Q.I. 2007

(9)

FACULTAD DE CIENCIAS EXACTAS Y NATURALES
UNIVERSIDAD DE BUENOS AIRES

Departamento de Quimica Inorgánica, Analítica y Química Física

Ciudad Autónoma de Buenos Aires, 25 de octubre de 2007

Señor Secretario/a Académico/a
de la Facultad de Ciencias
Exactas y Naturales
S/D

Tengo el agrado de dirigirme al señor Secretario Académico a efectos de comunicarle el desarrollo del curso de post-grado y/o doctorado que se dictará en este Departamento durante el ...2do..... cuatrimestre de 2007.

1- Denominación del Curso: ***X-ray photoelectron spectroscopy // Espectroscopia fotoelectrónica de rayos X (XPS)***

1a- Carácter del Curso:
(para Doctorado: ampliar conocimientos, actualización, extensión profesional)

2- Fecha de iniciación: 12 al 16 de noviembre de 2007.

3- A dictarse en: **Depto. de Qca. Inorgánica, Analítica y Qca. Física**

4- Responsable (s): Dra. Maria Afonso dos Santos e Ing. Michel Genet
(si no revistan en la Facultad, adjuntar nota solicitando la autorización pertinente, la que comprenderá el dictado del Curso y la firma de las Actas de Examen pertinentes).
(Además agregar curriculum vitae resumido, debidamente firmado por el Director de Departamento o por el interesado).

5- Cantidad de horas semanales: 30 hs. totales

5a- Nro. de horas semanales de clases teóricas: 15 hs.

5b- Nro. de horas semanales de clases de problemas:

5c- Nro. de horas semanales de trabajos prácticos: 15 hs.

6- Condiciones de ingreso: Tener título de grado y/o estudiante avanzado con las materias de fisicoquímica aprobadas o equivalentes.

7- Nro. de alumnos (mínimo y máximo):

8- Forma de evaluación: Exposición de un seminario y examen final.

8a- Certificado de aprobación: SI-~~NO~~ (tachar lo que no corresponda)

9- Puntaje propuesto de acuerdo con el carácter del curso: 1,5 (uno y medio)

10- Nro. de código: nuevo

11- Se acompaña despacho de la Sub-Comisión Departamental con V°.B°. del Director de Departamento.

12- Se propone un arancel de .150.....módulos, teniendo en cuenta como base el valor de $ .....(el que rija en ese momento).

Dr. FERNANDO V. MOLINA
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DEPTO. QUÍMICA INORGÁNICA
ANALÍTICA Y QUÍMICA FÍSICA

D. ESTRIN

AVE COMISION DE DOCTORADO

FACULTAD DE CIENCIAS EXACTAS Y NATURALES
UNIVERSIDAD DE BUENOS AIRES

Departamento de Quimica Inorgánica, Analítica y Química Física

CARRERA: Doctorado en Ciencias Químicas

CUATRIMESTRE: Segundo **AÑO:** 2007

CODIGO DE CARRERA: 51

MATERIA: ***X-ray photoelectron spectroscopy*** **CODIGO:** nuevo

PUNTAJE: 1,5 (uno y medio)

PLAN DE ESTUDIO: --------

CARÁCTER DE LA MATERIA: --------

DURACIÓN: 1 semana.

HORAS DE CLASE SEMANAL:

- **Teóricas:** 15 hs.
- **Prácticas:** 15 hs.

TOTAL: 30 hs.

CARGA HORARIA TOTAL: 30 hs.

ASIGNATURAS CORRELATIVAS: Tener título de grado y/o estudiante avanzado con las materias de físicoquímica aprobadas o equivalentes.

FORMA DE EVALUACIÓN: Exposición de un seminario y examen final.

PROGRAMA ANALÍTICO:

Abstract

There is a growing interest in characterizing the surface of materials: atomic and molecular composition, properties, organisation of their constituents in space. This course will be focused on X-ray photoelectron spectroscopy (XPS - ESCA). This technique, developed in the 1960's, is applicable to all kinds of materials and in all research areas. The number of papers, in which XPS is involved, continues to progress from year to year.

