

# **Multi-scale dynamics of structured polymeric materials**

**DECEMBER 6-7, 2010, PARIS, FRANCE**

**International workshop  
The Michelin Materials Science Chair at ESPCI ParisTech**

**Amphithéâtre Langevin  
École supérieure de physique et de chimie industrielles de la Ville de Paris  
(ESPCI ParisTech)**





## Seminar Program

### Monday December 6<sup>th</sup>

9:00 **Jacques Prost (ESPCI ParisTech)**

Opening and introduction

9:20 **Marc Couty (Michelin)**

Keynote : Future research in Materials Science at Michelin

#### **SESSION 1 : New trends in polymeric, colloidal and molecular glasses**

10:00 **Kurt Binder, Johannes Gutenberg-University (Germany)**

Phase behavior of polymer-containing systems: recent advances by computer simulation

10:40 Coffee break

11:00 **Mark Ediger, University of Wisconsin (USA)**

Direct measurement of molecular mobility in actively deformed polymer glasses

11:40 **Alexei Sokolov, The University of Tennessee (USA)**

Cooperativity and heterogeneities in dynamics of glass-forming systems: new insight

12:20 Lunch break : Buffet and poster session

15:30 **Kenneth S. Schweizer, University of Urbana (USA)**

Predictive theories of slow relaxation, physical aging and mechanical response of glassy polymer and colloidal materials

16:10 **Juan Colmenero, Universidad del Pais Vasco (Spain)**

Chain dynamics in dynamically asymmetric polymer blends

16:50 Coffee break

#### **SESSION 2 : From molecular dynamics to mechanical properties of polymers**

17:10 **Mark O. Robbins, Johns Hopkins University (USA)**

Strain hardening and crazing in amorphous polymers: effects of entanglements and molecular orientation

17:50 **Jean-Louis Barrat, Université Claude-Bernard (France)**

Microscopic and mesoscopic approaches to the deformation of amorphous materials



## December 7th

- 9:00 **Tom McLeish, University of Durham (UK)**  
Bottom-up molecular rheology with full industrial complexity in branched polymers
- 9:40 **Tristan Baumberger, Université Pierre et Marie Curie (France)**  
Multi-scale, slow crack dynamics in soft polymer networks
- 10:20 Coffee break and poster session
- 11:20 **Marc Daniel (Michelin)**  
Keynote: Materials for a sustainable mobility
- 12:00 Lunch break: buffet

### SESSION 3: Polymer dynamics at interfaces

- 13:30 **Kay Saalwächter, Martin-Luther-Universität (Germany)**  
Confinement effects on segmental and chain dynamics in polymer melts and elastomers
- 14:10 **Charles F. Zukoski, University of Urbana (USA)**  
Characterization of polymer segment-particle surface interaction strength from suspension microstructure and its role in nanocomposite stability
- 14:50 Coffee break
- 15:10 **Julian Oberdisse, Université de Montpellier (France)**  
Reinforcement in nanocomposites with tunable structure: observation of chains in crowded environments
- 15:50 **Didier Long, CNRS-Rhodia (France)**  
How do the mechanical properties of confined polymers depend on the strength of the polymer/substrate interactions: linear and plastic behavior?
- 16:30 **Christine Bénard (Michelin)**  
Conclusions
- 17:00 End of workshop



## Posters

### 1 - Micromechanisms and macroscopic behaviour of a highly-filled elastomer

Aurélie Azoug

Laboratoire de Mécanique des Solides, UMR 7649  
Ecole Polytechnique, France  
[azoug@lms.polytechnique.fr](mailto:azoug@lms.polytechnique.fr)

The propellant is an energetic highly-filled elastomer used in rocket propulsion. Research in this field of activity aims at developing propellant compositions that provide a high quantity of energy in service. Hence, the material is designed to show an energetic performance, not a mechanical one. In order to reach this performance level, the filler fraction introduced is more important than the one in a classic carbon black filled elastomer. Consequently, propellants are called highly-filled elastomers. However, the mechanical behaviour of the material has to allow manufacturing and ensure integrity in use.

The aim of this study is to understand the physical origin of the macroscopic non linearities of the mechanical behaviour. The links between micromechanisms and mechanical properties are explored on various scales using different experimental methods. The study starts with the formulation level and aims to reach the macroscopic scale. As a comprehensive vision of the influence of the structure on the behaviour is desired, a design of experiments is used and 23 materials are studied.

Relaxation in nuclear magnetic resonance (NMR) gives access to material behaviour on the proton scale. The application of NMR to propellants is explored according to the specific characteristics of these materials. More precisely, heterogeneities of the polymer network and the sol fraction are studied. Besides, the evolution of the relaxation times  $T_2$  while stretching the sample is assessed.

On a macroscopic scale, dynamic mechanical analysis (DMA) tests are performed. The measurements focus on the influence of prestrain on the behaviour. On one hand, the linear behaviour of the materials resulting from the design of experiments is characterized. On the other hand, the effect of prestrain on the non linear behaviour is quantified. Micromechanisms leading to the non linearity due to prestrain are discussed and compared with NMR results.



## 2 - Aspects of polymer dynamics in three- and two-dimensional polymer melts

Jörg Baschnagel

Institut Charles Sadron, Strasbourg, France  
[jorg.baschnagel@ics-cnrs.unistra.fr](mailto:jorg.baschnagel@ics-cnrs.unistra.fr)

We present results from computer simulations and theoretical studies for the chain conformation and polymer dynamics of three-dimensional (3D) and two-dimensional (2D) polymer melts. In 3D, we combine elements from polymer theory (excluded volume effects and dynamicRPA) with mode-coupling theory to discuss the dynamics of the center of mass (CM) of a polymer in the melt. For intermediate times (shorter than the entanglement time) the theory predicts a power-law decay of the velocity auto-correlation function (VCAF) of the CM, i.e.  $VCAF(t) \sim t^{-5/4/N}$  ( $N$  being the chain length) and thus a subdiffusive increase of mean-square displacement (MSD) of the CM,  $MSD(t) \sim t^{3/4/N}$ . We discuss the strengths and the weaknesses of the theory by comparing its predictions to results from molecular-dynamics (MD) simulations of bead-spring models. We also present results on strictly two-dimensional polymer melts. In 2D, the chains adopt compact, segregated conformations with an irregular (fractal) chain contour. Using MD simulations and scaling arguments we discuss the conformational dynamics of the chains. The relaxation of the chains is well described by a model where shape fluctuations occur in an amoeba-like fashion through the advancing and retracting of contour "lobes". This relaxation behavior and the incompressibility of the melt lead to a power-law decay of the VCAF of the CM, i.e.  $VCAF(t) \sim t^{-6/5/N^{1/2}}$ .



### **3 - New hybrid Siloxane / Polysaccharides Based Sol-Gel Matrices : Synthesis and Properties**

**Christophe Bliard**

**CNRS UMR 6229, Institut de Chimie Moléculaire de Reims, France**

[christophe.bliard@univ-reims.fr](mailto:christophe.bliard@univ-reims.fr)

In this communication we present the synthesis of new hybrid materials constituted of a dual siloxane-polysaccharidic based materials by inter intertwining/cross-linking two polymeric epoxy-silane/polysaccharide based networks in aqueous solution ; using the carbohydrate framework as the building template for the siloxane polymerization.

The advantage of cross-linkable sol-gel matrices over traditional sol-gel chemistry methods are primarily the use of low temperature processing to prepare the material, the opportunity to incorporate useful organic functionality into the final matrix, modified mechanical properties and partial and adjustable biodegradability. Depending on the starting silanes, the polysaccharides these gels are cross-linked in a number of ways, to produce materials with unique, innovative and potentially valuable properties.



## **4 - Effect of displacement rate on fracture behaviour of carbon black filled natural rubber**

**Manuela Boggio**

Politecnico di Milano - Dip. Chimica, Materiali e Ingegneria, Italy  
[manuela.boggio@mail.polimi.it](mailto:manuela.boggio@mail.polimi.it)

The fracture behaviour of carbon black filled vulcanized natural rubber compounds is strongly related to its structure and to the structure's changes which can occur when the compound is strained. Some of the phenomena occurring may be influenced by the applied strain rate, in particular, the ones taking place at the filler/polymer interface where molecules have a restricted mobility.

