



Advanced spectroscopy of molecular materials: Application to environmental and pharmaceutical compounds

le jeudi 21 mai 2015 – Salle de réunion de l'UFR de Chimie, Bât. C8

Matin de 09h00 à 12h00

09h00 Francesca Ingrosso, Université de Lorraine, SRSMC

Understanding solvation for a ‘greener’ chemistry: a contribution from theoretical approaches

09h30 Ari Seitsonen, Ecole Normale Supérieure, Paris

H₂O-CO₂ mixtures at supercritical conditions: A molecular dynamics study

10h00 Benjamin Hanoune, Université de Lille1, Sciences et Technologies, PC2A

Interpretation of the Raman spectrum of formaldehyde aqueous solutions through *ab initio* molecular dynamics simulations and quantum chemistry calculations

10h30 Coffee Break

11h00 Robert Georges, Université de Rennes1, IPR

Growth of water-containing clusters in supersonic expansions

11h30 Arnaud Desmedt, Université de Bordeaux1, ISM

Guest-water interactions in clathrate hydrates: from van der Waals to hydrogen bondings

Après-midi de 14h00 à 17h00

14h00 Emeline Dudognon, Université de Lille1, Sciences et Technologies, UMET

Pharmaceuticals solid state manipulation

14h30 Mark Eddleston, University of Cambridge

Transmission electron microscopy of pharmaceutical materials

15h00 Coffee Break

15h30 Delphine Vardanega, Université de Lille1, Sciences et Technologies, PhLAM, PCMT

Molecular Dynamics study of organic aerosols: influence of humidity

16h00 Yeny Tobon Correa, Université de Lille1, Sciences et Technologies, LASIR

Physical and chemical properties of individual atmospheric particles

16h30 François-Alexandre Miannay, Université de Lille1, Sciences et Technologies, LASIR

Searching for new improved exchange media for solar cells

Organisation

A. Idrissi (LASIR)

F. Affouard (UMET)

B. Chazallon (PhLAM)

LASIR

UMET

PhLAM