A sample, introduced in an ultra high vacuum chamber, is irradiated with an X-ray beam. The kinetic energy of emitted electrons of all elements (except H and He) present at the surface (analyzed depth between 1 and 10 nm) is measured with a precision of about 0.2 eV. Shape and position of peaks

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depend on the chemical state of the element (the so-called "chemical shift" effect). Area of peaks used in combination with elemental sensitivity factors allow to calculate elements concentrations with a detection limit of a few tenths of mole percent. A detailed analysis of certain well-resolved peaks allows quantifying the chemical functions present at the surface. On most recent systems the lateral resolution is about 15 µm and 5 µm in spectroscopic and imaging modes, respectively.

Data interpretation will be illustrated by some recent results obtained in very different areas: from steel corrosion to bio materials, from minerals to food products.

All exercises will start on raw data with the objective to perform more and more sophisticated interpretation by successive steps corresponding to the different parts of the course. Some data treatment will be performed with the help of dedicated software.

CONTENT

Part 1. Principles

- Introduction
- XPS at UCL
- Historic timeline
- Photoelectric effect
- Surface sensitivity
- Brief survey of some other surface characterization techniques (ToF-SIMS, AFM, static and dynamic contact angle measurement)

Part 2. Instrumentation

- Summary of Part 1
- Work "in front" of a virtual XPS system:
  Chambers, vacuum, analyser and lenses, detector, charge stabilisation, accessories, specimen preparation, using synchrotron radiation.

Part 3. Basic methodology and information

- Summary of Part 2
- Overview of an XPS spectrum: energy referencing, charging effect, background, main peaks and satellites, peak width, chemical shift.
- Bases of quantification: from general to simplified equations, common practice.
- Angle resolved XPS.

Exercise 1

a) Peaks attributions on survey scans recorded on very different samples with both Al and Mg anodes. Tables with lines positions will be provided.
b) Students will be asked to bring or imagine 4 or 5 series of very different samples. A discussion will be initiated on:
   - The interest or not of performing an XPS analysis on these samples
   - How to prepare samples

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- How to select a coherent series of samples to obtain as reliable results as possible
- How to control surface charging, what peaks to record …

Part 4. Data interpretation

- Summary of Part 3
- Background subtraction
- Quantification
- Peak decomposition
- Reference data (polymers, biochemical and inorganic compounds)
- Data interpretation through simulation
- Analytical performances
- How a critical examination of peak shape can contribute to a reliable XPS analysis (decomposing peaks, reconstructing peaks, overlapping peaks, comparing peaks areas)
- From functional analysis toward molecular composition, application to microbial cells
- General conclusions

Exercise 2

- Quantification from survey scan and individual peaks
- Peaks decomposition
- Interpretation of chemical shifts

Case study 1.

"Nature, quantification and destiny of organic contamination on surfaces studied by XPS."

Rock around the carbon:

- A binding energy reference
- A constituent of the organic contamination. Including a detailed study of organic contamination on metal and oxide surfaces
- A key element to characterize surfaces.

Exercise 3

A series of spectra recorded on stainless steel immersed in synthetic fresh water, simulating river water, will be provided. A detailed study of carbon, oxygen and metal peaks will be performed. Background subtraction on metal peaks will be discussed as well as pitfalls of quantification.

Case study 2.

"Advantages and limitations of Low Temperature XPS: application to the oil-water interface."

Exercise 4

Correlations between peaks components and tentative interpretation

A series of spectra recorded on different samples will be provided: pure materials, surface modified materials, materials associated with another constituent. Groups of tudents will be asked to identify materials from spectra, and to comment their choice.

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Exercise 5

Four series of very recently recorded raw XPS spectra will be provided to groups of students. Each series will include a pure clay mineral and the same mineral with a pesticide adsorbed at different pH. The main goal will be to perform the different steps of the data treatment and to discuss results with respect to the research objectives of Prof Maria Dos Santos Afonso.

Bibliography

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Ing. Michel Genet

Dra. Maria Afonso dos Santos

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