

European FP7 ITN contract "LASSIE"
LABORATORY ASTROCHEMICAL SURFACE SCIENCE IN EUROPE
Grant Agreement #238258

LASSIE 2013 Summer School*
"State-of-the-art Astrochemistry"
Paris Observatory
77 Av. Denfert-Rochereau, Paris 75014
4th to 6th September 2013

Participants reception: Tuesday 3rd, from 6 to 8 PM at the Paris Observatory

Registration is free and open now with deadline August 1st 2013,
but the sooner the better as the participation is limited up to 50 participants.

This Summer School takes place just before the IVC19 Conference (including Astrosurf 2013)

Organized by Prof. JL Lemaire

Local ESRs: L. Gavilan -summer school website-, I. Oueslati, R. Tchalala, M. Minissale

- * **Attendance of LASSIE ESRs and ERs is part of their duties.**
(a training certificate will be delivered)
- * **Past LASSIE members are invited to participate.**
- * **Non-LASSIE participants are also welcome.**
- * **NB: 50 participants maximum**

General lectures are designed both for theoreticians and experimentalists in a common room while specialized lectures will take place as parallel sessions.

Lectures on Theory

D. Billy (ISMO, Orsay, Fr)
S. Bromley (IQTUB, Barcelona, Sp)
Y. Ellinger (LCT, UPMC Paris, Fr)
A. Kara (UCF, Orlando, USA)
B. Kerkeni (LPMC Tunis, Tu & UPMC Paris, Fr)
M. Watkins (UCL, London, UK)

4 general lectures and 8 specialized ones

DB (1 gen + 1 spec lectures)

Elementary processes on surfaces: adsorption and molecular formation on dust grains of the interstellar medium

Abstraction Reactions: Eley-Rideal, Langmuir-Hinshelwood Mechanisms for Heterogeneous Catalysis

Focus on hydrogen interaction with carbonaceous dust grains (graphenic surfaces, PAH)

adsorption, desorption processes

molecular formation mechanisms

electronic structure determination

dynamics (reaction probability, energy release in the substrate, internal and kinetic energy of the nascent molecules)

SB (1 gen + 1 spec lectures)

General lectures On modelling:

- Structure of nanoscale dust precursors

- Dust nucleation pathways from the bottom-up

YE (1 gen + 1 spec lectures)

- *General lecture*: Molecule surface interactions: from adsorption to chemical reactions.

- *Specialized lecture*: Molecule surface interactions: from adsorption to chemical reactions.

AK (1 gen + 2 spec lectures)

- Electronic structures calculations of molecules adsorbed on metallic surfaces: role of steps and kinks

- Simulations of temporal and spatial evolution: Self-Learning Kinetic Monte Carlo (application to the treatment of the evolution of dust grains after inter-grains collisions)

- A real space method to calculate the vibrational dynamics and thermodynamics of low dimensional systems and systems with no long-range order

BK (1 gen + 1 spec lectures)

- Quantum Dynamics Study of the Langmuir-Hinshelwood H+H Recombination Mechanism and H₂ Formation on a Graphene Model Surface.

- Energetic Pathways Towards H₂ Formation on an Ultrasmall Silicate Nanocluster Dust Precursor

MW (2 spec lectures)

- Introducing CP2K, a "Swiss army knife" for atomistic simulation.

- CP2K hands on - molecules, surfaces and crystals.

Lectures on Experiment

C. Jäger (AIU, Jena, D)
H. Oughaddou (ISMO, Orsay, Fr)
F. Salama (NASA-AMES, USA)
G. Vidali (Syracuse, USA)
H. Zacharias (WWU, Münster, D)
N. N. (Europe)

4 general lectures and 8 specialized ones

CG (2 Lectures)

- Overview of laboratory experiments on dust condensation and processing, and on spectral properties and spectroscopic tools

HO (1 Lecture)

- Analytical tools for chemical characterization of Nano-materials. Interaction of atoms with graphenic and silicenic structured surfaces.

N. N. (1 lecture)

- *General lecture*: Physical and chemical characterization of surfaces at different scales

Introduction to surface analysis, Laboratory conventional techniques, Synchrotron based techniques (X-ray microscopy, Photoemission X, Absorption X, X-ray diffraction and scattering)

FS (2 Lectures)

- Lab. studies of Diffuse Interstellar molecules and comparison to astronomical observations - Tracing PAHs in the diffuse ISM.

- Lab. studies of the formation of carbon molecules and grains in the outflow of carbon stars - Linking the Gas and Solid Phases of Cosmic Dust.

GV (3 Lectures)

- *General lecture*: Formation of molecules in space; survey of the molecular universe; role of molecules in the ISM; most significant observational and theoretical results

- Specialized lectures: Experiments of formation of molecular hydrogen, water and other molecules on grain analogues; comparison with observations, theory and computer simulations of the chemical evolution of space environments (Part I and II)

HZ (3 Lectures)

- *General lecture*: Basics of surface science and surface reaction dynamics

- *General lecture*: Light sources in the UV, VUV and XUV - lamps, synchrotrons, lasers, High Harmonic generation, Free electron lasers

- Specialized lectures: Dynamics of hydrogen reactions" (thermal at high T or light-induced on metals and graphite); Electronic properties of graphene" (static and dynamic); Thermal desorption spectroscopy" (in general and applied to astrochemically relevant surfaces and molecules)

Tutorial on software

3 specialized lectures

- * BK -- A hands-on tutorial using Gaussian:
 - Simulation of Nanoclusters with the Gaussian Package and visualization
 - Physisorption, Chemisorption, Recombination, Desorption and Reaction Paths
- * MW -- A hands-on tutorial using CP2K : Large scale DFT simulations of water ice surfaces.
- * SB -- A hands-on tutorial using VASP: Surface energies and surface-adsorbate interactions

Tutorial on instrumentation

3 specialized lectures

- * BRUKER (S. Lesko): Some examples of scientific results obtained with the BRUKER instrumentation (AFM)
- * BRUKER (J.C. Boulou): Some examples of scientific results obtained with the BRUKER instrumentation (IR spectroscopy)
- * HIDEN ANALYTICAL (Y. Gonzalvo): Some examples of scientific results obtained with the HIDEN instrumentation

About communicating in science

Chris Sterken (Vrije Universiteit Brussel, Be)

3 general lectures

- Writing a Scientific Paper I. The writing process

Based on my direct personal experience as an author, referee, editor, and PhD thesis supervisor, I present some advice and guidelines on writing scientific papers. This lecture copes with the preparation of manuscripts, with the handling of copyrights and permissions to reproduce, with communicating with editors and referees, and with avoiding common errors.

- Writing a Scientific Paper II. Communication by Graphics

This talk discusses facets of visual communication by way of images, graphs, diagrams and tabular material. Design types and elements of graphical images are discussed, along with advice on how to create graphs, and on how to read graphical illustrations. This is done in astronomical context, using case studies and examples of good and bad graphics. Special attention is given to the verity of graphical content, and to misrepresentations and errors in graphics and associated basic statistics. Dangers of dot joining and curve fitting are discussed, with emphasis on the perception of linearity, the issue of nonsense correlations, and the handling of outliers.

- Writing a Scientific Paper III. Ethical Aspects

The main theme of this lecture is truthful communication of scientific results, but also correct measurement of the work of scientists. The following bibliometric parameters are explained: the journal impact factor, citation index and the Hirsch index. These bibliometric indices and indicators are illustrated with examples derived from bibliometric analyses of the astronomical literature. The biases of these bibliometric indices, and the use and abuse of bibliometrics are illustrated.