

# Global Initiative of Academic Networks(GIAN)

MHRD, Govt. of India

Department of Physics, Guru Nanak Dev University,  
Amritsar-143005, Punjab, India

## Local-and Nano-Structure Determination of Complex Nanostructured Materials using Scattering Methods

Aug.29-Sep.2,2017

### Overview

Modern materials, under study for next generation technologies such as energy conversion and storage, environmental remediation and health, are highly complex, often heterogeneous and nano-structured. A full understanding of the structure requires us to go beyond crystallography and to study the local structure, which is a major experimental challenge. There are recently emerging powerful experimental and theoretical developments that are bringing us close to being able to address this problem, ranging from powder to single-particle methods. This course will give an overview of the total scattering and atomic pair distribution function (PDF) analysis methods for studying structure at the nanoscale. Students will learn about the cutting edge applications of these methods, but also will learn the basic theory behind them, and receive practical hands-on instruction in the computational methods used to apply them.

### Objectives

Upon completion of the course, participants will:

1. Be familiar with the power and application of total scattering and PDF methods to study nanostructure in materials.
2. Understand the basic scattering theory that underpins this field.
3. Be very familiar with basic usage of software programs used to carry out Total Scattering and PDF analysis data reduction and modeling.
4. Have an appreciation of the advanced techniques that are emerging for this activity and the scientific problems that they are appropriate for.

### Course Outline

Date	Lecture & Tutorial Topics
29-08-2017	<ol style="list-style-type: none"><li>1. Scientific overview. The nanostructure inverse problem. Review of successes and challenges. Examples of application and importance of nanostructure determination</li><li>2. Introduction to basic pedagogy of the course. Basic principles of x-ray and neutron scattering: sources, measurements, detectors, geometries</li><li>3. Scattering theory basics</li></ol>
30-08-2017	<ol style="list-style-type: none"><li>1. Scattering theory advanced, leading to the Debye Scattering equation and PDF equations</li><li>2. Obtaining F(Q) and the PDF from scattering data: practical and examples. Use of xPDFsuite and PDFgetX3</li></ol>
31-08-2017	<ol style="list-style-type: none"><li>1. Obtaining the PDF from models: practical using PDFgui</li></ol>
01-09-2017	<ol style="list-style-type: none"><li>2. Advanced PDFgui usage: practical</li></ol>
02-09-2017	<ol style="list-style-type: none"><li>1. Beyond Small Box modeling: Use of Diffpy-CMI</li><li>2. Cutting edge research studies using total scattering and PDF methods</li></ol>
Intended audience for this course	<ol style="list-style-type: none"><li>1. Students at all levels (B.Sc./MSc/MTech/PhD) of Physics and Chemistry, including Material Science and Nanoscience and Nanotechnology etc.</li><li>2. Faculty from academic and technical institutions.</li><li>3. Researchers/Post-docs/ Research associates from Universities, Govt. and R&amp;D laboratories.</li></ol>
Fees	Participants from abroad: US \$ 200 Industry/ Research Organizations: Rs. 5000/- Academic Institutions: BSc Students: Rs. 500/- MSc Students: Rs. 1000/- PhD Students: Rs. 1500/- Faculty members: Rs. 2000/-

The course will consist of lectures and hands-on computer exercises. Homework assignments will also be assigned for students to work through outside of class.



### Faculty:

**Professor Simon Billinge:** Prof. Billinge has more than 20 year experience developing and applying techniques to study local structure in materials using x-ray, neutron and electron diffraction. He earned his Ph.D in Materials Science and Engineering from University of Pennsylvania in 1992. After 13 years as a faculty member at Michigan State University, in 2008 he took up his current position as Professor of Materials Science and Applied Physics and Applied Mathematics at Columbia University and Physicist at Brookhaven National Laboratory, USA. Prof. Billinge has published more than 200 papers in scholarly journals. He is a fellow of the American Physical Society and the Neutron Scattering Society of America, a former Fulbright and Sloane fellow and has earned a number of awards including being honored in 2011 for contributions to the USA as an immigrant by the Carnegie Corporation of New York, the 2010 J. D. Hanawalt Award of the International Center for Diffraction Data, University Distinguished Faculty award at Michigan State, the Thomas H. Osgood Undergraduate Teaching Award. He is Section Editor of Acta Crystallographica Section A: Advances and Foundations. He regularly chairs and participates in reviews of major facilities and federally funded programs.

### Course-Co-ordinator:



**Professor Atul Khanna:** Prof. Khanna has more than 20 year experience in studying structure-property co-relations in oxide glasses and thin films using X-ray and neutron diffraction, Solid State Nuclear Magnetic Resonance and Raman spectroscopic techniques, and has published 65 papers in international journals. Prof. Khanna got his MSc degree in Physics from the Indian Institute of Technology, Delhi in 1991 and worked as a Scientific Officer in the Technical Physics and Prototype Engineering Division of Bhabha Atomic Research Centre, Mumbai during the years: 1991-1993. He earned his Ph.D in Applied Physics from Guru Nanak Dev University, Amritsar in 1998 and carried out post-doctoral research at the University of Arkansas, Fayetteville, USA during 2004-2006. He has been honored with Young Scientist Award in Physics by Indian Science Congress Association, Kolkatta for the year 2000-2001 and the Vocational Excellence Award and the Nation Builder Award by Rotary International, District 3070 in 2015. He is working on several projects funded by national agencies such as UGC, DAE, IUAC and CSIR.

Contact:

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For more details and online registration please visit:

[www.gian.iitkgp.ac.in](http://www.gian.iitkgp.ac.in)

**REGISTRATION CUM ACCOMODATION REQUEST FORM**

**Local-and Nano-Structure Determination of Complex Nanostructured Materials using Scattering Methods**

**Aug. 29- Sept. 2, 2017**

**Department of Physics, Guru Nanak Dev University  
Amritsar-143005, Punjab (India)**

**Designation/ Professional Title:.....**

**Name (Block Letters): .....M/F: ..... ..**

**Organization: .....**

**Address:**

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**Tel.:.....Mobile.....**

**E-mail: .....**

**Accommodation Required (Yes/ No): .....**

**The Registration fee of Rupees .....has been paid via Demand Draft No..... in favour of The Registrar, Guru Nanak Dev University, Amritsar-143005. Through online/offline banking bearing Transaction No. .... to Punjab & Sind Bank, Guru Nanak Dev University Campus, Guru Nanak Dev University, Amritsar.**

**Demand Draft/ Fee Receipt have been enclosed herewith.**

**Date:**

**Signature**