,000/-• Medium and large companies/ others: Rs. 4,000/-



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Introduction

X-ray diffraction is a tool for the investigation of the structure of matter. X-rays are scattered by interaction with the electrons of the atoms in the material being investigated. The technique began when von Laue discovered that crystals diffract x-rays in 1912. Since then it has been applied to chemical analysis, stress and strain measurement, the study of phase equilibria, measurement of particle size, as well as crystal structure.

To describe a material uniquely, generally two pieces of information are required: what are the elements present and how are they arranged. The first question is usually answered by chemical analysis techniques and gives the ratio of the elements present in the material. This is a chemical formula often called the chemical stoichiometry. The chemical formula does not describe how the atoms are arranged in space or with respect to each other. X-ray diffraction can be used to tell different crystal structures apart.

The purpose of the X-ray workshop is to provide participants with a fundamental understanding of the theoretical basis as well as the practical applications and implementation of powder diffractometry in today's laboratory. This knowledge and understanding is applicable whether the attendee works in academia, industry, or government laboratory, or whether they are a student, professor, researcher, or analyst.

The workshop will be conducted by an NCL scientist having vast experience working in X-ray diffraction techniques.

Course Outline

- Production and properties of X-rays: continuous and characteristic radiation, absorption, scatter and diffraction
- Production of monochromatic X-radiation: choice of source conditions, use of beta-filters, proportional detectors and pulse height selection, monochromators, use of the Si(Li) and Ge(Li) detectors
- Constituents of the diffraction pattern: expected reflections, Miller indices, unexpected reflections, effect of scatter and fluorescence, factors affecting peak positions and intensities
- The powder diffractometer: optical arrangement, factors affecting instrumental profile widths; choice and function of divergence slits, calibration and alignment, detectors, X-ray optics
- Acquisition of good diffraction data: specimen requirements, preparation techniques, use of standards, and proper operation of powder diffractometers
- Qualitative phase identification: the **Powder Diffraction File™**, quality of reference patterns, the Alphabetical, Hanawalt, and Fink Indexes, automated methods.
- Industrial applications of X-ray powder diffraction

Time	Session title	Lead	Venue
8.30 to 9:00	Registration		Foyer, Learning Center, VC
9:00 to 9:15	Introduction to the course and faculty	Dr. V Premnath	Training room, VC
9:15 to 10:30	Introduction and basic principles of XRD; General terms and essential concepts; Sample preparation; Quick overview of XRD; Typical data recorded	Dr. Rahul Banerjee	Training room, VC
10:30 to 11:00	Tea & Group Photograph		Foyer, Learning Center, VC
11:00 to 11:30	Instrumentation; Types of detectors	Dr. Rahul Banerjee	Training room, VC
11:30 to 12:00	Basic Maintenance of XRD; Trouble shooting processes	Dr. Rahul Banerjee	Training room, VC
12:00 to 13:00	Practical applications of XRD; Method development strategies. Best practices, Few special applications illustrated with real case studies.	Dr. Rahul Banerjee	Training room, VC
13:00 to 13:45	Lunch		Cafeteria , VC
13:45 to 14:00	Introduction to practical session Instructions, Learning points, Making groups, Assigning tasks	Dr. Rahul Banerjee	Training room, VC
14:00 to 16:00	Practical Session Instrument parts <ul style="list-style-type: none"> • Sample preparation • Samples analysis • Data interpretation exercise • Calculations • Discussions to close workshop 	Mr. Tanay Kundu Mr. Bishnu Biswal Dr. Rahul Banerjee	PAML, NCL
16:00 to 16:30	Tea		Foyer, Learning Center, VC
16:30 to 17:00	Closure – Feedback, Certificate distribution	Dr. V Premnath	Training room, VC

Anchor Faculty	
	<p>Dr. Rahul Banerjee Scientist, Polymers & Advanced Materials Laboratory, National Chemical Laboratory,</p> <p>Rahul Banerjee received his PhD degree from University of Hyderabad, Hyderabad in 2006 under the supervision of Prof. Gautam R. Desiraju. After a postdoctoral work in UCLA with Prof. Omar M. Yaghi (2006-2008), he joined CSIR-National Chemical Laboratory, Pune, India in 2008 as a Scientist. His research interests include the study of structural chemistry with the flavor of chemical synthesis to design new materials for hydrogen storage and carbon sequestration. Additionally, his group is also engaged in design and synthesis of lightweight materials for hydrogen storage, carbon capture and proton conduction. Dr. Banerjee is an editorial board member and associate editor of CrystEngComm. He also serves as a co-editor of Acta Crystallographica Section E since 2011.</p>
Other Faculty	<p>Dr V. Premnath is Scientist, Complex Fluids and Polymer Engineering Group at NCL, Pune, Head, NCL Innovations and Director, Venture Center. He specializes in Polymer Science and Engineering.</p> <p>Mr. Tanay Kundu is currently a senior research fellow at National Chemical Laboratory, Pune, pursuing PhD under the guidance of Dr. Rahul Banerjee. He has contributed to more than 15 scientific articles with reviews and patents. His research interest includes synthesis of amino acid and peptide based molecules, their metal mediated assemblies and properties. His instrumental expertises are on single crystal XRD and powder XRD.</p> <p>Mr. Bishnu Biswal is a research fellow at National Chemical Laboratory, Pune, pursuing his PhD under the guidance of Dr. Rahul Banerjee. His research interest includes Crystalline porous nanomaterials: Synthesis, Characterization and Applications.</p> <p>Mrs. Sujaya Ingale and Ms. Edna Joseph shall organize and assist in lab demos.</p>



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Course includes

- Course notes (hard copy) including slides, case studies, application notes
- Lab demo
- Access to restricted website with online compilation of resources for XRD
- One-on-one feedback on data interpretation exercise
- Certificate of Participation issued by Venture Center
- Course includes tea and lunch at Venture Center cafeteria

About the organizers

About Venture Center

Entrepreneurship Development Center (Venture Center) – a CSIR initiative – is a Section 25 company hosted by the National Chemical Laboratory, Pune. Venture Center strives to nucleate and nurture technology and knowledge-based enterprises by leveraging the scientific and engineering competencies of the institutions in the Pune region in India. The Venture Center is a technology business incubator supported by the Department of Science & Technology's National Science & Technology Entrepreneurship Development Board (DST-NSTEDB). Venture Center's focuses on technology enterprises offering products and services exploiting scientific expertise in the areas of materials, chemicals and biological sciences & engineering. For more information, visit <http://www.venturecenter.co.in/>

About SPIRIT at National Chemical Laboratory, Pune

SPIRIT stands for Sustainable Polymer Industry through Research, Innovation and Training. SPIRIT is a Centre of Excellence in Polymers sponsored by the Department of Chemicals and Petrochemicals, Government of India, at the CSIR-National Chemical Laboratory, Pune. More information: <http://www.pamlab.org/spirit/>