



University of Puerto Rico – Mayagüez Campus

Department of Chemical Engineering

PO Box 9046

Mayagüez, PR 00681-9046

Phone: (787) 832-4040 – Exts. 2568,2587

Fax: (787) 265-3818

Website: <http://atomo.uprm.edu/inqu/>

## **Syllabus & Instructor Information Sheet Form**

### **A. COURSE SYLLABUS**

#### **1. General Information:**

Course Number: InQu 6038

Course Title: X-ray Characterization of Materials

Credit-Hours: 3

#### **2. Course Description:**

Study of the use of X-rays for the characterization of materials. Study of the fundamentals of space groups and the theory, applications, and experimental considerations of diverse techniques such as: single crystal and powder X-ray diffraction, small angle scattering, amorphous scattering, X-ray fluorescence, and X-ray absorption. Discussion of the relation between these techniques and other materials characterization techniques.

#### **3. Pre-requisites:**

Graduate students and senior undergraduate students in a science or engineering major with permission of the director.

#### **4. Co-requisites:**

None

#### **5. Textbook, Supplies and Other Resources:**

• Textbook: \* V. Pecharsky, P. Zavalij, (2005). "Fundamentals of Powder Diffraction and Structural Characterization of Materials", 1st ed.: Springer.

#### **Reference Materials:**

- \*\* A.C. Thompson, D. Vaughan, (2001) "X-ray Data Booklet" 2<sup>nd</sup> Ed.: Lawrence Berkley National Laboratory
- B.E. Warren (1990) "X-ray Diffraction": Dover Publications There is no newer version.
- D.C. Koningsberger, R. Prins, Editors,(1988) "X-ray Absorption: Principles, Applications, Techniques of EXAFS, SEXAFS, and XANES": John Wiley and Sons. There is no newer version.
- \* E. Prince, editor, (2004). "International tables for crystallography. Vol. C, mathematical, physical and chemical tables": Wiley-VCH.
- \* Y.Waseda, (2002). "Anomalous X-ray scattering for materials characterization : atomic-scale structure determination": Springer.
- "Crystallography Reports" and "Crystallography Reviews"- Available through the UPRM Library online database
- \* These books are available in the library.

\*\* This booklet is available free of charge from the Lawrence Berkeley National Laboratory. Can be obtained through <http://xdb.lbl.gov/>

#### **6. Purpose:**

#### **7. Course Goals:**

**By the end of the course students should be able to:**

- Identify crystal unit cells and basic symmetry operations in crystalline materials.
- Analyze X-ray diffraction patterns to obtain structural information.
- Propose X-ray techniques needed to obtain desired information.
- Identify the interaction of X-rays with matter in the different techniques.
- Identify experimental considerations for each technique and application studied.
- Review and discuss current literature on X-ray characterization.

#### **8. Requirements:**

All students are expected to bring a solid basic Mathematical and Physics background.

## **9. Laboratory/Field Work (If applicable):**

No laboratory or field work in this course.

## **10. Department/Campus Policies:**

- 10a. Class attendance:** Class attendance is compulsory. The University of Puerto Rico, Mayagüez Campus, reserves the right to deal at any time with individual cases of non-attendance. Professors are expected to record the absences of their students. Frequent absences affect the final grade, and may even result in total loss of credits. Arranging to make up work missed because of legitimate class absence is the responsibility of the student. (Bulletin of Information Undergraduate Studies, pp 39 1995-96)
- 10b. Absence from examinations:** Students are required to attend all examinations. If a student is absent from an examination for a justifiable reason acceptable to the professor, he or she will be given a special examination. Otherwise, he or she will receive a grade of zero of "F" in the examination missed. (Bulletin of Information Undergraduate Studies, pp 39, 1995-96)
- 10c. Final examinations:** Final written examinations must be given in all courses unless, in the judgment of the Dean, the nature of the subject makes it impracticable. Final examinations scheduled by arrangements must be given during the examination period prescribed in the Academic Calendar, including Saturdays. (see Bulletin of Information Undergraduate Studies, pp 39, 1995-96).
- 10d. Partial withdrawals:** A student may withdraw from individual courses at any time during the term, but before the deadline established in the University Academic Calendar. (see Bulletin of Information Undergraduate Studies, pp 37, 1995-96).
- 10e. Complete withdrawals:** A student may completely withdraw from the University of Puerto Rico, Mayagüez Campus, at any time up to the last day of classes. (see Bulletin of Information Undergraduate Studies, pp 37, 1995-96).
- 10f. Disabilities:** All the reasonable accommodations according to the Americans with Disability Act (ADA) Law will be coordinated with the Dean of Students and in accordance with the particular needs of the student. After identifying himself (herself) with the instructor and the institution, students with disabilities will receive reasonable academic accommodation in their courses and evaluations. For more information please contact Services to Students with Disabilities in the Students Dean Office, (Q-019), 787-265-3862 either 787-832-4040 x 3250 or 3258.
- 10g. Ethics:** Any academic fraud is subject to the disciplinary sanctions described in article 14 and 16 of the revised General Student Bylaws of the University of Puerto Rico contained in Certification 018-1997-98 of the Board of Trustees. The professor will follow the norms established in articles 1-5 of the Bylaws.