In this work the influence of strain rate on fracture phenomenology and fracture toughness was investigated performing video-recorded fracture tests. A pure shear test configuration using suitable specimen geometry was adopted and the J-integral fracture mechanics approach applied. The fracture toughness data were analyzed considering the input energy as made of two components, one stored and one dissipative. To separate energy into these components appropriate "loading-unloading" tensile tests were performed on unnotched pure shear specimens. Results on fracture toughness rate dependence have then been interpreted considering the possible effects of strain rate on the so-called non-catastrophic dissipative events occurring at the filler/polymer interface.



## 5 - Viscoelastic behaviour of elastomers from uncured to cured state

Salvatore Coppola

Polimera Europa S.p.A., Ravenna, Italy  
[salvatore.coppola@polimerieuropa.com](mailto:salvatore.coppola@polimerieuropa.com)

In the tire industry, the pure polymer seems to be just a minority ingredient of a complex material, the tire compound, which is composed of two or three polymers and a number of other materials like fillers, plasticizers, oil, vulcanization accelerators, sulfur. Nevertheless, the nature of the pure polymer(s) in terms of MMD and architecture can still have significant effects on the rheological behaviour of the uncured and even the cured compound. The rheology of uncured rubber is important for the processability while the dynamic-mechanical properties of cured rubber are crucial for the tire performance (in particular, grip and rolling resistance). This work aims at building a bridge between the structure of the base polymers and the properties of polymeric networks in view of tyre applications. To do this, we studied the viscoelastic behavior of pure polymer samples before and after vulcanization.

The pure polymers used in this work are Styrene-Butadiene Rubber samples characterized by different molecular architecture in terms of polydispersity and branching patterns. A thorough analysis of linear viscoelasticity is reported for all the samples. Transient non linear experiments are used to find out the relationships between long term relaxation and processability. The non-linear viscoelastic behavior was also used to investigate the influence of the polymer matrix on typical properties of rubber in the post-cure state (Mullins effect). The rheological behavior of pure polymers in the uncured and cured state was compared with predictions of Wagner's models.



## 6 - Characterization of the process zone near the crack tip in filled elastomers

**S. Mzabi<sup>1</sup>, C. Boue<sup>2</sup>, F. Martin<sup>1</sup>, M. Portigliatti<sup>3</sup>, D. Berghezan<sup>3</sup>, C. Creton<sup>1</sup>**

<sup>1</sup> Laboratoire PPMD – ESPCI-CNRS-UPMC, Paris, France

<sup>2</sup> LPEM – ESPCI-CNRS-UPMC, Paris, France

<sup>3</sup> Michelin, CERL Ladoux, F-63040 Clermont Ferrand, France

The prediction of phenomena like fatigue crack propagation in filled elastomers is still very challenging today mainly because the LEFM approach, usually used for studying stress fields near a crack tip, has significant limitations for these materials. The mechanical properties of filled elastomers at large strains and in cyclic loading are complex and poorly known due to the non-linearity of the material properties, the Mullins effect and the viscoelasticity. This in turns results in a poor knowledge of stress and strain fields close to the crack tip.

We have developed different experimental techniques to characterize the material behaviour near the crack tip, combining time resolved optical observations, digital image correlation methods, IR images of the temperature field and SEM images to characterize the deformations near the crack tip. We proved the existence of a localized process zone and propose a new approach defining a local energy release rate  $g_{local}$  as the governing parameter controlling the crack propagation rate in fatigue.



## 7 - Modelling the Rheology of Carbon Nanotube Suspensions in Linear Regime

Camilo Cruz

Laboratoire de Procédés et Ingénierie en Mécanique et Matériaux, ENSAM, Paris, France  
[camilo.cruz@ensam.eu](mailto:camilo.cruz@ensam.eu)

Carbon nanotubes (CNT) are roughly very long cylinders formed by rolled-up graphite sheets, with diameters of around 1nm and very high aspect ratios, going from 100 to 700. CNTs exhibit excellent mechanic, thermal and electrical properties. A large number of envisaged applications require dissolving CNTs and processing them in liquid phase. Pristine CNTs tend to agglomerate into bundles due to strong covalent attraction forces between tubes. In order to prevent such agglomeration and promote solubility, CNT are sometime chemically functionalized. This work is particularly dedicated to the modelling of the rheological behaviour of diluted suspensions of functionalized single-walled CNTs into a Newtonian solvent.

When a diluted suspension of functionalized single-walled CNTs is subjected to a small-amplitude oscillatory deformation test, a mild elasticity is measured in the tested frequencies range. Today, the physical origin of this response is not absolutely clear. Several hypotheses have been suggested as responsible of that non-negligible elastic contribution : existence of a weak CNT network, electrostatic repulsion between CNTs and intrinsic CNT bending dynamics. Recently, using a semi-flexible filament model perfectly straight (i.e. without defects) to mimic the single-walled CNT structure, Pasquali found an elastic response when a diluted suspension is dynamically solicited. However, CNTs contain defects that can induce a natural bent tubular structure, with angles varying from 0° to 34°. This work looks for elucidating the effect of a bent structure on the dynamics of a single-walled CNT in diluted suspension using Brownian dynamics (BD) simulations.

We introduced a naturally non-straight configuration to the semi-flexible filament model in order to take into account the existence of bent junctions in the single-walled CNT structure. To perform the BD simulations this semi-flexible filament model was discretized as a non-freely jointed multi bead-rod system with a natural non-straight configuration. In such discrete model the rod length represents the persistent length of the CNT under flow conditions. Using a BD approach the stress relaxation and the dynamic mechanical response of bent single-walled CNTs in diluted suspensions were studied. Non-negligible differences between a straight system and a non-straight one were observed, a meaningful fact that supports the pertinence of consider the defects for explaining the dynamics of a single-walled CNT in suspension. The dynamic response of the proposed model showed the activation of a mild elasticity at intermediate frequencies. The bending rigidity constant and the number of rods were found to be the main model parameters.



## 8 - Rheology investigation of magnetic field responsive biopolymer based materials

Cecilia Galindo-Gonzales

Matière et Systèmes Complexes UMR 7057, CNRS & Université Paris Diderot-Paris 7, France  
[cecilia.galindo-gonzalez@univ-paris-diderot.fr](mailto:cecilia.galindo-gonzalez@univ-paris-diderot.fr)

In the last few years, a new kind of “smart materials”, known as “Field-Responsive Fluids” has received increasing attention. The main feature of these materials is the possibility of controlling some of their properties by means of external fields. Within this sort of materials, magneto-responsive soft matter presents high potential for biomedical and engineering applications.

The aim of our work is to elaborate and to study new magneto-responsive biopolymer-based materials suitable for novel high technology applications in materials industry, drug and biotechnology industries, as well as medical and environmental technology. Specifically, these magnetic field responsive complex biopolymer-based structures consist of magnetic nanoparticles introduced in biopolymer networks.

As a previous step in the study of these magnetic sensitive biopolymers, the analysis of sodium alginate/ferrofluid blends provides useful information. In this way, their rheological behavior is studied, both in the absence of a magnetic field and when an external magnetic field is applied. For this purpose, a new device consisting of a magnetorheological set up was developed. The shear viscosity and the ionotropic gelation of sodium alginate/ferrofluid blends are modulated by the strength of magnetic field.



## **9 - Control of fatigue damage mechanisms in neat and short glass fiber reinforced polyamide**

**Naji Hussein**

[naji.hussein-exterieur@eu.rhodia.com](mailto:naji.hussein-exterieur@eu.rhodia.com)

The growing number of applications of short glass fiber reinforced (SGFR) polyamide 6,6 under cyclic loading in automotive as well as other industries in recent years has led to an increased interest in understanding their fatigue resistance.

In this study, tensile fatigue tests were performed on standard specimens of 30 wt% fiber glass reinforced polyamide 6.6 in the dried state. It was observed that the number of cycles to failure is dependent upon applied stress. A linear correlation of cyclic creep rate and number of cycle to failure was found. We presented also 3 steps in fatigue, and we proved that the critical damage occurs during the second step when the macroscopic mechanical properties evolve linearly with the logarithm of number of cycles. Finally we showed the interaction of creep and fatigue in comparison with static loading.



