

MONDAY, 17th SEPTEMBER

ELYSE, Laboratoire de Chimie Physique, Bâtiment 349, Salle Magat, Basement

1st session

Chair: **B. Lösekrug**

- 9:30 Opening remarks
M. Suhm
- 9:35 Natural Abundance Deuterium 1D and 2D NMR in Chiral Oriented Solvents : Development and Applications in Chemistry.
P. Lesot
- 10:05 Development of single-site catalysts in olefin polymerization: examples of the use of lanthanide catalysts for the design of new materials.
C. Boisson
- 10:35 Characterization of smooth PMMA films laser deposited at 248 nm.
B. Lösekrug
- 10:55 COFFEE BREAK

2nd session

Chair: **M. Albrecht**

- 11:10 Infrared multi photon dissociation spectroscopy: structure of protonated peptides, DNA strands and drugs in the gas phase.
G. Grégoire
- 11:40 Solid-state NMR spectroscopy applied to the full-length KcsA-Kv1.3 potassium channel in lipid bilayers.
R. Schneider
- 12:00 Calculation of entropies based on MD trajectories.
U. Hensen
- 12:20 LUNCH

3rd session

Chair: **K. Le Barbu-Debus**

- 14:40 Infrared Spectroscopy with ab initio molecular dynamics simulations - Applications to peptide building blocks.
M. P. Gaigeot
- 15:10 Secondary structures of peptide chains isolated in the gas phase: IR/UV double resonance spectroscopy and quantum chemistry calculations.
M. Mons
- 15:40 Photoinduced hydrogen atom transfer in the gas phase.
I. Bloch Nielsen
- 16:00 How much can the ionization potential of sodium be influenced by methanol solvation?
I. Dauster
- 16:20 BREAK
- 16:45 SEPARATE STUDENTS' AND PROFESSORS' MEETINGS
- 17:30 POSTER SESSION / BUFFET STYLE DINNER

Posters:

- M. Albrecht**
M. Baldus
A. Bögehold
R. Briquel
A. Cimas
A. Mahjoub
U. Nergui
J. C. Pouilly
S. Seyffarth
R. Tuckermann
- Spectroscopy of strongly bound hydrogen-bonded clusters.
Solid-state NMR: A spectroscopic technique to study structure and dynamics of molecular complexes at atomic resolution.
Investigation of biomolecular aggregation and polymers by liquid beam desorption mass spectrometry.
Synthesis of end-functionalized polyethylenes. Application to the elaboration of ethylene/polar monomers copolymers.
Car Parrinello molecular dynamics applied to the infrared investigation of phosphorylated amino acids.
Chiral recognition in jet-cooled complexes.
Some characterization of ethene and acrylic acid copolymer.
InfraRed Multi Photon Dissociation Spectroscopy: Structure of protonated peptides, DNA strands and drugs in the gas phase.
Laser deposition of PMMA at high temperatures
FTIR spectroscopy of pure and binary mixed nanoparticles of H₂O and NH₃.

TUESDAY, 18th SEPTEMBER

ELYSE, Laboratoire de Chimie Physique, Bâtiment 349, Salle Magat, Basement

1st session

Chair: **A. Bögehold**

- 9:30 Performances and limits of FCS and FRAP for the study of molecular diffusion inside biofilms and polymer inclusion membranes.
K. Steenkeste
- 9:50 Photofragmentation of biomolecules by multi-coincidences methods.
B. Lucas
- 10:10 The role of photoelectrons in atmospheric pressure photoionisation and their implication in electron capture dissociation of peptides.
A. Giuliani
- 10:40 COFFEE BREAK

2nd session

Chair: **U. Hensen**

- 11:10 Jet-FTIR-spectroscopy of proline esters, their aromatic homologs and their aggregates.
S. Hesse
- 11:30 The microsolvation of alkali atoms in polar solvent clusters. New insights from the sodium-methanol system.
T. Zeuch
- 11:50 UV photoisomerisation in cryogenic matrices of malonaldehyde and acetylacetone. Approach of the reactional pathways.
S. Coussan
- 12:20 LUNCH
- 14:00 Beginning of lab visits
- Evening STUDENT / PI DINNERS