

# NTNU

# **BY COMPLEX OF A Structure of Complex Physical Phenomena in Materials** Pontifícia Universidade Católica do Rio de Janeiro, Brazil, February 17-22, 2014

The scope of the workshop: Scientific tutorials, talks and posters on soft and complex matter phenomena in materials and related phenomena and methods, such as flow of complex fluids in confined and complex environments including the physics of drops, emulsions, foams, granular systems, porous structures, micro-channels and micro-fluidics. In particular we will in this context have a special focus on physical phenomena underlying (Enhanced) Oil Recovery ((E)OR),.







## Invited speakers:

Vladimir Alvarado (Univ. Wyoming, USA) Wilson Barros (UFPE-Recife, Brazil) Daniel Bonn (Univ. Amsterdam, Netherlands) Heloisa Bordallo (Univ. Copenhagen, Denmark) Oliver Chao (Exploratory Unit, Sanofi R&D) Paul Dommersnes (Univ. Paris 7, France) Roosevelt Droppa Jr. (UFABC - Sao Paulo, Brazil) Antonio Figueiredo (Univ. Sao Paulo. Brazil) Azarmidokht Gholamipour-Shirazi (PUC-Rio de Janeiro, Brazil) Irep Gozen (Harvard Univ., USA) Kenneth D. Knudsen (Inst. for Energy Tech., Norway) Reidar Lund (Univ. Oslo, Norway) Yves Meheust (Univ. Rennes 1, France) Geraldo Jose da Silva (Univ. Brasilia, Brazil) Paulo R. de Souza Mendes (PUC-Rio de Janeiro, Brazil) Pavlo Mikheenko (Univ. Oslo, Norway) Wilson Ortiz (UFScar - SP, Brazil) Zbigniew Rozynek (Polish Acad. Sciences, Warsaw, Poland) Patrick Tabeling (ESPCI-ParisTech, France)

**Organizers:** Marcio Carvalho (PUC-Rio de Janeiro, Brazil) Jon Otto Fossum (NTNU-Trondheim, Norway)

## **Practical information to participants:**

The 4 day workshop will take place at Pontifícia Universidade Católica do Rio de Janeiro, Rua Marquês de São Vicente 225, Rio de Janeiro, Brazil, February 17-22, 2014..

For further information about the workshop, and for submission of contributions, contact Marcio Carvalho (<u>msc@puc-rio.br</u>) or Jon Otto Fossum (<u>jon.fossum@ntnu.no</u>). <u>Registration deadline for submission of contributed poster</u> abstracts is February 1, 2014. Submission should include title + coauthors/affiliations + ½ page abstract.











## Abstracts from

# 3<sup>rd</sup> International Workshop on

## **Complex Physical Phenomena in Materials**

Pontificia Universidade Católica do Rio de Janeiro - PUC-Rio, Brazil, February 17- 22, 2014

### Foreword

Welcome to the **3<sup>rd</sup> International Workshop on "Complex Physical Phenomena in Materials**" at Pontificia Universidade Católica do Rio de Janeiro - PUC-Rio, Brazil, February 17-22, 2014.

The 1<sup>st</sup> International Workshop on "Complex Physical Phenomena in Materials", held in *Recife*, Brazil, from December 14-17 2010, and organized by Prof. Mario Engelsberg, from the Physics Department of UFPE, Recife, Brazil, and by Prof. Jon Otto Fossum from the Department of Physics at NTNU, Trondheim, Norway, grew out of good and productive scientific collaborations. As it turned out, that 1<sup>st</sup> Workshop went well beyond the context of this bilateral collaboration and served as a venue for discussions on a wider range of complex phenomena in materials.

The 2nd International Workshop on "Complex Physical Phenomena in Materials" in Porto de Galinhas - PE, Brazil, January 31- February 3, 2012, was organized by Prof. Giovani Vasconcelos from the Physics Department of UFPE, Recife, Brazil, and by Prof. Jon Otto Fossum from the Department of Physics at NTNU, Trondheim, Norway. In the 2<sup>nd</sup> Workshop, we tried to follow the same guiding principles as for the 1<sup>st</sup> Workshop. We also tried to expand its scope not only with respect to the scientific contributions themselves but also including a roundtable session to discuss the translation of academic research within complex matter physics into industrial applications.

In organizing this 3<sup>rd</sup> International Workshop on "Complex Physical Phenomena in Materials", we expand the scope even further, and this time we have made it into a PhD level school in addition to being a regular Workshop. This 3<sup>rd</sup> Workshop is thus part of a "package" in the following way:

(i) Monday February 17<sup>th</sup> 2014: Short course on MRI (Wilson Barros UFPE and Daniel Bonn Univ. Amsterdam) for participating Master/PhD students; (ii) Tuesday February 18<sup>th</sup> - Friday February 21<sup>st</sup>: "3<sup>rd</sup> International Workshop on Complex Physical Phenomena in Materials"; (iii) Saturday February 22<sup>nd</sup> 2014: Short course on Finite Element Methods (Marcio Carvalho PUC-Rio) for participating Master/PhD students; (iv) Continued distance training via Skype of participating Master/PhD students during the following couple of weeks.

The total package (2 short courses + workshop) will constitute the total curriculum for a PhD/Master level course (7.5 CTS) at NTNU scheduled for this semester, course number FY8203 "Soft Condensed Matter". At the end of the short courses + workshop + distance training, participating students will have to pass a "distance" home-exam in order to get the CTS registered. The FY8203 course is open to any student that wish to participate, from anywhere in the world, the only requirement is being present at the lectures in Rio during the period February 16-23, taking part in the distance training, and passing the final exam.

The success of the two previous workshops was a clear evidence of the importance of having meetings that promote interactions between scientists from (seemingly) different fields and from different working environments (universities, research institutes, and industry research centers). In this 3<sup>rd</sup> Workshop, the central overall topic is on soft and complex matter phenomena in materials and related phenomena and methods. In particular we will have a focus on physical phenomena underlying (Enhanced) Oil Recovery ((E)OR), such as the physics of flow of complex fluids in confined and complex environments (e.g. the physics of drops, emulsions, foams, granular systems, porous structures, micro-channels and micro-fluidics).

This 3<sup>rd</sup> Workshop is made possible because of grants from the Norwegian agencies RCN (Research Council of Norway) - Petromaks2 Program, and SIU, and from the Brazilian agencies CAPES and CNPq, as well as from IBM-Brazil and from PUC-Rio Dept. of Mech. Eng. Proex Program, from CAPES. We gratefully thank all our sponsors.

The last sentence of the Foreword to the Book of Abstracts of the 1st Workshop in Recife in 20110 stated: "*We hope that this is not the last workshop of its kind*." It turned out not to be the last, and we have already secured partial funding from RCN – Petromaks2 for the 4<sup>th</sup> Workshop in the series to take place in Recife in 2016.