## 10 - Friction mechanisms at soft polymer interfaces

C. Cohen, E. Degrandi, F. Restagno, C. Poulard, L. Leger

Laboratoire de Physique des Solides, Université Paris-Sud 11, CNRS UMR 8502,  
Bâtiment 510, 91405 Orsay cedex, France

We shall present series of experiments, conducted on model systems based on polydimethylsiloxane (PDMS) cross linked elastomers, and aimed at identifying the molecular mechanisms of friction. Two systems will be presented: interfaces between PDMS chains end grafted or strongly adsorbed on silica surfaces, and interdigitated into the PDMS elastomer, and micropatterned PDMS elastomers, in both cases put into contact with a smooth PDMS surface which can be slide at chosen velocity with respect to the surface. The first system exemplifies the high sensitivity of friction to tiny details in the molecular organization of the surface anchored chains, demonstrating that friction force measurements can be used to trace back the dynamic mechanical response of polymer layers confined at solid interfaces. The second system shows that surface roughness deeply affects friction: first, the contact zone slits into full and partial contact zones whose relative areas depend on the sliding velocity, leading to a strong non linear friction, and second, when the patterning leads to protruding features which can be tilted with respect to normal to the surface, friction anisotropy appears, which can be tuned by a proper adjustment of the geometry of the pattern.



## 11 - Multiscale dynamics in structured polymeric materials

Eric Leroy

GEPEA, Nantes, France

[Eric.Leroy@univ-nantes.fr](mailto:Eric.Leroy@univ-nantes.fr)

Thermoplastic starch (TPS) plasticized by 1-Butyl-3-methylimidazolium Chloride ([BMIM]Cl) was obtained by melt processing. The resulting electrically conductive TPS samples were less hygroscopic than glycerol plasticized TPS. Despite this lower water uptake, [BMIM]Cl seems to be intrinsically a more efficient plasticizer of starch. [BMIM]Cl plasticized TPS samples show a much higher elongation at break in the rubbery state than the glycerol plasticized TPS samples. Their unusually low rubbery Young's modulus for thermoplastic starch (0.5 MPa) suggests a strong reduction of hydrogen bonds between the starch chains due to the presence of the ionic liquid. A detailed IR spectroscopy analysis supports this interpretation.



## 12 - Effects of Strong Confinement on the Glass Transition Temperature in Simulated Atactic Polystyrene Films

Alexey Lyulin

Eindhoven University of Technology, The Netherlands  
[a.v.lyulin@tue.nl](mailto:a.v.lyulin@tue.nl)

The determination of the glass transition temperature ( $T_g$ ) in confined ultrathin films is still weak link in condensed matter physics. In a case of polymer films a physical picture is getting even more complex since it involves different relaxation times of polymer-chain segments. We have performed molecular-dynamics simulations to explore the influence of confinement on a  $T_g$  for supported atactic polystyrene thin films of different thickness ( $1 \div 10$ ) nm and different strength of attraction to the substrate, ( $0.1 \div 3.0$ ) kcal/mol. The simulated films have been equilibrated in a melt at 540 K and further cooled down with a constant cooling velocity below the  $T_g$  value to the room temperature, 300 K. Based on the density measurements we have defined three layers (substrate, middle and surface) for each film. We found that for the whole film the average  $T_g$  value remains almost constant for films down to 2 nm thickness that is, in our simulations, comparable with the gyration radius, 1.5 nm. For thicker films the  $T_g$  value is completely defined by the cohesive interactions between monomers in the middle of the film. Adhesion to the substrate plays role for films where the cohesive interactions in the middle of the film can be neglected. For the middle layer itself the  $T_g$  does not depend on the total film thickness, whereas the surface layer remains liquid-like in the whole temperature range ( $300 \div 540$ ) K. For such stratified structure we have also defined mechanical properties of polystyrene films, which are also discussed.



## 13 - Stress Relaxation of Carbon-Black Natural Rubber Compounds

Claudia Marano

Politecnico di Milano, Milan, Italy  
[claudia.marano@polimi.it](mailto:claudia.marano@polimi.it)

When a rubber is strained, changes in its structure may occur. These changes may be related to rubber crystallization and, in carbon black filled compounds, also to filler particles de-bonding from each other or from the polymer chains. In this work the strain-induced structure modification was studied performing stress relaxation tests on carbon-black filled natural rubber compounds. Uniaxial tensile test were performed on compounds differing in CB content. The unfilled natural rubber was studied too. Samples were first strained, at constant strain rate, up to a strain value ranging from 0.2 to 5.5. Stress was then let to relax. A normalized stress, that is the ratio between the actual stress and the maximum applied stress, was considered to analyse the kinetics of relaxation as a function of the applied strain and the carbon black content. A correlation between the relaxation kinetics and the structural changes in the rubber compounds was attempted.



## 14 - Liquid Crystalline Magnetic Materials

**Monique Mauzac**

CNRS, Laboratoire des IMRCP, Toulouse, France  
[mauzac@chimie.ups-tlse.fr](mailto:mauzac@chimie.ups-tlse.fr)

We presented a new composite obtained by dispersing metallic cobalt nanorods which are strong nanomagnets in a liquid crystal silicone matrix. The liquid crystal order is maintained in the presence of the nanorods and the magnetic properties are improved compared to the properties of the same nanorods in an inert matrix. Coupling the inherent advantages of magnetic nanoparticles and liquid crystal groups result in materials with interesting magnetic properties and orientational behaviour, while providing mechanical properties, which are mandatory for applications, such as actuators.



## **15 - Fatigue behavior in filled rubber: study of the mechanical damage dynamics**

**Luisa Munoz Mejia**

[luisa-fernanda.munoz-mejia-exterieur@eu.rhodia.com](mailto:luisa-fernanda.munoz-mejia-exterieur@eu.rhodia.com)

The filled rubbers are fundamental materials in the structure of modern tires. Traditionally, they are composed of an elastomeric matrix and filled with carbon black. In our case, we study rubber filled with silica particles which are employed in truck tires, particularly in the tread which assures the contact between the vehicle and the road. The silica reducing the rolling resistance contributes to decrease the fuel consumption and the CO<sub>2</sub> discharged, without negative effects on the grip. In real rolling conditions (110 km/h) a truck tire is submitted to vibrations of some 15 Hz on the sidewall and usually accompanied by temperature rise up to 80°C. This solicitation leads most often to material wears by fatigue. The goal of this work is to understand the behavior of filled rubbers under fatigue solicitation. Identification of the most relevant parameters involved in the dynamic damage of elastomers. Characterization of the mechanical damage dynamics from crack growth rate on rubber blends with modifiable properties (rubber matrix, filler type, filler rate and cross-linking) Performance confrontation of fillers: Silica vs. Carbon black.



## 16 - Contact imaging of frictional interfaces between rubbers and rough surfaces

Danh Toan Nguyen

Laboratoire PPMD, ESPCI ParisTech, France  
[danh-toan.nguyen@espci.fr](mailto:danh-toan.nguyen@espci.fr)

Friction is one of the most longstanding problems in Physics. One of the major origins of the complexity of this problem comes from the roughness of the contacting surfaces. When macroscopic bodies are pressed together, contact only occurs at localized spots between surface asperities. Friction thus involves the shearing of a myriad of micro-contacts which are distributed over length scales ranging from micrometers to nanometres. Although widely debated, the manner in which these micro-contacts locally dissipate energy remains obscure. This problem is especially relevant to the adhesion and friction of tire/road systems which involve surfaces with roughness distributed over many length scales. We have developed a method to measure local friction of rubbers by means of a contact imaging approach. Silicon rubber substrates marked on their surface are prepared in order to measure the displacement field induced by the steady state friction of a glass sphere. The deconvolution of this displacement field then provides a spatially resolved measurement of the actual shear stress distribution at the contact interface. This approach thus provides insight into the local friction law, i.e. the relationship between the actual normal stress and shear stress at the frictional interface. Within the framework of this study, it is used to discuss the friction of rubbers against statistically rough surfaces.



