

# Structure solution, refinement and interpretation of difficult inorganic structures by Jana2006

## Overview

Jana2006 is a crystallographic program for solution, refinement and interpretation of difficult structures, especially modulated structure. It calculates structures from powder as well as single crystal data measured with X-ray or neutron diffraction. The structure solution can be performed using in built charge flipping algorithm or by calling an external direct methods program. The program can handle multiphase structures and twins structures. The program has powerful transformation tools for symmetry (group-subgroup relations) relations. Wide scale of constrains and restrains are available including a powerful rigid body approach and possibility to define a local symmetry affecting only part of the structure. It can also handle magnetic structures. The recent development of Jana2006 deals with structure from electron diffraction.

The primary objectives of the course are as follows: familiarise the participants to the scope of Jana2006, solution of simple 3d inorganic structures together with twinning and handling twinning by Jana2006, presenting an overview of disordered crystal structures, rigid body refinements and application of local symmetry, providing hands on experience to crystallographic problems and their solutions, through case studies.

Course participants will learn these topics through lectures and case studies. Assignments will be shared to stimulate research motivation of participants.

<b>Modules</b>	<b>A: Structure solution, refinement and interpretation of difficult inorganic structures by Jana2006 : Feb 18, 2019 - Feb 22, 2019</b> <b>Number of participants for the course will be limited to fifty.</b>
<b>You Should Attend If...</b>	You are a student (BTech/MSc/MTech/PhD) or faculty from academic institutions and technical institutions willing to have/improve their knowledge of structure determination of inorganic structure by Jana2006  You are a metallurgical and/or materials engineer or a research scientist (Chemistry, Physics, and Materials science) interested in understanding the .knowledge of structure solution and refinement by Jana2006.
<b>Fees</b>	The participation fees for taking the course is as follows: <b>Participants from abroad : US \$300</b> <b>Industry/ Research Organizations: Rs. 10,000/-</b> <b>Teachers/Faculty Members: Rs. 5,000/-</b> <b>Students: Rs.1,500/-</b> The above fee includes all instructional materials, materials for tutorials and assignments, 24 hr free internet facility. The participants will be provided with accommodation on payment basis.

## The Faculty



**Dr. Lukas Palatinus** is a senior researcher at the Department of Structure Analysis in Institute of Physics of the CAS, Czech Republic. He has been mainly focusing on the methodology and software development in the field of structure solution and refinement. His research topics include especially incommensurately modulated structures, structure solution by charge flipping and structure solution from electron diffraction data and dynamical structure refinement.



**Dr. Partha Pratim Jana** is an Assistant Professor at Indian Institute of Technology Kharagpur. His research interest revolves around synthesis, crystal structures, physical properties, and theoretical investigation of intermetallic phases.

## Course Co-ordinator

**Prof. Partha Pratim Jana**  
Department of Chemistry  
IIT Kharagpur, India-721302  
email: [ppj@chem.iitkgp.ac.in](mailto:ppj@chem.iitkgp.ac.in)  
Office: 03222-283330  
E-mail: [ppj@chem.iitkgp.ac.in](mailto:ppj@chem.iitkgp.ac.in)  
<http://www.gjan.iitkgp.ac.in/GREGN>