Welcome to Rio de Janeiro.

Marcio Carvalho (PUC-Rio, Brazil) and Jon Otto Fossum (NTNU, Norway)



Jon Otto Fossum (NTNU, Norway)

Marcio Carvalho (PUC-Rio, Brazil)

## **Workshop Program**

## 3<sup>rd</sup> International Workshop on "Complex Physical Phenomena in Materials", Pontifícia Universidade Católica do Rio de Janeiro - PUC-Rio, Brazil, Feb. 17- 22, 2014.

The workshop, and the two associated short courses (Monday Feb. 17th (NMR) and Saturday Feb 22nd (FEM)), will take place at the AMEX auditorium at IAG building, Pontificia Universidade Católica do Rio de Janeiro (PUC-Rio), Rua Marquês de São Vicente 225, Gávea, Rio de Janeiro, Brazil.

All days Feb. 16 – Feb. 21, buses will depart from Hotel Debret in Avenida Atlantica in Copacabana at 0715 am sharp.

Monday Feb. 17th: NMR short course, buses depart from Hotel Debret 0800 am. Saturday Feb. 22nd: FEM short course, buses depart from Hotel Debret at 0800 am.

	Feb 18, 2014 (Tue.)	Feb. 19, 2014 (Wed.)	Feb. 20, 2014 (Thu.)	Feb. 21, 2014 (Fri.)
0715	Buses depart from Hotel Debret	Buses depart from Hotel Debret	Buses depart from Hotel Debret	Buses depart from Hotel Debret
0800-0810	Welcoming remarks: Marcio Carvalho and Jon Otto Fossum Paulo Roberto de Souza Mendes	Wilson Ortiz & Pavlo Mikheenko	Paul Dommersnes	Patrick Tabeling
0810-0845				
0845-0930			Zbigniew Rozynek	
0930-0940		Coffee break	Coffee break	Coffee break
0940-1000	Coffee break	Contec break	Contec break	Contec break
1000-1010	Contec break	Roosevelt Droppa & Geraldo Jose da Silva	Alexander Mikkelsen	- Vladimir Alvarado
1010-1020	Daniel Bonn			
1020-1105			Irep Gozen	
1105-1130			Oliver Chao	
1130-1140		- Leander Michels		Azarmidokht Gholamipour-Shirazi
1140-1150	Alexandra Alicke			
1150-1200			Discussions	
1200-1400	Lunch Garota da Gavea	Lunch Garota da Gavea	Lunch Garota da Gavea	Lunch Garota da Gavea
1400-1445	Reidar Lund	Heloisa Bordallo	Antonio Figueiredo	Yves Meheust
1445-1530				Marcio Carvalho
1530-1600	Coffee break	Coffee break	Coffee break	Coffee break
1600-1620	Poster presentations	Pavlo Mikheenko	Azarmidokht Gholamipour-Shirazi	Ranena Ponce
1620-1640		Wilson Ortiz	Kenneth D. Knudsen	Raphael da Silva Alvim
1640-1700		Maycon Motta		James Moraes de Almeida
1700-1705	Poster session	Mathias Steiner		Katherine Aurand
1705-1720			Johann Penuela	
1720-1725		Discussions		Marcel Moura
1725-1740			Simone Bochner	
1740-1745				Closing remarks: Jon Otto Fossum
1745-1800			Discussions	
1800	Transport to Hotel Debret	Transport to Hotel Debret	Transport to Hotel Debret or to Academia de Cachaca	Transport to Hotel Debret
1900-		Workshop dinner in Copacabana: Palace Churrascaria	Suggested happy hour in Academia de Cachaca	

## **Short Courses:**

Monday - February 17 – Short Course on Magnetic Resonance Imaging 0900-1600: Wilson Barros (UFPE) (+Daniel Bonn (Univ. Amsterdam)) 0800: Departure from Hotel Debret, 1700: Reurn to Hotel Debret



Prof. Wilson Barros (UFPE)

Saturday - February 22 – Short Course on Finite Element Methods 0900-1600: Marcio Carvalho (PUC-Rio) 0800: Departure from Hotel Debret, 1700: Reurn to Hotel Debret



Prof. Marcio Carvalho (PUC-Rio)

Workshop:

## Tuesday - February, 18 - "Mechanics and Kinetics of Complex Fluids"

## 0715: Departure from Hotel Debret

8:00 - 8:10 Marcio Carvalho and Jon Otto Fossum: *Welcome* 

8:10 - 9:40 Paulo Roberto de Souza Mendes (PUC-Rio) *Thixotropy* 

## 9:40 - 10:10 COFFE BREAK

**10:10 - 11:40** Daniel Bonn (Univ. Amsterdam) *Why is (wet) granular rheology so complicated?* 

**11:40 - 12:00** Alexandra Alicke (PUC-Rio) *Rheological characterization of waxy crude oils* 

12:00 - 14:00 LUNCH

**14:00 - 15:30** Reidar Lund (Univ. Oslo) *Filming Kinetic Processes on the Nanoscale using Small-angle X-ray & Neutron Scattering* 

## 15:30 - 16:00 COFFE BREAK

**16:00 - 18:00 POSTER SESSION** Poster presentations 3 minutes per poster: 2 ppt slides per presenter to be handed in on Tuesday morning.

**1800: Departure from PUC** 

## Wednesday - February, 19 - "Condensed Matter Physics and Methods"

## 0715: Departure from Hotel Debret

8:00 - 9:30

Wilson Ortiz (UFSCar) and Pavlo Mikheenko (Univ. Olso) Superconductivity: brief history, materials and practical uses

## 9:30 - 10:00 COFFE BREAK

**10:00 - 11:30** Roosevelt Droppa (UFABC) and Geraldo Jose da Silva (UnB) *On x-ray methods in soft matter* 

**11:30 - 11:50** Leander Michels (NTNU) Intercalation and Retention of Carbon Dioxide in Synthetic Fluorohectorite Clay at Near-Ambient Conditions

## 12:00 - 14:00 LUNCH

**14:00 - 15:30** Heloisa Bordallo (Univ. Copenhagen) *Looking at hydrogen motions in confinement: The uniqueness of Quasi-Elastic Neutron Scattering* 

## 15:30 - 16:00 COFFE BREAK

**16:00 - 16:20** Pavlo Mikheenko (Univ. Olso) *Complex flux flow in superconducting films* 

**16:20 - 16:40** Wilson Ortiz (UFSCar) *Guidance of flux avalanches in microstructured superconducting films* 

**16:40 - 17:00** Maycon Motta (UFSCar) Enhanced pinning in superconducting thin films with graded pinning landscapes

**17:00 - 17:20** Mathias Steiner (IBM) Directed assembly of aligned carbon nanotube arrays in solution

**1800: Departure from PUC** 

19:00 -..... Workshop Dinner

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## Thursday - February, 20 - "Interface, Droplets and Suspensions"