## 17 - Etude mécanistique des matériaux polymères biodégradables

Nadia Ouddai

Université de Batna, Algeria  
[ouddai\\_nadia@yahoo.fr](mailto:ouddai_nadia@yahoo.fr)

La polymérisation par voie radicalaire est un procédé de préparation industriel, pratique et relativement peu coûteux, de polymères dont le squelette macromoléculaire contient exclusivement des atomes de carbone. Les polymères préparés par polycondensation : d'autres atomes que le carbone (« hétéroatomes ») sont introduits dans le squelette macromoléculaire, sous la forme de groupements fonctionnels (voir figure1) dont la présence permet de nommer le polymère formé : polyester, polyamide, etc. Cette différence de structure entre polyvinyliques et polycondensats peut se traduire par des différences de propriétés physicochimiques mais une conséquence plus "pratique" est la différence de comportement vis à vis de la dégradation chimique. En effet, la liaison carbone-carbone est d'une si grande stabilité, que les polymères polyvinyliques présentent une grande inertie à la dégradation, voire à la biodégradation. Ceci n'est pas le cas des polycondensats qui sont susceptibles de subir des réactions de coupures ioniques, par exemple une hydrolyse basique. Conférer un tel caractère de dégradabilité aux polyvinyliques se révèle d'un grand intérêt pratique si l'on pense aux problèmes d'environnement.



## 18 - LAOS: a new signature for the mechanics of filled elastomers

Aurélie Papon

PPMD, ESPCI ParisTech, France

[aurelie.papon@espci.fr](mailto:aurelie.papon@espci.fr)

At high strains, filled elastomers show not only a decrease in their storage modulus - the Payne effect, but also a non linear behavior - strain hardening. We show in this study that the two effects can be separated thanks to Large Amplitude Oscillatory Shear experiments. The stress signal of filled elastomers consisting of a dispersion of silica particles into a polymeric matrix was decomposed into an elastic and viscous part and we could observe simultaneously a strain hardening and the Payne effect. The strain hardening is most probably due to a finite extensibility phenomenon of the polymer chains confined between solid particles, where the strain is the largest. The strain amplification factors extracted from fittings were in good agreement with the geometrical structure of the samples and well correlated with the Payne effect. ethanol as solvent of dopant and surfactant.



## **19 - Low field NMR investigation of nanocomposites: polymer dynamics and network effects**

**Aurélie Papon**

PPMD- ESPCI ParisTech, France  
[aurelie.papon@espci.fr](mailto:aurelie.papon@espci.fr)

The dynamics of the polymer matrix in filled elastomer is modified by the presence of solid particles. We used NMR to investigate model filled samples consisting in a dispersion of grafted silica particles into an elastomeric matrix. Exploiting Magic Sandwich Echo experiments, we were able to determine the fraction of polymer with a slower dynamics and to correlate it to the silica specific surface. This fraction of immobilised polymer - due to a gradient of glass transition temperature around the solid particles - depends not only on the temperature, but also on the grafting agent used. Moreover, if the grafting agent introduces a covalent bond between the silica and the polymer, Multiple Quantum experiments indicate that the cross-link density of the elastomer matrix is locally increased in the vicinity of the particles. This is an observation that was not made in any conventional filled elastomer system. We attribute this to the good particle dispersion, the homogeneous surface grafting density, and the consequently large volume fraction of affected material. It remains to be investigated in how far this effect is relevant for the reinforcement mechanisms in conventional (aggregated) filled elastomers, where this fraction is obviously much smaller.



## 20 - <sup>33</sup>S Solid State NMR and First Principle Calculations

Thomas Poumeyrol

CEMHTI – CNRS, Orléans, France

[thomas.poumeyrol@cnrs-orleans.fr](mailto:thomas.poumeyrol@cnrs-orleans.fr)

Sulfur atoms are widely present in many compounds and materials of the chemical, biochemical and rubber industries. In spite of its broad range of application, very few NMR studies have been dedicated to the investigation of the local environment of sulfur in the solid state. This is due to the very low NMR receptivity of the only NMR active isotope of sulfur which make it very difficult to be studied by NMR : sulfur-33 is a 3/2-spin nucleus with a low gyromagnetic ratio (3.272 MHz/T), a low natural abundance (0.76%) and a relatively large quadrupolar moment (-0.06780 barn) giving rise to a significant quadrupolar broadening of the <sup>33</sup>S resonances. We performed natural abundance <sup>33</sup>S solid state NMR experiments on several crystalline sulfates and on dimethyl sulfone at magnetic fields of 9.4 T and 17.6 T. The use of both a high magnetic field (17.6 T) and the QCPMG[1] sequence, which gives rise to significant enhancement of the <sup>33</sup>S signal, allowed us to record <sup>33</sup>S solid state NMR spectra with good signal to noise ratio for experimental time ranging from 1 to 16 hours. At lower magnetic field (9.4 T), we have used the Double Frequency Sweeps technique[2] in addition to the QCPMG sequence to further enhance the <sup>33</sup>S NMR signal. For the studied compounds, NMR parameters such as isotropic chemical shifts, chemical shift anisotropies and quadrupolar coupling constants were measured from static and MAS NMR spectra recorded at two magnetic fields. The parameters determined experimentally were then compared to those obtained from first principle calculations using the Density Functional Theory and GIPAW[3] method included in the CASTEP software.

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## 21 - Effet des solvants polaires et non polaires sur les propriétés barrière et choc du polyamide 66

Agustin Rios De Anda

Laboratoire Polymères et Matériaux Avancés (UMR5268), Lyon, France  
[agustin.riosdeanda-exterieur@eu.rhodia.com](mailto:agustin.riosdeanda-exterieur@eu.rhodia.com)

L'effet de la présence de solvants polaires et apolaires dans le polyamide 66 sur un ensemble de propriétés incluant la sorption et la perméabilité ainsi que la résistance à l'impact est étudié. Une spécificité des polyamides est leur sensibilité à l'eau et aux solvants polaires (comme l'éthanol), à cause de l'affinité de ces solvants pour les groupes amides. Les solvants polaires se substituent aux interactions entre groupes amides et cassent le réseau de liaisons hydrogène initialement présent, ce qui conduit à une baisse importante de la température de transition vitreuse ( $T_g$ ). Les solvants non polaires (comme le toluène ou l'isooctane) ne présentent pas d'affinité particulière avec les groupes amides et ne gonflent le polyamide qu'en quantité très limitée, mais ils conduisent néanmoins eux aussi à une chute significative de  $T_g$ .

Dans un premier temps, la modulation de la température de transition vitreuse du polyamide par la sorption de différents solvants polaires (eau, éthanol) et apolaires (toluène et isooctane), ainsi que par des mélanges de ces solvants est étudiée. Ensuite, les propriétés barrière à ces différents solvants sont caractérisées par des mesures de sorption et de perméation, et la résistance à l'impact est évaluée sur des échantillons secs ou gonflés par des essais de choc entaillé dans différentes conditions de sollicitation (température, vitesse). Une discussion des relations entre mobilité moléculaire /performance choc et température de transition fragile/ductile est enfin proposée.



## 22 - Tuning the Dispersion of Magnetic Fillers in Nanocomposites

Anne-Sophie Robbes<sup>1,2</sup>, Fabrice Cousin<sup>1</sup>, Jacques Jestin<sup>1</sup>, Florian Meneau<sup>2</sup>, Olivier Sandre<sup>3</sup>,  
Didier Gigmes<sup>4</sup> and François Boue<sup>1</sup>

<sup>1</sup> Laboratoire Léon Brillouin (LLB), CEA Saclay, 91191 Gif-Sur-Yvette

<sup>2</sup> Synchrotron Soleil, L'Orme des Merisiers, Saint Aubin, BP 48, 91192 Gif-Sur-Yvette Cedex

<sup>3</sup> PECSA, CNRS UMR 7612, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris Cedex 05

<sup>4</sup> Laboratoire Chimie Provence, UMR 6264, Av. Escadrille Normandie, 13397, Marseille Cedex 20  
[anne-sophie.robbes@cea.fr](mailto:anne-sophie.robbes@cea.fr)

During the past two decades, many industrial applications have encouraged research toward developing methods to reinforce polymer materials with nanoparticles as fillers. One of the key points to improve the mechanical properties is to play on the local structure of the filler. We present here new nanocomposites made of spherical magnetic nanoparticles of maghemite ( $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>) dispersed in a polystyrene (PS) matrix. Thanks to the magnetic susceptibility of the nanoparticles, we're able to build anisotropic structures of controlled morphology by applying an external magnetic field during the material processing. We obtain a material with anisotropic macroscopic mechanical properties. The structure of the composites without external magnetic field [1] obtained with a combination of scattering (Small Angle Neutron and X Ray Scattering) and imaging (Transmission Electronic Microscopy) experiments have shown the formation of compact aggregates (called primary aggregates) at short range. These aggregates form elongated supra-aggregates of finite size at longer range, which are connected for highest nanoparticles concentrations, forming a filler network. Whatever the nanoparticles' size (from 6.7nm to 10nm), the size of the primary aggregate doesn't change ( $\approx$ 17nm) but its compactness is decreasing when increasing the size of the filler. This property permit us to build various controllable anisotropic filler structures by applying an external magnetic and by playing with the magnetic susceptibility of the nanoparticles (which strongly increases with the size) and with the nanoparticles concentration (above or beside the network threshold). During the uni-axial stretch experiments, the resulting materials have shown anisotropic macroscopic mechanical properties more or less pronounced depending on the anisotropic structures formed at the nanoscale. We have obtained composites which have a reinforcement factor four times higher when they are stretched in a direction parallel to the applied magnetic field than perpendicular to the magnetic field. In order to modify the dispersion of the fillers, we have grafted PS chains from the surface of the nanoparticles by adapting a nitroxide mediated polymerization processing from [2] and we have studied the dispersion of such grafted nanoparticles inside the matrix.



