THEMATIC SCHOOL

Catalyst Characterization and Modeling

1) Transmission Electron Microscopy for Catalysis

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2) XPS Spectroscopy
Principle and fundamentals of the technique- Application examples

Professor Delphine FLAHAUT
Université de Pau et des Pays de l'Adour, Pau

3) Characterization of Organometallic Nanoparticles: Synergy between Theory and Experiments

Professor Romuald POTEAU

Université Paul Sabatier, Toulouse

1) Transmission Electron Microscopy for Catalysis

I - The Transmission Electron Microscope

I.1 Description of the machine
I.2 TEM vs STEM
I.3 Aberrations and corrections

II - Image formation for atomic observations

II.1 TEM mode : HRTEM
II.2 STEM mode : STEM-HAADF

III - Chemical analysis in a TEM

III.1 EELS : electron energy loss spectrocopy
III.2 EDS : erngy dispersive x-ray spectroscopy

IV - In operando experiments

IV.1 Liquid cell : study of particle formation inside the TEM
IV.2 Gaz cell : behaviour of the particles under O_2, H_2 ..
IV.3 Dynamical TEM : synthesis of particles thanks to laser beam impulsion

2) XPS Spectroscopy
Principle and fundamentals of the technique- Application examples

I. XPS history

I.1. Photoelectric effect
I.2. High resolution X-ray photoemission
I.3. ESCA- Electron Spectroscopy for Chemical Analysis
I.4. Development of X-ray photoelectron spectroscopy

II. XPS principle

II.1. Surface analyses techniques
II.2. Photoelectronic spectroscopies
II.3. XPS – A surface sensitive technique?
II.4. Analysis capabilities
II.5. XPS photoionization process
II.6. Evaluation of the binding energy

III. XPS spectra

III.1. XPS wide scan data
III.2. XPS core level spectrum
III.3. Peak intensity
III.4. XPS background
III.5. Line shape
III.6. Valence level

IV. XPS instrumentation

IV.1. Spectrometer architecture
IV.2. Binding energy measurement
IV.3. Sample preparation
IV.4. Charge effects: insulating/conductive materials

V. XPS for chemical investigation

V.1. Chemical shift for chemical state analysis

V.2. Secondary structures

VI. XPS quantitative analysis

VI.1. Peak Intensity
VI.2. Thickness determination of a homogeneous overlayer/layer
VI.3. XPS compositional depth profiling

VII. Perform an XPS analysis

VII.1. Data acquisition
VII.2. Decomposition procedure
VII.3. Informations from XPS peaks

VIII. XPS technique: applications

VIII.1. Study of the surface reactivity by coupling gas probes adsorption/XPS
VIII.2. Interfacial layers: valence spectra calculation

3) Characterization of Organometallic Nanoparticles: Synergy between Theory and Experiments

I - Structure of the metal core: WAXS experiments and reverse Monte-Carlo methods

II - *in silico* titration of surface or subsurface species by *ab initio* thermodynamics methods

III - Coordination of surface species: assignment of NMR and IR data by DFT

IV - Relation between the electronic structure of metal NPs and their catalytic properties.

Prerequisites: basic knowledge in MO theory, thermodynamics, spectroscopy