THE PARTNERSHIP FOR INTERNATIONAL RESEARCH AND EDUCATION AT THE UNIVERSITY OF CALIFORNIA
ELECTRON CHEMISTRY AND CATALYSIS AT INTERFACES

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SEMINAR ANNOUNCEMENT

Advanced solid-state NMR as a key tool for the deeper understanding of heterogeneous catalysts

Régis M. Gauvin
CNRS and University of Lille, France

Date: Monday, August 18, 2014
Place: ESB 2001
Time: 4:00PM

Among the various approaches to heterogeneous catalysts preparation, the grafting of organometallic species onto inorganic supports is most attractive: This may in principle afford surface species with precisely controlled coordination sphere, for which structure-activity and –selectivity relationships may be drawn to some extent. However, this implies thorough understanding of the inorganic interface chemistry, of the grafting reaction, and of the surface species' structural features.

Solid-state MAS NMR is a technique of choice for the study of immobilized inorganic or organometallic centers, down to the molecular level. The vast number of NMR active nuclei allows for deep studies to be carried out. These involve the recording not only of simple 1D spectra but also of 2D homo- and heteronuclear correlation spectra. In this latter case, one can gather precious information, such as proximity or connectivity between given nuclei. Furthermore, in the case of quadrupolar nuclei such as ^{17}O or ^{27}Al, precious information can be extracted from NMR parameters beyond chemical shift, such as quadrupolar coupling and chemical shift anisotropy, for instance. When combined with DFT calculations, this turns into a very informative analytical package.

In this seminar, selected examples will illustrate the input of solid-state NMR to the field of supported catalysis:

- Surface-selective ^{17}O labelling of silica provides information on the interactions between grafted organometallic fragments and the support;[1]
- Structural assignment of silica-supported tungsten oxo (organometallic) species for alkene metathesis can be achieved thanks to ^{17}O NMR;[2]
- Selective and efficient ^{1}H-^{27}Al heteronuclear correlations provide a fresh view on the alumina hydroxyl groups network and on its surface chemistry.[3]

[1] N. Merle, J. Trébosc, A. Baudouin, I. Del Rosal, L. Maron, K. Szeto, M. Genelot, A. Mortreux, M. Taoufik, L. Delevoye, R. M. Gauvin, *J. Am. Chem. Soc.* **2012**, *134*, 9263.
[2] N. Merle, G. Girard, N. Popoff, A. De Mallmann, J. Trébosc, E. Berrier, J.-F. Paul, I. Del Rosal, L. Maron, R. M. Gauvin, L. Delevoye, M. Taoufik, *Inorg. Chem.* **2013**, *52*, 10119.
[3] M. Taoufik, K. C. Szeto, N. Merle, I. Del Rosal, L. Maron, J. Trébosc, G. Tricot, R. M. Gauvin, L. Delevoye, *Chem. Eur. J.*, **2014**, *20*, 4038.

Refreshments will be served before the seminar
To meet with Régis Gauvin on August 18, please contact Lela Castillo:
lela@engineering.ucsb.edu