## 23 - Atomistic Simulation of the Glass Transition

Armand Soldera

University of Sherbrooke, Québec, Canada  
[Armand.Soldera@USherbrooke.ca](mailto:Armand.Soldera@USherbrooke.ca)

To describe the vast domain of relaxation times occurring at the glass transition, molecular modelling was revealed to be a strongly beneficial tool to complement existing theoretical models. In fact, among the different kinds of simulations, the coarse-grained approach remains the most appropriate technique to deal with the “time spreading” phenomenon. Alternatively, atomistic simulation (AS) is more appropriate when treating the effect of small variations in the atomistic architecture of the repeat unit. However, transition temperatures that are usually related to  $T_g$ s have been determined using this approach. The restricted description of the phase space (domain of times covered by AS, typical length, number of limited points in the configurational space) questions the adequacy of  $T_g$  determined by AS  $AS g T$  compared to those experimentally determined  $exp. g T$ . A procedure is then proposed that yields reproducible  $AS g T$  for a series of vinylic polymers at different cooling rates. Some of the properties that can be revealed from this atomistic simulation are the link with  $exp.g T$  through the well-established WLF equation, the mechanical properties, the different contributions of the variation of the heat capacity at  $g T$ , presence of other characteristic temperatures, effect of the polymer chain tacticity...



## 24 - Adhesives with a gradient of viscoelasticity

François Tanguy

PPMD-SIMM ESPCI ParisTech, France

[francois.tanguy@espci.fr](mailto:francois.tanguy@espci.fr)

A good pressure-sensitive-adhesive is obtained when the material has a liquid-like behavior to create easily a molecular contact and dissipate energy upon debonding and an elastic behavior to resist shear forces over long times. This dual property is especially important on rough surfaces and low energy surfaces. A novel strategy to improve adhesives is here to create a gradient in the viscoelastic properties to obtain a more dissipative behavior near the adhesive/adherend interface and an elastic behavior in the bulk. Bi-layer adhesives have already been studied and show some interesting properties [1].

We focus here on acrylate polymers (butyl acrylate-co-acrylic acid, BA-AA) for applications as Pressure Sensitive Adhesives (PSA) prepared both by emulsion polymerization and by solution polymerization. Two approaches to create a gradient of viscoelasticity are studied. First, we design bi-layer adhesives based on water-borne adhesives (in collaboration with DOW Chemical). Then, we attempt to create a continuous gradient in the film by using a gradient in cross-linking using BA-AA copolymer, synthesized in solution [2].

So far, adhesive properties of the homogeneous materials were tested with a custom-designed probe tack method [3], in which the debonding process between a steel probe and a smooth adhesive film is precisely studied. The linear viscoelastic properties and the large strain properties of the films were tested with linear rheology, extensional rheology and tensile test.

This work is part of the EU integrated project (MODIFY).

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## 25 - Evaluation of a tube-based constitutive equation using rheometry and fieldwise measurements

Rudy Valette

CEMEF Mines-ParisTech, France  
[rudy.valette@mines-paristech.fr](mailto:rudy.valette@mines-paristech.fr)

A polydisperse case of an entangled linear polymer melts constitutive equation is studied. This model, based on the model proposed by Dhole S.D., Leygue A., Bailly C. and Keunings R. (J. Non-Newt. Fluid Mech., 161, 10:18, 2009: "A single segment differential tube model with inter-chain tube pressure effect") is tested on a polystyrene in shear (capillary rheometry), uniaxial extension (extensional rheometry) and planar extension in a complex flow (fieldwise measurements in a contraction flow) for different level of strain rates. It was found that this model is predictive for all rheometrical flows investigated. It was also shown that the model gives good predictions in a more complex flow characterized by a strong, non-homogeneous planar extensional contraction flow.



## 26 - Resistance to tear propagation in reinforced natural rubber

Arnaud Vieyres

Laboratoire Polymères et Matériaux Avancés, Lyon, France

[arnaud.vieyres-exterieur@eu.rhodia.com](mailto:arnaud.vieyres-exterieur@eu.rhodia.com)

Our study focuses on tear resistance of reinforced elastomers made of synthetic or natural rubber and precipitated silica or carbon black as reinforcing fillers. Single edge notched tensile tests are performed. In filled natural rubber samples, the tear follows an unusual propagation path : it rotates and propagates along the stress direction. This tear rotation phenomenon only occurs in reinforced natural rubber, whose matrix crystallizes under traction. Our aim is to describe and better understand the tear bifurcation phenomenon which is related to the material anisotropy induced by reinforcing fillers and strain-induced crystallites.

The initiation statistics and propagation dynamics of tear rotations are observed during the tests. The number and length of tear rotations are correlated to experimental conditions such as speed and temperature. The strain field in the vicinity of the propagation front is measured by image correlation especially when the tear rotates. The crystallization at the tear tip due to local strain amplification is characterized with an X-ray microdiffraction technique. We study the relationships between the tear rotations length and the size of the crystallized zone.



## **27 - Computational Mesoscopic Determination of Mechanical Behaviour of Textile Composite Reinforcements**

**Samia Zouaoui**

**University of MOSTAGANEM, Algeria**  
[souma\\_zouaoui@yahoo.fr](mailto:souma_zouaoui@yahoo.fr)

The knowledge of the mechanical behaviour of woven fabrics is necessary in many applications in particular for the simulation of textile composite forming. This mechanical behaviour is very specific due to the possible motions between the fibres and the yarns. In this paper, the mechanical behaviour is analysed from virtual tests on the Representative Unit Cell. These virtual tests avoid performing tricky experimental tests. The presented 3D finite element analyses involve two main specific aspects. Firstly the yarn that is made of thousand of fibres is modelled as a continuous medium but its constitutive law has to take its fibrous nature into account. For that reason a rate constitutive equation using a specific objective stress rate is used. It is based on the rotation of the fibre. Secondly the boundary conditions have to render the periodicity at large deformations and, in some cases, the evolution of contacts between neighbouring yarns during the motion. The analysis is performed for two unit cells and two tests (shear and biaxial tension). Both results are in good agreement with the experiments, but the use of one of the cells turns out to be much easier.



## 28 - Reactive Mixing at the Silica-Silane-Elastomer Interfaces

**Camille Willer, Laurent Petitjean, Franck Vilmin, Nicolas Malicki, Sebastien Brun, Anne Veyland, Fabien Gaboriaud\***

Manufacture Française des Pneumatiques Michelin, Clermont Ferrand, France  
[fabien.gaboriaud@fr.michelin.com](mailto:fabien.gaboriaud@fr.michelin.com)

Elastomer-filler mixing involves several processes at the macroscopic level (e.g. agglomerate dispersion, filler wetting) down to the molecular one (e.g. chemical reactions, filler-elastomer interactions, filler flocculation). Among the important physico-chemical characteristics of elastomer and filler, the chemical nature of filler surface sites, the morphology of filler, the functionalization and the microstructure of elastomers play an important role in the composite mixing and its resulting properties. However, the molecular understanding of filler dispersion in polymer matrix is still a challenging problem.

In the context of “green tire”, silica is extensively used in combination with a coupling agent. The role of the coupling agent is to improve the interactions between the hydroxylated silica surface and the elastomer matrix. The molecular mechanisms and the structural characteristics of the silica-elastomer interfaces are still under debate. In particular, the impact of the co-condensation of silane molecules, the balance between the chemisorption and/or physisorption of silane grafted to silica, and the released of free sulphur are important questions to address. However, the combination of experimental and theoretical tools at different scales will help to improve our understanding of the key processes responsible of the properties of such composite materials.