#### 0715: Departure from Hotel Debret

**8:00 - 8:45** Paul Dommersnes (Univ. Paris 7) *Introduction to Electrohydrodynamics* 

8:45 - 9:30 Zbigniew Rozynek (Polish Acad. Sciences) *Electrohydrodynamic structuring of colloidal armoured drops* 

#### 9:30 - 10:00 COFFE BREAK

**10:00 - 10:20** Alexander Mikkelsen (NTNU) *Quincke – Electrohydrodynamic drop rotation* 

**10:20 - 11:05** Irep Gozen (Harvard Univ.) *Thermal migration of molecular lipid films* 

**11:05 - 11:50** Oliver Chao (Sanofi - Paris) *Lipid droplets in living cells* 

12:00 - 14:00 LUNCH

**14:00 - 15:30** Antonio Figueiredo (USP) *Nonlinear optical properties of magnetic colloids investigated with the z-scan technique* 

## 15:30 - 16:00 COFFEE BREAK

**16:00 - 16:20** Azarmidokht Gholamipour-Shirazi (PUC-Rio) *Micrometer-Sized Pickering Emulsions Stabilized by Laponite Nanoparticles* 

**16:20 - 17:05** Kenneth Knudsen (Inst. for Energy Technology) *Association structures of oil-water mixtures* 

**17:05 - 17:25** Johann Penuela (PUC-Rio) Drop break up in turbulent in the flow of diluted o/w emulsions through an orifice

**17:25 - 17:45** Simone Bochner (PUC-Rio) *Slot coating flow of particle suspensions* 

**1800: Departure from PUC** 

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# Friday - February, 21 - "Complex flows in micro channels and porous media"

#### 0715: Departure from Hotel Debret

#### 8:00 - 9:30

Patrick Tabeling (ESPCI-Paris) Introduction to Microfluidics

## 9:30 - 10:00 COFFE BREAK

**10:00 - 11:30** Vladimir Alvarado (Univ. Wyoming) *Complex Fluids and Interfaces and Waterflooding Enhancement Connections (EOR)* 

## 11:30 - 11:50

Azarmidokht Gholamipour-Shirazi (PUC-Rio) A Tale of Two Applications of Microfluidics: Kinetics Measurement and Alzheimer Diagnosis

#### 12:00 - 14:00 LUNCH

**14:00 - 14:45** Yves Meheust (Univ. Rennes 1) *The flow of an aqueous foam through a two-dimensional porous medium* 

**14:45 - 15:30** Marcio Carvalho (PUC-Rio) *Flow of oil-water emulsion through porous media (EOR)* 

## 15:30 - 16:00 COFFE BREAK

**16:00 - 16:20** Ranena Ponce (PUC-Rio): *Reservoir simulation of flow of complex fluids (EOR)* 

**16:20 - 16:40** Raphael da Silva Alvim (UFABC) *Multiscale modeling of clay surfaces and interaction with SiO2 nanoparticles for EOR applications* 

## 16:40 - 17:00

James Moraes de Almeida (UFABC) Molecular confinement of fluids on amorphous sílica nanopores

## 17:00 - 17:20

Katherine Aurand (NTNU) An overview of core flooding experiments investigating the application of hydrophilic silica nanofluids for enhanced oil recovery (EOR)

**17:20 - 17:40** Marcel Moura (University of Oslo) *Pressure driven drainage of fluid from a quasi-two-dimensional porous media* 

**17:40 - 17:50** Jon Otto (NTNU): *Closing remarks* 

**1800: Departure from PUC** 

## Poster presenters (8 submitted posters):

**Leander Michels** (Dept. of Physics, NTNU – Trondheim, Norway) EXAFS and XRD studies of water intercalation in synthetic nanosilicate Ni-Fluorohectorite

**Sylvia M. Mutisya** (NanoPetro, Centro de Ciências Naturais e Humanas , Universidade Federal do ABC, Santo André, SP, Brazil) *Multi-scale simulations of cement based materials.* 

**Giovanni Grassi** (Instituto de Física, Universidade de Brasília, Brasília – DF, Brazil and Dept. of Physics, Norwegian University of Science and Technology, Trondheim, Norway) *Cation Exchange in a Synthetic Clay Mineral* 

**Everton Carvalho dos Santos** (Dept. de Física, IGCE - Universidade Estadual Paulista – UNESP – Rio Claro - SP, Brazil) *Negative Differential Resistance in Ludwigite Fe3O2BO3* 

**Zbigniew Rozynek** (Dept. of Physics, Norwegian University of Science and Technology, Trondheim, Norway and Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland) *Electrohydrodynamic controlled assembly and fracturing of thin colloidal particle films confined at drop interfaces* 

**Marzena Prus** (Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland) Janus colloidal shells by microfluidics: Preliminary results on shell fabrication and sintering

**Marlon Ivan Valerio Cuadros** (Universidade Federal de São Carlos, SP, Brasil) Unraveling the behavior of a single superconducting weak-link using magneto-optical imaging

**Cicero Inacio da Silva** (PGNMA, NanoPetro-Universidade Federal do ABC, Santo André-SP, Brazil) *Combined GISAX and modeling studies on the wettability phenomena in Oil-Rock-Brine interface for Enhanced Oil Recovery applications* 

# Abstracts

# **Talks and posters**



## **Group Photo:**



## Tuesday - February, 18 - "Mechanics and Kinetics of Complex Fluids"

## 8:10 - 9:40

## Thixotropy

## Paulo Roberto de Souza Mendes Pontificia Universidade Católica do Rio de Janeiro, Rio de Janeiro, RJ, Brazil

Elasto-viscoplastic materials are structured materials that, when submitted to stresses below a threshold limit -- usually called the *yield stress* -- behave as a viscoelastic solid. When the yield stress is surpassed, a major microstructure collapse occurs which causes a steep viscosity decrease, and the mechanical behavior becomes predominantly viscous. Paints, medicines, biological fluids, drilling muds, cements, slurries, pastes, gels, among many other materials of practical interest present this kind of behavior. Most of these materials possess some degree of thixotropy, meaning that their microstructure requires a finite amount of time to respond to stress changes. In this lecture, we survey different manners that have been employed to model the mechanical behavior of these materials. Then we describe a novel constitutive model for these materials, and illustrate its performance by presenting predictions for a wide range of flow situations. Finally, we present a novel experimental technique involving large-amplitude oscillatory shear (LAOS) that can be used to determine the mechanical behavior of this type of materials.