### **10 h. Student Attendance and Behavior**

- *Class attendance is compulsory.*
- *Students are expected to dress properly for class.*
- *Smoking, eating, or drinking in the classroom will not be allowed.*
- *Bringing cell phones and beepers to class is not recommended. If you must do so, make sure that they are turned off when you enter the classroom.*
- *Leaving the classroom in the middle of class is disruptive to both the teacher and other students. If you must leave before the scheduled end of class, make sure that it is for a justifiable reason.*
- *Many of the class materials will be distributed electronically through your campus email address. Please make sure you access your email regularly.*

## **11. Course Outline and Schedule:**



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## B. INSTRUCTOR INFORMATION SHEET

### 1. General Information:

Instructor's Name: **Dr. María M. Martínez Iñesta**  
Title: Assistant Professor  
Office: IQ-205-I  
Phone: 787-832-4040 ext. 3605

Class Meeting Hours: Mo-We: 9:00 – 10:20 am  
Office Hours: Mo 10:30-12:00 pm  
E-mail: [mariam.martinez@upr.edu](mailto:mariam.martinez@upr.edu)

### 2. Course Description:

Study of the use of X-rays for the characterization of materials. Study of the fundamentals of space groups and the theory, applications, and experimental considerations of diverse techniques such as: single crystal and powder X-ray diffraction, small angle scattering, amorphous scattering, X-ray fluorescence, and X-ray absorption. Discussion of the relation between these techniques and other materials characterization techniques.

### 3. Purpose:

### 4. Course Goals:

By the end of the course students will be able to:

- Identify crystal unit cells and basic symmetry operations in crystalline materials.
- Analyze X-ray diffraction patterns to obtain structural information.
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- Identify the interaction of X-rays with matter in the different techniques.
- Identify experimental considerations for each technique and application studied.
- Review and discuss current literature on X-ray characterization.

### 5. Instructional Strategy:

A combination of lectures with special homeworks and project.

### 6. Evaluation/Grade Reporting:

1 partial examination	100 points
Quizzes/Homework	100
Project	100
1 Final Exam	<u>100</u>
	400 points

### 7. Deadlines for Assignments:

Assignments should be turned in on scheduled dates. It is the instructor's prerogative whether to accept and/or penalize assignments that are turned in past the deadline.

### 8. Student Assistance (If applicable): Refer to Section A, item 10

### 9. Attendance and Behavior: Refer to Section A, item 10

The instructor reserves the right to offer a make-up exam to any student that fails to take an exam at the scheduled date. Make-up exams are limited to one per semester. The student must provide documented evidence of the reasons why he or she was absent to the exam in question, and these reasons will only be considered if they represent strictly an emergency. The student has a maximum of **one week** after the scheduled exam to notify an absence to the professor and provide the corresponding documentation.

### 10. Instructor Responsibilities (If applicable): Refer to Institution Manual

## 11. Course Outline:

X-ray production and interaction with matter

X-ray Scattering and Diffraction Basics

Symmetry Operations

Single Crystal X-ray Diffraction: Experimental Setup and Applications

Powder X-ray Diffraction: Experimental Setup and Applications

Small Angle X-ray Scattering: Experimental Setup and Applications


Amorphous X-ray Scattering Methods: Experimental Setup and Applications

Comparison of X-ray and Neutron and Electron Scattering Methods

X-ray Absorption Basics; EXAFS, SEXAFS and XANES: Experimental Setup and Applications

X-ray Fluorescence: Experimental Setup and Applications

Submitted by:



María M. Martínez-Iñesta, *Ph.D.*

Assistant Professor

Approved by:



David Suleiman, *Ph.D.*

Director