## **29 - A new approach to the rheological behaviour of elastomer / filler composites in fully developed flows**

**Marie Lenoble, Vincent Pelissier**

**Manufacture Française des Pneumatiques Michelin, Clermont Ferrand, France**

The work presented here brings a physico-chemical description of the rheological behaviour of reinforcing fillers / elastomer composites in fully developed flows as measured by capillary rheometry.

Notions of elastomer rheology, filler volume fraction, effective filler volume fraction, maximum volume fraction of the filler and strain amplification are combined in a simple model. This model gives the rheology of the composite from the rheology of the elastomer, with a single parameter related to the effective volume fraction of the filler in the composite.

This model fits the experimental data at low shear but deviations occur at higher shear rates. The limits of this approach and the ways of improvement (hard sphere or soft sphere description, filler disagglomeration under shear, viscosity divergence exponent ...) are discussed in the poster



## 30 - Polymers Structure Design for Traction Performance

**N. Coste<sup>(1)</sup>, R. Matmour<sup>(1)</sup>, A. Roy<sup>(2)</sup>, R. Schach<sup>(1)</sup>**

<sup>(1)</sup> **Manufacture Française des Pneumatiques Michelin, Clermont Ferrand, France**

<sup>(2)</sup> **ENSCP trainee (april - july 2010)**

Taken into account the road indenters' size, we can approximate traction to a  $10^3 - 10^7$  Hz frequency solicitation for the rubber materials. The traction performance could be related to the dissipation potential associated to the glass transition phenomenon in other words, depends on the Temperature Time Superposition behaviour (TTS).

To be able to identify the structural parameters of polymer that control the TTS, we have studied different structures with original backbone and different side groups. We verify first that TTS behaviour depends on the polymer backbone nature. The side group effect is studied for two polymer's family that presents different TTS: Polyacrylates and Polymethacrylates. For both, there is no effect of the alkyl side group on the TTS.

In addition, the slow and arrhenian temperature dependence of Polymethacrylates relaxation time could be related to the merging of the  $\alpha$  and  $\beta$  relaxation.



## 31 - Strain hardening in PMMA/silica nanocomposites

J. Jancar\*, L. Recman, E. Jancarova

Institute of Materials Science, Brno University of Technology, Czech Republic

[jancar@fch.vutbr.cz](mailto:jancar@fch.vutbr.cz)

The effect of adding rigid silica nanoparticles on the strain hardening modulus,  $G_H$ , of the PMMA was investigated under compressive loading over a wide range of silica volume fraction and strain rate for temperature below and above the  $T_g$  of PMMA. For any given silica  $v_f$  investigated, the  $G_H$  increased with the logarithm of strain rate linearly with the slope increasing with filler volume fraction,  $v_f$ . With increasing temperature, the  $G_H$  was observed to decrease. The WLF type equation was utilized to assemble the  $G_H - \log(d\varepsilon/dt)$  master curves. The dependence of the logarithm of the shift factor,  $a_H$ , for  $T_g$  as the reference temperature on the reciprocal temperature,  $1/T$ , was linear for neat PMMA and became increasingly non-linear with increasing  $v_f$ . Prediction of the  $G_H$  vs  $v_f$  dependence based on the simple volume replacement Guth-Gold model was in agreement with the experimental data for the temperature well in the glassy region. Substantial deviation from this model, occurring at temperatures near the  $T_g$ , suggested that the properties of the matrix became strongly affected by the filler due to chain stiffening resulting from retarded chain dynamics and altered conformation statistics.

Recently, the existence of a scaling has been proposed between the strain hardening modulus ( $G_H$ ) and the flow stress ( $\sigma_{flow}$ ) in glassy polymers over wide temperature and strain rate intervals. In an effort to overcome the shortcomings of the network model of strain hardening, computer simulation has been used to support this claim the most. In this communication, experimental evidence is presented supporting the scaling of  $G_H$  with  $\sigma_{flow}$  for neat and silica filled PMMA. The  $G_H$ , measured over a wide range of temperatures and strain rates, has been correlated with rejuvenated yield stress ( $\sigma_{yR}$ ) and yield stress ( $\sigma_y$ ). It is shown that both parameters scale linearly with the  $G_H$  over a broad range of temperatures and strain rates for both neat PMMA and its silica nanocomposite. In contrary to some computer simulations, no difference in the slope of the  $G_H - \sigma_{flow}$  dependence has been observed when the  $\sigma_{flow}$  has been varied by varying temperature or strain rate. It is proposed that the scaling of  $G_H$  with  $\sigma_{flow}$  has its origin in the similarity in nature of the molecular mechanism of yielding considered a cooperative flow of ensembles of chains and the view of chain entanglements as dynamically rearranging ensembles of cooperatively relaxing chain segments.



## Participants

### A

ADAM BERRET Matthieu  
ANDRE Stéphane  
ARBE Arantxa

[matthieu.adam-berret@cea.fr](mailto:matthieu.adam-berret@cea.fr)  
[stephane.andre@ensem.inpl-nancy.fr](mailto:stephane.andre@ensem.inpl-nancy.fr)  
[a.arbe@ehu.es](mailto:a.arbe@ehu.es)

CEA  
LEMETA, Nancy  
University of the Basque  
Country, San Sebastian  
Ecole Polytechnique, Palaiseau

AZOUG Aurélie (P)

[azoug@lms.polytechnique.fr](mailto:azoug@lms.polytechnique.fr)

### B

BANC Amélie  
BARITAUD Claire  
BASCHNAGEL Jorg (P)  
BATISTAKIS Chrysostomos  
BEAKOU Alexis  
BENARD Christine  
BERGHEZAN Daniel  
BERRIOT Julien  
BILGER Nicolas  
BIZET Stéphane  
BLIARD Christophe (P)  
BOGGIO Manuela (P)  
BOKOBZA Liliane  
BRULE Benoit  
BULTERS Markus  
BURHIN Henri

[amelie.banc@univ-montp2.fr](mailto:amelie.banc@univ-montp2.fr)  
[claire.baritaud@fr.michelin.com](mailto:claire.baritaud@fr.michelin.com)  
[jorg.baschnagel@ics-cnrs.unistra.fr](mailto:jorg.baschnagel@ics-cnrs.unistra.fr)  
[c.batistakis@tue.nl](mailto:c.batistakis@tue.nl)  
[Alexis.Beakou@ifma.fr](mailto:Alexis.Beakou@ifma.fr)  
[christine.benard@fr.michelin.com](mailto:christine.benard@fr.michelin.com)  
[daniel.berghezan@fr.michelin.com](mailto:daniel.berghezan@fr.michelin.com)  
[julien.berriot@fr.michelin.com](mailto:julien.berriot@fr.michelin.com)  
[nicolas.bilger@e-xstream.com](mailto:nicolas.bilger@e-xstream.com)  
[stephane.bizet@arkema.com](mailto:stephane.bizet@arkema.com)  
[christophe.bliard@univ-reims.fr](mailto:christophe.bliard@univ-reims.fr)  
[manuela.boggio@mail.polimi.it](mailto:manuela.boggio@mail.polimi.it)  
[liliane.bokobza@espci.fr](mailto:liliane.bokobza@espci.fr)  
[benoit.brule@arkema.com](mailto:benoit.brule@arkema.com)  
[markus.bulters@dsm.com](mailto:markus.bulters@dsm.com)  
[henri.burhin@dynisco.com](mailto:henri.burhin@dynisco.com)

University of Montpellier  
Michelin, Clermont-Ferrand  
Institut Charles Sadron, Strasbourg  
University of Eindhoven  
IFMA, Clermont-Ferrand  
Michelin, Clermont-Ferrand  
Michelin, Clermont-Ferrand  
Michelin, Clermont-Ferrand

ARKEMA  
University of Reims  
Politecnico di Milano  
ESPCI ParisTech  
ARKEMA  
DSM  
DYNISCO

### C

CANTALOUBE Bernard  
CHATEAUMINOIS Antoine  
CHAZEAU Laurent  
CHENAL Jean marc  
CICCOTTI Mattéo  
CLOITRE Michel  
COPPOLA Salvatore (P)  
COSTE Nathalie  
COUTY Marc  
CRETON Costantino (P)  
CRIE Alice  
CRUZ Camilo (P)

