



## Interdisciplinary Workshop on Nanobiohybrids: Vlasta Bonačić-Koutecký 75th Birthday Honor

November 19th 2018, Conference Room, Institute of Analytical Sciences  
Université Claude Bernard Lyon1

The development of cluster science takes place from the beginning at the interface of Physics and Chemistry. From the 90' the clusters physics has stimulated a new vision in material science at nanoscale. In chemistry, the clusters are very important for catalysis and reactivity and on fundamental aspect to understand binding energy and geometry beyond the surface structuration in nanoparticles. The collaboration between theoreticians and experimentalists were crucial for the advance of the field.

More recently, the search for new properties has led to the combination of atomic clusters with ligands, biomolecules, including nanoalloys and supra-crystals of clusters etc. These *nanobiohybrids* have attracted a great attention as biosensing materials and as promising targets in medical diagnostics and biomedicine. This exponential development brings together chemists, physicists, biologists with many challenging theoretical and experimental breakthroughs.

Vlasta Bonačić-Koutecký, Professor of Theoretical Chemistry has been very active in all these researches since the end of the 80'. After a master in Zagreb, she got a PhD in USA (Johns Hopkins University, Baltimore), V. Bonačić-Koutecký move then to Berlin where she became a reference in the theoretical calculations of clusters, including geometric structure, optical spectroscopy, reactivity, dynamics properties. Recently she developed the theoretical investigation of nanobiohybrids and established an Interdisciplinary Laboratory in Split. She obtained in 2015 a Center of excellence for science and technology – integration of Mediterranean region – STIM in Split. Her laboratory is also associated with ILM in a LIA (Laboratoire International Associé). In 2009, she was awarded a Honoris Causa Doctorate from Université Claude Bernard Lyon1.

V. Bonačić-Koutecký reaches 75 in 2018. Therefore considering her exceptional career and the general interest of her scientific field, a workshop on nanobiohybrids is organized in honor of V. Bonačić-Koutecký. The purpose is to discuss and enlighten the challenges of nanobiohybrids.



Université Claude Bernard  Lyon 1



# Program

**8h45** – Welcome from UCBL and FRAMA – *Marie-France JOUBERT and Alfonso SAN MIGUEL*

Address from Humboldt University – *Michael LINSCHELD*

**9h05** - Introduction - *Michel BROYER*

*Chair: Philippe DUGOURD*

**9h15** : **Richard PALMER** – Swansea University, The United Kingdom.

*Atomic structure, dynamics and scale-up of deposited clusters for biomedical and catalytic applications.*

**9h45** : **Jiří PITTNER** – Czech Academy of Sciences, Czech Republic.

*DMRG-externally-corrected coupled cluster methods - a computational tool for strongly correlated molecular systems.*

**10h15** : **Roland MITRIĆ** – Würzburg University, Germany.

*Light-induced function in supramolecular systems.*

**10h45** – COFFEE BREAK

*Chair: Christian BORDAS*

**11h15** : **Fernand SPIEGELMAN** – Université de Toulouse, France.

*Structural and electronic aspects of metal nanoparticles: a theoretical approach from small clusters to bulk.*

**11h45** : **Patrice MELINON** – Université de Lyon, France.

*Superlattices based from clusters: a way for new materials.*

**12h15** : **Florent CALVO** – Université de Grenoble, France.

*Size-induced submersion of alkali clusters into helium nanodroplets.*

**12h45** - LUNCH

*Chair: Claire LOISON*

**14h00** : **Josef MICHL** – University of Colorado, USA and Czech Academy of Sciences, Czech Republic.

*Delocalization of sigma electrons as a function of conformation.*

**14h30** : **Thorsten BERNHARDT** – Ulm University, Germany.

*Biomimetic gas phase clusters: Catalytic activation of water and nitrogen.*

**15h00** : **Piercarlo FANTUCCI** – University of Milano, Italy.

*Computational molecular models of natural metal enzymes. The Ni-Fe and Fe-Fe hydrogenases.*

**15h30** – COFFEE BREAK

*Chair: Patrick RAIROUX*

**16h00** : **Miroslav RADMAN** – French Academy of Sciences, France and Mediterranean Institute for Life Sciences (MedILS), Croatia

*Biology of aging and diseases needs chemistry and physics.*

**16h30** : **Jean-Pierre WOLF** – University of Geneva, Switzerland.

*Ultrafast molecular control and biological function.*

**17h00** : **Ludger WOESTE** – Free University of Berlin, Germany.

*Wave packets : Theory and Experiment.*

**17h30** – Closing speech – *Vlasta BONAČIĆ-KOUTECKÝ*

Participation, **including coffee breaks and lunch**, is free of charge, but the inscription is mandatory at the following link:

<https://www.inscription-facile.com/form/hAE0B2SUzKiOgRsV2cU>

**The workshop is limited to 70 persons.**

### **Workshop Venue and Travel Information**

How to reach us :

Institute of Analytical Sciences – UMR 5280

5, rue de la Doua

69100 Villeurbanne, France

Phone: +33 (0)4 37 42 35 35

GPS : N 45° 46' 45.45" E 4° 52' 28.52"

Itinerary by tramway:

From railway station Part-Dieu :

Exit station through «porte Vivier Merle»

Take line T1 tramway, direction «IUT – Feyssine»

Get off at «INSA – Einstein» station

Take avenue Albert Einstein and follow rue de la Doua on 400m.

Duration : about 30 minutes

### **Scientific committee**

Michel Broyer (chair)

Ludger Woeste (co-chair)

Marion Girod

Philippe Dugourd

### **Local organization committee**

Rodolphe Antoine

Clothilde Comby-Zerbino

Luke MacAleese

Isabelle Russier-Antoine

