

## INSTITUTE OF CHEMICAL PROCESS FUNDAMENTALS

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# Lectures (October 2013 - January 2014)

(Thursday, 13:30 h, ICPF, Zasedací síň ÚCHP)

10.10.	Ing. Jiří Sobek, Ph.D. (ICPF AS CR, Environmental Process Engineering Laboratory)
	Microwave technologies
24.10.	Ing. Mgr. Ondřej Kaman, Ph.D. (Institute of Physics AS CR, v. v. i.)
	Complex magnetic nanoparticles
14.11.	Mgr. Michal Fárník, Ph.D., DSc. (J. Heyrovský Institute of Physical Chemistry, AS CR, v. v. i.)
	Aerosol particles in molecular beams: pickup of molecules, chemistry and photochemistry
28.11.	Ing. Petr Stavárek, Ph.D. a Ing. Jiří Křišťál, Ph.D. (ICPF AS CR, Department of Separation Processes)
	F <sup>3</sup> Factory - motivation, results and experience from EU project
12.12.	Prof. RNDr. Robert Ponec, DrSc. (ICPF AS CR, Department of Catalysis and Reaction Engineering)
	Modern theoretical methods for the analysis of chemical bonding
9.1.	Ing. Pavel Novák (ICPF AS CR, Department of Multiphase Reactors)
	Effect of physical and chemical factors on the beer gushing intensity
23.1.	Mgr. Klára Hilscherová, Ph.D. (Research Centre for Toxic Compounds in the Environment - RECETOX, Faculty of Science, Masaryk University, Brno)
	Endocrine disruption as an important mechanism of toxicity of chemicals and their mixtures

### Ing. Jiří Sobek, Ph.D.

## **Microwave technologies**

In a lecture will be presented developed microwave processes in our laboratory - such as the preparation of dried surfactants, the microwave decontamination of soils, the asphalt repair technology and the microwave technology for recycling of PET bottles.

Ing. Mgr. Ondřej Kaman, Ph.D.

### **Complex magnetic nanoparticles**

Complex nanoparticles based on ferromagnetically or ferrimagnetically ordered phases have become a traditional topic of both basic and applied research which might lead for instance to applications in analytical chemistry, magnetic separations and also in biological research and medicine. The crucial issue for any use of magnetic nanoparticles in a biological system is a suitable shell providing a stable and biologically inert or even biocompatible barrier between the core and the surroundings. At the same time, the cores have to possess well adjusted magnetic properties in order to fulfil specific requirements of various applications like magnetic resonance imaging (MRI) or magnetic fluid hyperthermia (MFH). However, for the basic research the most important attributes of the studied material include the size and shape distributions of the magnetic cores since these extrinsic properties significantly affect its magnetic behaviour. The last point will be discussed on selected examples from the study of nanoparticles based on perovskite manganite  $La_{1-x}Sr_xMnO_3$  and spinel phase of the composition  $Co_{1-x-y}Zn_xFe_{2+y}O_4$ . The talk will be particularly dedicated to the relation between magnetic properties and structure being influenced by surface and finite size effects. Furthermore, the preparation and properties of complex materials employing magnetic cores and hybrid silica shells will be illustrated with respect to possible applications.

#### Mgr. Michal Fárník, Ph.D., DSc.

## Aerosol particles in molecular beams: pickup of molecules, chemistry and photochemistry

Molecular beams in vacuum provide a unique tool for detailed investigations of aerosol particles at the molecular level. An overview of molecular beam experiments with clusters which are performed in Prague will be presented and we will cover several topics. First, we discuss studies of atmospherically relevant clusters including (i) photochemistry of hydrogen halides on ice nanoparticles leading to radical H<sub>3</sub>O generation, and photochemistry of CFCs; (ii) pickup of atmospheric molecules on ice nanoparticles having surprising consequences for nucleation of atmospheric aerosols, (iii) studies of mixed nitric acid - water nanoices.

Ing. Petr Stavárek, Ph.D. a Ing. Jiří Křišťál, Ph.D.

## **F**<sup>3</sup> Factory - motivation, results and experience from EU project

The  $F^3$  – Factory (<u>www.f3factory.com</u>) project funded from EC 7<sup>th</sup> Framework Programme finished this year. It was a collaborative research project among 30 academic institutions and

industrial partners from 9 EU member countries. The aim was to develop the new modular continuous technologies for chemical processes to create " $F^3$  Factory plant" which is more competitive than the traditional technologies.

At ICPF we were involved a subproject focused on the anionic surfactant making. Our project was solved in the international team with partners from KIT (Karlsruhe, Germany), Britest (UK) and industrial partner Procter&Gamble (Brussels, Belgium). We were developing new reactors for two crucial steps in the surfactant making process:  $SO_2$  to  $SO_3$  oxidation and sulf(on)ation reaction. The results obtained and experience gained from the close cooperation within international team will be shared during the presentation.

Prof. RNDr. Robert Ponec, DrSc.

### Modern theoretical methods for the analysis of chemical bonding

Lecture contributes to summary overview of the original theoretical methods (i.e. population analysis, analysis of domain averaged Fermi holes) developed in our laboratory over past 10-15 years. These approaches will be presented on examples of possible utilization at analysis and interpretation of bonding ordering both in stable molecules and for description of the electron reorganization during chemical reactions.

Ing. Pavel Novák

## Effect of physical and chemical factors on the beer gushing intensity

Gushing is a negative phenomenon characterized by spontaneous overfoaming of beer after opening a bottle or can. Despite long-term research it is still not possible to predict its occurrence or to suppress it. The first aim of this work was to find a gushing-active matrix on which it would be possible to observe the influence of physical factors and the influence of the addition of hop compounds. The solution of bovine serum albumin of concentration 0.5 g/l was determined as the most convenient matrix. In this solution micelles of albumin are formed which act like nucleation sites for the formation of gushing foam. This solution was used to estimate the influence of pH and the suppressing effect of increased pressure over the solution on gushing. Further, the influence of hop bitter compounds and essential oils (linalool) on gushing was studied. All measurements were carried out in for this purpose specially constructed apparatus consisting of a pressure column, a high-speed camera and a pressure probe.

Mgr. Klára Hilscherová, Ph.D.

## Endocrine disruption as an important mechanism of toxicity of chemicals and their mixtures

Many can act as disruptors of endocrine system and mimic or antagonize functions or biosynthesis of endogenous hormones and thus negatively affect hormonal regulation in organisms. Endocrine disruption is connected with many effects in organism, such as immunosuppression, carcinogenicity, reproductive and developmental toxicity, embryotoxicity and others. This lecture will summarize approaches and outcomes of a number of studies focused on endocrine disruptive compounds realized in the Research Centre for Toxic Compounds in the Environment (RECETOX)