[bernard.cantaloube@fr.michelin.com](mailto:bernard.cantaloube@fr.michelin.com)  
[antoine.chateauminois@espci.fr](mailto:antoine.chateauminois@espci.fr)  
[laurent.chazeau@insa-lyon.fr](mailto:laurent.chazeau@insa-lyon.fr)  
[jean-marc.chenal@insa-lyon.fr](mailto:jean-marc.chenal@insa-lyon.fr)  
[matteo.ciccotti@espci.fr](mailto:matteo.ciccotti@espci.fr)  
[michel.cloitre@espci.fr](mailto:michel.cloitre@espci.fr)  
[salvatore.coppola@polimerieuropa.com](mailto:salvatore.coppola@polimerieuropa.com)  
[nathalie.coste@fr.michelin.com](mailto:nathalie.coste@fr.michelin.com)  
[marc.couty@fr.michelin.com](mailto:marc.couty@fr.michelin.com)  
[costantino.creton@espci.fr](mailto:costantino.creton@espci.fr)  
[alice.crie@mines-paristech.fr](mailto:alice.crie@mines-paristech.fr)  
[camilo.cruz@ensam.eu](mailto:camilo.cruz@ensam.eu)

Michelin, Clermont-Ferrand  
ESPCI ParisTech  
INSA, Lyon  
INSA, Lyon  
ESPCI ParisTech  
ESPCI ParisTech  
Polimeri Europa  
Michelin, Clermont-Ferrand  
Michelin, Clermont-Ferrand  
ESPCI ParisTech  
Ecole Mines ParisTech  
ENSAM, Paris

### D

DALMAS Florent  
DANIEL Marc  
DE FOCATIIS Davide  
DIANI Julie  
DOMENEK Sandra  
DRONET Séverin  
DUCOURET Guylaine  
DURAND Graziella

[dalmas@icmpe.cnrs.fr](mailto:dalmas@icmpe.cnrs.fr)  
[marc.daniel@fr.michelin.com](mailto:marc.daniel@fr.michelin.com)  
[davide.defocatis@nottingham.ac.uk](mailto:davide.defocatis@nottingham.ac.uk)  
[julie.diani@paris.ensam.fr](mailto:julie.diani@paris.ensam.fr)  
[sandra.domenek@agroparistech.fr](mailto:sandra.domenek@agroparistech.fr)  
[severin.dronet@fr.michelin.com](mailto:severin.dronet@fr.michelin.com)  
[guylaine.ducouret@espci.fr](mailto:guylaine.ducouret@espci.fr)  
[durand@campus.colas.fr](mailto:durand@campus.colas.fr)

CNRS, Thiais  
Michelin, Clermont-Ferrand  
University of Nottingham  
ENSAM, Paris  
Agro ParisTech, INRA  
Michelin, Clermont-Ferrand  
ESPCI ParisTech  
COLAS SA



## E

EVARD Guillaume [evrard@synchrotron-soleil.fr](mailto:evrard@synchrotron-soleil.fr) Synchrotron Soleil

## F

FAVROT Jean-Michel [jean-michel.favrot@fr.michelin.com](mailto:jean-michel.favrot@fr.michelin.com) Michelin, Clermont-Ferrand  
FRETIGNY Christian [christian.fretigny@espci.fr](mailto:christian.fretigny@espci.fr) ESPCI ParisTech

## G

GABORIAUD Fabien (P) [fabien.gaboriaud@fr.michelin.com](mailto:fabien.gaboriaud@fr.michelin.com) Michelin, Clermont-Ferrand  
GALINDO-GONZALEZ Cecilia (P) [cecilia.galindo-gonzalez@univ-paris-diderot.fr](mailto:cecilia.galindo-gonzalez@univ-paris-diderot.fr) University of Paris Diderot  
GAUTHIER Catherine [catherine.gauthier@insa-lyon.fr](mailto:catherine.gauthier@insa-lyon.fr) INSA, Lyon  
GENIX Caroline [caroline.genix@LCVN.univ-montp2.fr](mailto:caroline.genix@LCVN.univ-montp2.fr) LCVN, Montpellier  
GEORGE Matthieu [mgeorge@univ-montp2.fr](mailto:mgeorge@univ-montp2.fr) LCVN, Montpellier  
GERARD Pierre [pierre.gerard@arkema.com](mailto:pierre.gerard@arkema.com) ARKEMA  
GILORMINI Pierre [pierre.gilormini@paris.ensam.fr](mailto:pierre.gilormini@paris.ensam.fr) ENSAM, Paris  
GUILLERMO Armel [armel.guillermo@cea.fr](mailto:armel.guillermo@cea.fr) CEA, Grenoble  
GUY Laurent [laurent.guy@eu.rhodia.com](mailto:laurent.guy@eu.rhodia.com) RHODIA

## H-J-K

HALARY Jean-Louis [jean-louis.halary@espci.fr](mailto:jean-louis.halary@espci.fr) ESPCI ParisTech  
HUSSEIN Naji (P) [naji.hussein-exterieur@eu.rhodia.com](mailto:naji.hussein-exterieur@eu.rhodia.com) RHODIA  
HUYNH Hieu Thao [thao.huynh@lcpc.fr](mailto:thao.huynh@lcpc.fr) LCPC, Marne La Vallée  
JANCAR Joseph (P) [jancar@fch.vutbr.cz](mailto:jancar@fch.vutbr.cz) University of BRNO  
JANIN Claude [claud.janin@orange.fr](mailto:claud.janin@orange.fr) LRCCP  
KAUSCH Henning [kausch.cully@bluewin.ch](mailto:kausch.cully@bluewin.ch) EPFL, Lausanne

## L

LAUBRY Philippe [philippe.laubry@fr.michelin.com](mailto:philippe.laubry@fr.michelin.com) Michelin, Clermont-Ferrand  
LAUPRETRE Françoise [françoise.laupretre@orange.fr](mailto:françoise.laupretre@orange.fr) IFMA/LAMI  
LE CAM Jean-Benoit [lecam@ifma.fr](mailto:lecam@ifma.fr) Michelin, Clermont-Ferrand  
LE CHENADEC Yohan [yohan.le-chenadec@fr.michelin.com](mailto:yohan.le-chenadec@fr.michelin.com)  
LE GAL LA SALLE Eric [eric.legallasalle@icam.fr](mailto:eric.legallasalle@icam.fr)  
LEGER Liliane (P) [leger@lps.u-psud.fr](mailto:leger@lps.u-psud.fr) University of Paris Sud  
LEQUEUX François [françois.legeux@espci.fr](mailto:françois.legeux@espci.fr) ESPCI ParisTech  
LEROY Eric (P) [eric.leroy@univ-nantes.fr](mailto:eric.leroy@univ-nantes.fr) GEPEA, Nantes  
LOCATELLI Clementine [clementine.locatelli@espci.fr](mailto:clementine.locatelli@espci.fr) ESPCI ParisTech  
LYULIN Alexey [a.v.lyulin@tue.nl](mailto:a.v.lyulin@tue.nl) University of Eindhoven

## M

MALICKI Nicolas [nicolas.malicki@fr.michelin.com](mailto:nicolas.malicki@fr.michelin.com) Michelin, Clermont-Ferrand  
MARANO Claudia [claudia.marano@polimi.it](mailto:claudia.marano@polimi.it) Politecnico di Milano  
MARQUE Gregory [gregory.marque@edf.fr](mailto:gregory.marque@edf.fr) EDF, France  
MARTZEL Nicolas [nicolas.martzel@fr.michelin.com](mailto:nicolas.martzel@fr.michelin.com) Michelin, Clermont-Ferrand  
MAUZAC Monique (P) [mauzac@chimie.ups-tlse.fr](mailto:mauzac@chimie.ups-tlse.fr) CNRS  
MERABIA Samy [smerabia@gmail.com](mailto:smerabia@gmail.com) LPMCN, Lyon  
MEYRUEIX Rémi [meyrueix@flamel.com](mailto:meyrueix@flamel.com) Flamel Technologies, Lyon  
MICHELS Matthias [m.a.j.michels@tue.nl](mailto:m.a.j.michels@tue.nl) University of Eindhoven  
MIQUELARD-GARNIER Guillaume [guillaume.miquelard@espci.org](mailto:guillaume.miquelard@espci.org) CNAM, Paris  
MONNERIE Lucien [lucien.monnerie@orange.fr](mailto:lucien.monnerie@orange.fr)  
MONSALLIER Jean-marc [jean-marc.monsallier@crayvalley.com](mailto:jean-marc.monsallier@crayvalley.com) CRAY VALLEY  
MONTARNAL Damien [dmaien.montarnal@espci.fr](mailto:dmaien.montarnal@espci.fr) ESPCI ParisTech  
MORICEAU Christophe [christophe.moriceau@fr.michelin.com](mailto:christophe.moriceau@fr.michelin.com) Michelin, Clermont-Ferrand  
MOUSTY Hervé [herve.mousty@fr.michelin.com](mailto:herve.mousty@fr.michelin.com) Michelin, Clermont-Ferrand  
MUNCH Etienne [etienne.munch@fr.michelin.com](mailto:etienne.munch@fr.michelin.com) Michelin, Clermont-Ferrand  
MUNOZ Luisa (P) [luisa-fernanda.munoz-meija-exterieur@eu.rhodia.com](mailto:luisa-fernanda.munoz-meija-exterieur@eu.rhodia.com) RHODIA