Prof. Paulo Roberto de Souza Mendes

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#### 10:10 - 11:40

## Why is (wet) granular rheology so complicated? Daniel Bonn University of Amsterdam, Netherlands



Granular rheology is everywhere around us; the book by Duran quotes the stunning figure that the handling and transport of granular materials consumes roughly 10% of the world energy consumption. You might think that is a ridiculous figure, but if you think, for instance, about how much concrete is being manufactured and transported on this planet, that mining is an incredibly important industry, or that most of agriculture actually deals in some way with granular materials, you get a better feeling for how much energy is actually involved in dealing with these materials. I will discuss the rheology and mechanical properties of wet granular materials, and show why the behavior can be verv subtle. Once one understands the mechanical properties, I will show that one can use this knowledge to construct the perfect sandcastle, or to understand why the ancient Egyptians wetted the desert sand with water before sliding heavy stones over it.

Daniel Bonn

#### 11:40 - 12:00

## Rheological characterization of waxy crude oils Alexandra Alicke and Paulo Roberto de Souza Mendes Pontificia Universidade Católica do Rio de Janeiro, Rio de Janeiro, RJ, Brazil



It is well known that below the crystallization temperature the rheology of waxy oils changes from a Newtonian to an extremely complex non-Newtonian behavior, which is temperature- and shear-rate-history dependent. In this work, we describe an experimental protocol designed to ensure well-defined thermal and shear histories of a waxy crude oil sample to be submitted to rheological measurements. With the methodology used, repeatable and reliable results can be obtained in a rotational rheometer. We performed temperature ramps and stress-amplitude-sweep tests and compare the results obtained with the main trends observed, highlighting the effects of cooling and shear on the rheological properties of these oils.

Alexandra Alicke

#### 14:00 - 15:30

## Filming Kinetic Processes on the Nano-scale using Small-angle X-ray & Neutron Scattering Reidar Lund (Reidar.lund@kjemi.uio.no) Department of Chemistry, University of Oslo, 0315 Oslo

Time-resolved small-angle x-ray or neutron scattering techniques present powerful methods to probe kinetic processes in nanostructured systems directly on the relevant temporal and structural length scales. Examples include kinetics processes in self-assembled systems such as surfactant and block copolymers or nucleation & growth processes involved in the formation of nanoparticles. While the thermodynamics and structure have been studied extensively over the last decades, non-equilibrium kinetics and their dynamic properties are



much less known. This is mainly related to the difficulty to resolve structural changes in these systems on the relevant time scale of milliseconds-seconds using traditional methods. With the advent of more powerful sources and synchrotrons and high-flux reactors/spallation sources, small-angle x-ray & neutron scattering can nowadays resolve kinetic processes down to a few milliseconds on a routine basis. Coupled with appropriate sample environments; e.g. traditional mixing devices (e.g. stopped-flow apparatus) and /or designs for pump-probe type methods (spectrophotometers and lasers), the desired perturbation necessary to trigger and follow kinetic changes can be induced for a wide range of systems.

In this lecture we shall present an overview over smallangle scattering techniques, the principles of time resolved measurements and the theoretical modelling. We will explicitly compare various scattering techniques based on X-rays, light or neutrons and discuss their strengths or weaknesses. Examples will include equilibrium & non-equilibrium kinetics of micelles, nucleation and aggregation process involved in inorganic nanoparticles, light sensitive surfactant. In light of the results, current technical limitations and future challenges within the field will also be discussed.

- R. Lund; L. Willner and D. Richter. Adv. Polym. Sci., 2013, vol. 259, pp. 51–158.

- G. V. Jensen, R. Lund, J. Gummel, M. Monkenbusch, T. Narayanan, and J. S. Pedersen, J. Am. Chem. Soc., 2013, 135, 7214–7222.

- R. Lund, L. Willner, M. Monkenbusch, P. Panine, T. Narayanan, J. Colmenero, and D. Richter, Phys. Rev. Lett., 2009, 102, 188301.

- G. V. Jensen, R. Lund, J. Gummel, , T. Narayanan, and J. S. Pedersen, *to be submitted* 

Dr. Reidar Lund

## Wednesday - February, 19 - "Condensed Matter Physics and Methods"

## 8:00 - 9:30

## Superconductivity: brief history, materials and practical uses

Wilson Ortiz (UFSCar-Sap Paulo, Brazil) and Pavlo Mikheenko (Univ. Oslo, Norway)

Superconductivity - a macroscopic quantum phenomenon discovered more than one century ago - is a field including a huge variety of materials, many of which have encountered relevant practical applications. The first half of this Tutorial will be devoted to briefly review the history of Superconductivity, followed by an introductory discussion of the main features of superconducting materials and their uses in real life. The second part will discuss the feasibility of employing superconducting materials and techniques for a renewable energy economy.



Prof. Pavlo Mikheenko

Prof. Wilson A. Ortiz

## 10:00 - 11:30

## On X-ray methods in soft matter

G. J. da Silva<sup>1</sup> and R. Droppa Jr.<sup>2</sup> *1 Instituto de Física, Universidade de Brasília - UnB, Brasília-DF, Brazil 2 Centro de Ciências Naturais e Humanas , Universidade Federal do ABC – UFABC, Santo André-SP, Brazil* 

In this tutorial, we present the basic principles of X-ray diffraction and its application in soft condensed matter. The topics will follow the sequence: X-rays and their interaction with matter: polariza-tion factor, wave and photons. Kinematical scattering: from an electron to crystalline structures. Lattices and unit cells. Powder diffraction, temperature effects and synchrotron radiation sources. Be-sides the fundamentals of XRD theory, it will be addressed practical aspects and analysis methods of powder x-ray diffraction.

Bibliography:

[1] – Jens Als-Nielsen and Des McMorrow, Elements of Modern X-ray Physics, Second Edition, John Willey & Sons, United Kingdom, 2011.

[2] - Bertrand Eugene Warren, X-ray Diffraction, Dover Publications, New York, 1969.

[3] – Using Synchrotron X-ray Scattering to Study the Diffusion of Water in Weakly Sample-Hydrated Clay. Me-heust, Y., Sandness, B., Lovoll, G., Maloy, K. J., Fossum, J. O., da Silva, G. J., Mundim, M. S. P., Droppa Jr., R., Fonseca, D. M., Applied clay science, Japan, v. 12, p. 66-70, 2006.

[4] – Cation distribution in copper ferrite Nanoparticles of Ferrofluids: A synchrotron XRD and EXAFS investigation. Gomes, J. A., Sousa, M. H., da Silva, G. J., Tourinho, F. A., Mestinick Filho, J., Itri, R., Azevedo, G. A., Depeyrot, J. Journal of Magnetism and Magnetic Materials, v. 300, p. 213-216, 2006.