## N-O

NGUYEN Danh toan (P)  
OUDDAI Nadia (P)  
OULD OUALI Mohand

[danh-toan.nguyen@espci.fr](mailto:danh-toan.nguyen@espci.fr)  
[ouddai\\_nadia@yahoo.fr](mailto:ouddai_nadia@yahoo.fr)  
[m\\_ouldouali@mail.ummo.dz](mailto:m_ouldouali@mail.ummo.dz)

ESPCI ParisTech  
University of Batna, Algeria

## P

PAPON Aurélie (P)  
PELISSIER Vincent (P)  
PETITJEAN Laurent  
PITARD Domitille  
PONTON Alain  
PORTIGLIATTI Maude  
POUMEYROL Thomas

[aurelie.papon@espci.fr](mailto:aurelie.papon@espci.fr)  
[vincent.pelissier@fr.michelin.com](mailto:vincent.pelissier@fr.michelin.com)  
[laurent.petitjean@fr.michelin.com](mailto:laurent.petitjean@fr.michelin.com)  
[domitille.pitard@edf.fr](mailto:domitille.pitard@edf.fr)  
[alain.ponton@univ-paris-diderot.fr](mailto:alain.ponton@univ-paris-diderot.fr)  
[maude.portigliatti@fr.michelin.com](mailto:maude.portigliatti@fr.michelin.com)  
[thomas.poumeyrol@cnsr-orleans.fr](mailto:thomas.poumeyrol@cnsr-orleans.fr)

ESPCI ParisTech  
Michelin, Clermont-Ferrand  
Michelin, Clermont-Ferrand  
EDF  
University of Paris-Diderot  
Michelin, Clermont-Ferrand  
CNRS

## R

REGNIER Gilles  
RESTAGNO Frédéric  
RIOS DE ANDA Agustin (P)  
ROBBES Anne-Sophie (P)

[gilles.regnier@ensam.eu](mailto:gilles.regnier@ensam.eu)  
[restagno@lps.u-psud.fr](mailto:restagno@lps.u-psud.fr)  
[agustin.riosdeanda-exterieur@eu.rhodia.com](mailto:agustin.riosdeanda-exterieur@eu.rhodia.com)  
[anne-sophie.robbes@cea.fr](mailto:anne-sophie.robbes@cea.fr)

ENSAM, Paris  
LPS, Orsay  
LPMA, Lyon  
Synchrotron Soleil & Léon  
Brillouin Lab  
Michelin, Clermont-Ferrand  
Michelin, Clermont-Ferrand

ROBERT Pierre  
RONSIN Olivier

[pierre.robert-f086241@fr.michelin.com](mailto:pierre.robert-f086241@fr.michelin.com)  
[olivier.ronsin@fr.michelin.com](mailto:olivier.ronsin@fr.michelin.com)

Michelin, Clermont-Ferrand  
Michelin, Clermont-Ferrand

## S

SCHACH Régis  
SCHNELL Benoît  
SEEBOTH Nicolas  
SHI Peiluo  
SHIVOKHIN Maksim  
SOLDERA Armand  
SPIEGEL Stefan

[regis.schach@fr.michelin.com](mailto:regis.schach@fr.michelin.com)  
[benoit.schnell@fr.michelin.com](mailto:benoit.schnell@fr.michelin.com)  
[nicolas.seeboth@fr.michelin.com](mailto:nicolas.seeboth@fr.michelin.com)  
[peiluo.shi@espci.fr](mailto:peiluo.shi@espci.fr)  
[maksim.shivokhin@uclouvain.be](mailto:maksim.shivokhin@uclouvain.be)  
[Armand.Soldera@USherbrooke.ca](mailto:Armand.Soldera@USherbrooke.ca)  
[sspiegel@wiley-vch.de](mailto:sspiegel@wiley-vch.de)

Michelin, Clermont-Ferrand  
Michelin, Clermont-Ferrand  
Michelin, Clermont-Ferrand  
ESPCI ParisTech  
University of Louvain  
University of Sherbrooke, Canada  
Wiley-UCH, Macromolecular  
Journals  
DSM

STOLK Jan

[jan.stolk@dsm.com](mailto:jan.stolk@dsm.com)

DSM

## T to Z

TANGUY François (P)  
TENGE-GIRAULT Sylvie  
THUILLIEZ Julien  
TIGHZERT Lan  
TRAVERT Pierrick  
TRUYOL Albert  
VACHERAND Jean-Michel  
VALETTE Rudy (P)  
VAN MELICK Harold  
VAN RUYMBEKE Evelyne (P)  
VANCAEYZEELE Cedric  
VERGELATI Caroll  
VIEYRES Arnaud (P)  
VILMIN Franck  
WOUTERS Guy  
YANG Dongmei  
ZERLAUTH Pierre  
ZOUAOUI Samia (P)

[francois.tanguy@espci.fr](mailto:francois.tanguy@espci.fr)  
[sylvie.girault@espci.fr](mailto:sylvie.girault@espci.fr)  
[julien.thuilliez@fr.michelin.com](mailto:julien.thuilliez@fr.michelin.com)  
[lan.tighzert@univ-reims.fr](mailto:lan.tighzert@univ-reims.fr)  
[pierrick.travert@fr.michelin.com](mailto:pierrick.travert@fr.michelin.com)  
[altruyol@club-internet.fr](mailto:altruyol@club-internet.fr)  
[jean-michel.vacherand@fr.michelin.com](mailto:jean-michel.vacherand@fr.michelin.com)  
[rudy.valette@mines-paristech.fr](mailto:rudy.valette@mines-paristech.fr)  
[harold.melick-van@dsm.com](mailto:harold.melick-van@dsm.com)  
[evelyne.vanruymbeke@uclouvain.be](mailto:evelyne.vanruymbeke@uclouvain.be)  
[cedric.vancaeyzele@u-cergy.fr](mailto:cedric.vancaeyzele@u-cergy.fr)  
[caroll.vergelati@eu.rhodia.com](mailto:caroll.vergelati@eu.rhodia.com)  
[arnaud.vieyres-exterieur@eu.rhodia.com](mailto:arnaud.vieyres-exterieur@eu.rhodia.com)  
[franck.vilmin@fr.michelin.com](mailto:franck.vilmin@fr.michelin.com)  
[guy.wouters@exxonmobil.com](mailto:guy.wouters@exxonmobil.com)  
[dongmei.yang@espci.fr](mailto:dongmei.yang@espci.fr)  
[pierre.zerlauth@fr.michelin.com](mailto:pierre.zerlauth@fr.michelin.com)  
[souma.zouaoui@yahoo.fr](mailto:souma.zouaoui@yahoo.fr)

ESPCI ParisTech  
ESPCI ParisTech  
Michelin, Clermont-Ferrand  
University of Reims  
Michelin, Clermont-Ferrand  
Michelin, Clermont-Ferrand  
CEMEF, Ecole Mines ParisTech  
DSM  
University of Louvain  
University of Cergy-Pontoise  
RHODIA  
LPMA, Lyon  
Michelin, Clermont-Ferrand  
EXXONMOBIL Chemical Europe INC  
ESPCI ParisTech  
Michelin, Clermont-Ferrand  
University of Mostaganem, Algeria