[5] - Synchrotron x-ray scattering studies of water intercalation in a layered synthetic silicate. da Silva, G. J., Fossum, J. O., Dimasi, E., Maloy, K. J., Lutnaes, S. B. Physical Review E - Statistical Physics, Plasmas, Fluids and Related Inter-disciplinary Topics, EUA, v. 66, p. 01130(2002).11:30 - 11:50



Prof. Roosevelt Dropped

Prof. Roosevelt Droppa Jr.

Prof. Geraldo J. da Silva

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#### 1130-1150

## Intercalation and Retention of Carbon Dioxide in Synthetic Fluorohectorite Clay at Near-Ambient Condition

Leander Michels,<sup>1</sup> Henrik Hemmen,<sup>1</sup> Zbigniew Rozynek,<sup>2</sup> Karin H. Rustenberg,<sup>1</sup> Tomás S. Plivelic,<sup>3</sup> Geraldo José da Silva,<sup>4</sup> and Jon Otto Fossum.<sup>1</sup> <sup>1</sup>Department of Physics, Norwegian University of Science and Technology, Norway. <sup>2</sup>Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland <sup>3</sup>MAX IV Laboratory, Lund University, Lund, Sweden. <sup>4</sup>Instituto de Física, Universidade de Brasília, Brasília – DF, Brazil



We show using x-ray diffraction that gaseous CO<sub>2</sub> intercalates into the interlayer space of the synthetic smectite clay fluorohectorite at conditions close to ambient. The rate of intercalation is found to be dependent on the interlayer cation, with about one order of magnitude increased rate in Li-fluorohectorite compared to Na-fluorohectorite. We further show that Li-fluorohectorite is able to retain  $CO_2$  in the interlayer space at room temperature, which could have applications related to CO<sub>2</sub> capture, transport and storage. De-intercalation starts occurring at temperatures exceeding 30 °C for Li-fluorohectorite and -5 °C for Nafluorohectorite

Leander Michels

## 14:00 - 15:30

## Looking at hydrogen motions in confinement: The uniqueness of Quasi-Elastic Neutron Scattering

Heloisa N. Bordallo Niels Bohr Institute - University of Copenhagen bordallo@nbi.ku.dk

Why in a barren and hot desert, clays can contain a significant fraction of water? Why concrete cracks? How can we demonstrate that complexation of a molecular drug does not alter its conformation in a way that affects its functionality? In this talk we present results on various studies using Quasi-Elastic Neutron Scattering (QENS) aimed at clarifying these questions.

To allow for a better understanding of neutron scattering, a brief introduction to the basics of its theory will be presented. Following the theoretical part, experimental results dealing with the effects of confinement on the water dynamics caused by the interfaces in clays and chalks and the nano- and micro-pores of concrete and dental cement will be discussed in detail.

At the end, recent investigations using QENS and thermo analysis on the influence of complexation of the local anesthetics Bupivacaine (BVC.HCI) and Ropivacaine (RVC.HCI) into the cyclic  $\beta$ -cyclodextrin oligosaccharide will be presented.

To conclude, the perspectives that the European Spallation Source brings to this subject are considered.



Prof. Heloisa Bordalo

16:00 - 16:20

## **Complex flux flow in superconducting films**

P. Mikheenko<sup>1</sup>, J. I. Vestgården<sup>1</sup>, S. Chaudhuri<sup>2</sup>, I. J. Maasilta<sup>2</sup>, Y. M. Galperin<sup>1,3</sup> and T. H. Johansen<sup>1,4</sup>

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The transition to renewable energy and the search for solutions of environmental problems like reduction of CO<sub>2</sub> emissions require new approaches. One of them is massive use of superconductors and utilization of liquid hydrogen as main energy carrier, which simultaneously works as efficient coolant for superconductors [1]. In their turn, superconductors offer no or small energy losses, unsurpassed efficiency and unique applications. Superconductors are must-to-have materials for most of large scale energy projects and with the adaptation of liquid hydrogen as main energy carrier they can easily be



used in everyday life. However, whenever large densities of energy are used, there is danger of instabilities and superconductors are not the exceptions. In order to use them safely, the magnetic flux flow during the instabilities must be understood in minute details

Typically flux flow forms complex patterns known in thin films as dendritic flux avalanches [2]. They propagate in the superconductor with the speed of tens kilometers per second and are big concern for many applications. Here we investigate the avalanches by magneto-optical imaging (MOI) combined with nanosecond time-scale pulse measurements [3]. Especially we design approach for putting barriers on the of propagating avalanches wav and unexpectedly uncover interesting behaviour that reminds penetration of the rays of light in the geometrical optics. The details of such behaviour will be explained.

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2. J. I. Vestgården, D. V. Shantsev, Y. M. Galperin and T. H. Johansen, Scientific Reports 2 886 (2012).

3. P. Mikheenko, A. J. Qviller, J. I. Vestgården, S. Chaudhuri, I. J. Maasilta, Y. M. Galperin and T. H. Johansen, Appl. Phys. Lett. 102 022601 (2013).

Prof. Pavlo Mikheenko

#### 16:20 - 16:40

### Guidance of flux avalanches in microstructured superconducting films

Wilson. A. Ortiz

Departamento de Física, Universidade Federal de São Carlos, São Carlos, SP, Brazil

In real applications of superconducting films, the availability of high critical currents (Jc) is a typical requirement, not necessarily for the purpose of transporting large current densities, but most likely because of the need to screen a substantial part of the applied magnetic field. The insertion of arrays of antidots (ADs) in a superconducting film can lead, at higher temperatures, to an increase of Jc. However, the existence of such pinning centers (PCs) facilitate flux channeling and, for temperatures below a characteristic threshold limit, unwanted instabilities of thermomagnetic origin lead to the occurrence of guided flux avalanches which, in the presence of ADs, occur for a wider interval of the applied magnetic field. A good compromise between the beneficial enhancement of Jc and the unavoidable increase of channeling when lattices of PCs are introduced, can be achieved by insertion of a non-periodic array of ADs, as previously pointed out by Silhanek et alli [Appl. Phys. Lett. 89, 152507, 2006]; and realized in practice by Motta and coworkers [Appl. Phys. Lett. 102, 212601, 2013], followed by other groups [Guenon et alli, Appl. Phys. Lett. 102, 252602, 2013; Wang et alli, Phys. Rev. B87, 220501, 2013]. The present contribution compiles recent results of a methodical study on superconducting systems with homogeneous and inhomogeneous distributions of ADs, as well as some others for which the shape of the ADs, or their separation, or even the symmetry of the lattice, varies from place to place along the film. The study was conducted on films of Nb and amorphous-MoGe, and includes magnetooptical imaging and measurements of the magnetic response in terms of temperature, applied magnetic field, amplitude of the AC excitation field and its frequency. For films decorated



Prof. Wilson. A. Ortiz

with ADs arranged in a regular mesh, avalanches are guided, forming patterns whose morphology is intimately related to the lattice symmetry and the shape of the holes [Motta et alli, unpublished]. For specimens decorated with non-periodic arrays of PCs, Jc is substantially enhanced and the avalanches take place at a reduced portion of the magnetic phase diagram [Motta et alli, Appl. Phys. Lett. 102, 212601, 2013]. Superconducting films with a small number of large holes (typically 4, symmetrically displayed) were also studied [Colauto et alli, Appl. Phys. Lett. 103, 032604, 2013], and the role of the tips of the holes on the morphology of secondary avalanches was demonstrated. In such configurations, circular perforations act as stop-holes, avoiding the appearance of secondary avalanches. A model considering the transport of supercurrents and heat transfer (within the sample and to the substrate), accounts for the morphology and time evolution of the avalanches actually observed [Vestgården et alli, Phys. Rev. B 85, 014516, 2012].

## 16:40 - 17:00

## Enhanced pinning in superconducting thin films with graded pinning landscapes

M. Motta<sup>1</sup>, F. Colauto<sup>1</sup>, W. A. Ortiz<sup>1</sup>, J. Fritzsche<sup>2</sup>, J. Cuppens<sup>3</sup>, W. Gillijns<sup>3</sup>, V. V. Moshchalkov<sup>3</sup>, T. H. Johansen<sup>4</sup>, A. Sanchez<sup>5</sup>, and A. V. Silhanek<sup>6</sup> <sup>1</sup> Departamento de Física, Universidade Federal de São Carlos, São Carlos, SP, Brazil <sup>2</sup> Department of Applied Physics, Chalmers University of Technology, GÄoteborg, Sweden <sup>3</sup> INPAC - Institute for Nanoscale Physics and Chemistry, Nanoscale Superconductivity and Magnetism Group, K.U.Leuven, Celestijnenlaan Leuven, Belgium <sup>4</sup> Department of Physics, University of Oslo, Norway <sup>5</sup> Departament de Física, Universitat Autµonoma de Barcelona, Barcelona, Spain <sup>6</sup> Département de Physique, Université de Liège, Belgium



magnetic flux is admitted into the sample in the form of quantized vortices. When superconducting currents are present, the vortices undergo a viscous motion which is prevented by the presence of pinning centers. A natural strategy in this attempt to anchor the flux lines is to spread, at random, small clusters of normal material, an approach adopted since long for superconducting alloys and reproduced more recently for high-temperature superconductors. Other commonly employed methods are the placement of arrays of holes (antidots) on the surface of superconducting films. In the present work, a graded distribution of ebeam lithographed antidots in superconducting thin films amorphous MoGe have been investigated by means of dc magnetization and magneto-optical imaging. The pinning landscape consists of a maximum density of antidots at the border of the sample which progressively decreases towards the center. At high temperatures and low fields where this graded distribution mimics the expected vortex distribution according to the Bean critical state model, a substantial increase of the critical current is observed with respect to a sample with periodically arranged antidots. At low temperatures and fields, the nonsamples also improves uniform the superconducting performance beyond that of a sample with periodically arranged antidots due to a strong suppression of thermomagnetic avalanches. These findings point out to the relevance of the, so far basically unexplored, non-uniform pinning landscape as a way to further increase the pinning properties of superconductors.

Dr. Maycon Motta

17:00 - 17:20

## **Directed assembly of aligned carbon nanotube arrays in solution** Mathias Steiner *IBM Research Brazil, Smarter Devices Group, Rio de Janeiro, Brazil*

In this presentation, I will report on the evaporation driven [1,2] and electric-field driven [3] assembly of aligned carbon nanotube arrays from aqueous solutions containing highly separated, 99% semiconducting carbon nanotubes. The aligned, semiconducting carbon



nanotube arrays constitute ideal building blocks for nano-electronic devices such as transistors [1,3] and light emitting p-i-n diodes [2]. I will discuss the experimental methods for manufacturing and characterization of solution-based carbon nanotube array devices. Also, I will outline some of the challenges that need to be addressed for future technological applications of carbon nanotube arrays.

[1] M. Engel, J. P. Small, M. Steiner, M. Freitag, A. A. Green, M. C. Hersam, and Ph. Avouris, "Thin Film Nanotube Transistors Based on Self-Assembled, Aligned, Semiconducting Carbon Nanotube Arrays," ACS Nano 2, 2445 (2008).

[2] M. Kinoshita, M. Steiner, M. Engel, J. P. Small, A. A. Green, M. C. Hersam, R. Krupke, E. E. Mendez, and Ph. Avouris, "The polarized carbon nanotube thin film LED," Opt. Express 18, 25738 (2010).

[3] M. Steiner, M. Engel, Y.-M. Lin, Y. Wu, K. Jenkins, D. B. Farmer, J. J. Humes, N. L. Yoder, J.-W. T. Seo, A. A. Green, M. C. Hersam, R. Krupke, Ph. Avouris, "High-frequency performance of scaled carbon nanotube array field-effect transistors," Appl. Phys. Lett. 101, 053123 (2012).

Dr. Mathias Steiner

## Thursday - February, 20 - "Interface, Droplets and Suspensions"

8:00 - 8:45

Introduction to Electrohydrodynamics Paul Dommersnes Matière et Systèmes Complexes, Université Paris 7 Diderot, , France



It is well known that electric fields can deform liquids, for example droplets tend to get stretched out by electric fields. Static electric fields can also in some cases induce steady electrohydrodynamic circulation flows in liquids. This lecture will give a brief introduction to electrohydrodynamics, with emphasis on the Taylor-Melcher leaky-dielectric model for emulsions droplets and particles [1,2,3]. Existing and potential applications of electrohydrodynamics to various technologies will also be discussed.

[1] Studies in electrohydrodynamics: The circulation produced in a Drop by an electric field G. Taylor, Proc. Royal Soc. London. Ser. A. Math. Phys. Sci. Vol. 291, p.159 (1966) [2] Electrohydrodynamics: A review of the role of interfacial stresses J. R. Melcher and G.I. Taylor, Annu. Rev. Fluid. Mech. Vol. 1: 111-146 (1969) [3] Electrohydrodynamics: The Taylor-Melcher leaky-dielectric model D. A. Saville, Annu. Rev. Fluid. Mech. Vol. 29: 27-64 (1997)

Prof. Paul Dommersnes

## 8:45 - 9:30

#### Electrohydrodynamic structuring of colloidal armoured drops

Zbigniew Rozynek<sup>1,2</sup>, P. Dommersnes<sup>3</sup>, A. Mikkelsen<sup>1</sup> L. Michels<sup>1</sup> and J.O. Fossum<sup>1\*</sup> <sup>1</sup>Dept. of Physics, Norwegian University of Science and Technology, Trondheim, Norway <sup>2</sup>Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland <sup>3</sup>Matière et Systèmes Complexes, Université Paris 7 Diderot, France <sup>\*</sup>Correspondence and requests for materials should be addressed to jon.fossum@ntnu.no

I will present how electric-field-based phenomena can be used to structure and dynamically control colloidal particle assemblies at drop surfaces, including (i) electrohydrodynamic convective assembly of jammed colloidal "ribbons", (ii) electro-rheological colloidal chains confined to a two-dimensional surface, (iii) spinning colloidal domains due to EDH flow instabilities, (iv) fabrication of patchy shells by means of electro-coalescence, (v) fracturing of colloidal thin films by electro-stretching, and finally (vi) an eye pupil-like effect obtained via reversible controlled change of two competing physical phenomena.





**Fig. 1.** Electric-field-assisted formation of (from left): a ribbon-like structure, an eye pupil-like effect, electro-rheological chains, 'shaking' of particles, and finally a very first moment of two drops coalescence leading to formation of Janus shell is captured.

<sup>1</sup> P. Dommersnes, Z. Rozynek, A. Mikkelsen, R. Castberg, K. Kjerstad, K. Hersvik, and J. O. Fossum, Nat. Commun. 4, 2066 (2013). Electrohydrodynamic driven assembly of particles on drop surfaces.

<sup>2</sup> Z. Rozynek, A. Mikkelsen, P. Dommersnes and J. O. Fossum, Nat. Commun. (revision submitted in Feb 2014).Electroformation of patchy colloidal capsules.

<sup>3</sup> Z. Rozynek, P. Dommersnes, A. Mikkelsen, L Michels and J. O. Fossum, Eur. Phys. J. - ST (submitted in Feb 2014). Electrohydrodynamic assembly and fracturing of collidal films.

<sup>4</sup> G. Taylor, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 291 (1425), 159 (1966). Electrohydrodynamics.

Dr. Zbigniew Rozynek

## 10:00 - 10:20

## Quincke – Electrohydrodynamic drop rotation

Alexander Mikkelsen<sup>1\*</sup>, Zbigniew Rozynek<sup>1</sup>, Paul Dommersnes<sup>1,2</sup> and Jon Otto Fossum<sup>1...</sup> <sup>1</sup> Department of Physics, NTNU, Trondheim, Norway. <sup>2</sup> Matière et Systèmes Complexes, Université Paris 7 Diderot, France. <sup>\*</sup>alexander.mikkelsen@ntnu.no, <sup>...</sup>jon.fossum@ntnu.no

The spinning of a rigid sphere in a uniform E-field has been known since Quincke [1] first developed the theory in 1896; if the induced dipole moment of a sphere is oriented opposite to the direction of the applied electric field, the unstable configuration becomes unstable above a critical E-field strength and a small perturbation is enough to displace the dipole and make the E-field rotate the sphere.

The physics of a Quincke rotating and weakly conducting drop is more complex since an applied E-field will deform the drop at any field strength. Taylor described the electrohydrodynamic deformation of a drop with the leaky dielectric model [2], while Salipante and Vlahovska [3] described how different liquid and size parameters affect the rotation.

We have studied how silicone oil drops covered with jammed micron sized PE particles and suspended in castor oil Quincke rotate compared to silicone oil drops without surface particles. Upon application of a uniform electric field, the shell slowly deforms into an ellipsoid before a Quinke rotation is initiated. Our experiments show that the critical electric



field strength  $E_c$  for the shell to Quincke rotate (750-800 V/mm) is remarkably lower than  $\underline{E}_c$  for pure silicone oil drops (300-350 V/mm).



Figure 1: Charge distribution in unstable equilibrium for a sphere suspended in a liquid having shorter relaxation time than the sphere. Above a critical field strength, constant rotation around an axis perpendicular to the electric field is induced by the misaligned dipole moment of the particle (right). The rotation can be either clock- or counterclockwise. Figure and caption adapted from[3].

1. Quincke, G., *Ueber Rotationen im constanten electrischen Felde*. Annalen der Physik, 1896. **295**(11): p. 417-486.

2. Taylor, G., *Studies in Electrohydrodynamics. I. The Circulation Produced in a Drop by Electrical Field.* Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 1966. **291**(1425): p. 159-166.

3. Salipante, P.F. and P.M. Vlahovska, *Electrohydrodynamics of drops in strong uniform dc electric fields*. Physics of Fluids, 2010. **22**(11).

Alexander Mikkelsen

#### 10:20 - 11:05

## **Thermomigration of molecular lipid films** Irep Gozen *Harvard Univ. Med. School.*

Living cells continuously probe their close-range environment and move accordingly in order to adjust to physical or chemical stimuli. Examples of such stimuli are a chemical concentration, temperature, or adhesion strength gradient. Movement in these gradients,



referred to as chemotaxis, thermotaxis or haptotaxis, respectively, benefits the cells in a particular way, for example by improving access to nutrients, creating connectivity or evading undesirable environmental conditions. Cell migration is a key mechanism in the function of immune system cells, sperm cells, wound healing and cancer cell metastasis.

The molecular machinery behind cell movement is complex. It involves a cascade of signaling events, structural elements, i.e., cytoskeleton filaments and motor proteins, as well as coordination of the extreme shape dynamics of the cell. There is a variety of experimental studies which, under laboratory conditions, focus on mimicking cell motility by exploiting a particular feature or component of the cellular machinery.

In the present study, we induce the migration of flat giant unilamellar vesicles (FGUVs), a variant of surface-supported lipid bilayer membranes, by generating a temperature gradient over a selected region on the membrane. Such gradient with a range of 20 µm has been achieved using a focused IR-B laser. The temperature gradient generated a surface adhesion gradient, along which FGUVs spontaneously relocated. We report on suitable lipid-substrate combinations, highlighting the critical importance of the electrostatic interactions between the engineered substrate and the membrane for reversible migration of intact vesicles. This is the first report on thermomigration of a supramolecular architecture. We also make use of the phenomenon to fabricate lipid nanotube networks in an entirely contactless manner.

Dr. Irep Gozen

## 11:05 - 11:50

## Lipid droplets in living cells

Oliver Chao, PhD Head/Emerging Biomedical Sciences, Exploratory Unit, Sanofi, France

Lipid droplets (LD) are ubiquitous in different tissues and cells, mainly composed of neutral lipids, as well as LD-specific proteins which interact with selective cellular components for designated functions. Extensive studies have demonstrated that LDs are not just 'fat particles' randomly assembled via hydrophobic interactions in the aqueous cellular environment. The formation of LDs is a well-regulated process, with sequential enzymatic reactions responding to distinctive stimulations. On the other hand, the reduction or utilization of LDs is also under tight control with *ad hoc* biochemical and biophysical signals.

The emerging important roles of LDs are beginning to be appreciated in a wider aspect of cellular functions. LDs can serve as lipid reservoirs to prevent toxicity elicited by excessive fats. LDs provide vital resources for cellular energy balance, as well as building blocks to sustain cell morphology. Consequently, dysregulation of LD metabolism underlies many human diseases, from diabetes/obesity to inflammation and cancer. Moreover, LDs have also been found to interplay with various pathogens (virus, bacteria) as entry point or gate-keeper. Conceivably, pharmaceutical development together with application on nanomaterials and microfluidic approaches to better monitor and manipulate LD are in progress.

For my presentation, I will elaborate and discuss the following subjects:

- 1. The biosynthesis of lipid droplets
- 2. Metabolisms of lipid droplets Lipolysis and lipophagy
- 3. LDs and the cellular energy homeostasis
- 4. Implications of LDs in human health and diseases



Dr. Oliver Chao

14:00 - 15:30

## Nonlinear Optical Properties of Magnetic Colloids Investigated with the Z-Scan Technique A.M. Figueiredo Neto Instituto de Física Universidade de São Paulo

In this talk we will present the investigation on the occurrence of the optical Kerr effect and two-photon absorption when an oil-based magnetic Fe<sub>3</sub>O<sub>4</sub> nanoparticles colloidal suspension is illuminated with high intensity femtosecond laser pulses. The frequency of the pulses is controlled and the Z-scan technique is employed in our measurements of the nonlinear optical Kerr coefficient (n<sub>2</sub>) and two-photon absorption coefficient ( $\beta$ ). From these values it was possible to calculate the real and imaginary parts of the third-order susceptibility. We observed that increasing the pulse frequency, additional physical processes take place, increasing artificially the absolute values of n<sub>2</sub> and  $\beta$ . The experimental conditions are discussed to assure the obtention of reliable values of these nonlinear optical parameters, which may be useful in all-optical switching and optical power limiting applications.

The free-carrier absorption cross-section  $\sigma$  of a magnetic colloid composed of magnetite nanoparticles dispersed in oil is also obtained by using the Z-scan technique in different experimental conditions of the laser beam. We show that it is possible to obtain  $\sigma$  with picosecond pulsed and millisecond chopped beams with pulse frequencies smaller than about 30 Hz. For higher pulse frequencies, the heating of the colloidal system triggers the appearance of the Soret effect. This effect artificially increases the value of  $\sigma$  calculated from the experimental results. The limits of the different experimental setups are discussed.



Prof. Antonio Figueiredo Neto

## 16:00 - 16:20

## Micrometer-Sized Pickering Emulsions Stabilized by Laponite Nanoparticles

Azarmidokht Gholamipour-Shirazi<sup>1</sup>, Marcio Carvalho<sup>1</sup>, Jon Otto Fossum<sup>2</sup> <sup>1</sup>PUC-Rio Dept. of Mech. Eng. Brazil, <sup>2</sup>NTNU Dept. of Physics, Norway

Oil-water Pickering emulsions were stabilized by nanosized Laponite particles. The effect of various parameters, such as nanoparticle concentration and stirring rate on the droplets' size and stability was investigated. The prepared emulsions were stable more than two weeks.



Azarmidokht Gholamipour-Shirazi

#### 16:20 - 17:05

## Association structures in oil-water mixtures

Kenneth D. Knudsen<sup>a</sup>, Sébastien Simon, Lilia Qassym<sup>b</sup>, Bicheng Gao<sup>b</sup>, Johan Sjöblom<sup>b</sup>
<sup>a)</sup> Physics Department, Institute for Energy Technology, N-2027 Kjeller, Norway.
<sup>b)</sup> Ugelstad Laboratory, Norwegian Univ- of Science and Technology, Trondheim, Norway



We show how scattering techniques are useful for studying nanosized particles, with particular emphasis on association structures formed in systems where oil and water interact. Tetra-acids are four-armed aliphatic molecules present in crude oil and responsible for severe flow reduction when accumulating at oil-water interfaces, eventually creating solid-like deposits. For the most abundant of these, the C<sub>80</sub>-tetraacid, a synthetic analogue has been made, allowing for detailed studies of aggregation and interactions. We also show how introduction of short-chained molecules (surfactants) can strongly modify the behaviour of these association structures.

Prof. Kenneth D. Knudsen

17:05 - 17:25

## ANALYSIS OF DROP BREAKUP PROCESS IN THE FLOW OF DILUTED O/W EMULSIONS THROUGH AN ORIFICE IN A PIPE.

Johann H. Penuela and Marcio S. Carvalho

Department of Mechanical Engineering, Pontificia Universidade Católica do Rio de Janeiro, Rio de Janeiro, RJ 22453, Brazil.

## Abstract.

An experimental device of an Oil-in-Water (O/W) dispersed flow has been used to analyze the drop break-up process of diluted emulsions induced by a cross sectional restriction in a pipe. Two mineral oils of moderate viscosity were dispersed in two different continuous phases, common water and a continuous phase formed by a mixture of substitute ocean water and STEOL® CS-330 (Stepan Company). The first objective of this work deals with the visualization of drop break-up of a single drop through the onfice by using an acrylic concentric orifice device and analysis of the images obtained from a high-speed camera. It was observed that entire drop break-up is taking place downstream of the orifice, rather than the initial acceleration zone upstream of the restriction. In addition, the visualization has allowed the identification of the break-up mechanism and some particular characteristics of the flow for various systems with different interfacial tension values. Results are in agreement with the previous observations made by Percy and Sleicher (A.I.Ch.E. Journal, 29 (1983) 161-164) and Galinat et al. (Chemical Engineering Science, 60 (2005) 6511 - 6528). The relative influence of dispersed phase viscosity and interfacial tension on maximum stable drop diameter was studied for diluted emulsions (5% vol. basis) of both mineral oils dispersed in the substitute ocean water continuous phase. Analysis of the data revealed that maximum stable drop sizes were in the inertial sub range, characterized exclusively by the energy dissipation rate per unit mass c. A linear mechanistic model for the inertial sub range, which account for drop interactions with turbulent velocity fluctuations in the flow and based in Kolmogorov's theory of isotropic turbulence, were developed to aid in data interpretation and provide a basis for correlation. The models were adjusted using a Non-Linear Optimization tool based in the Generalized Reduced Gradient (GRG2) code. From the Root Mean Squared Difference (RMSD) values as a measure for model's precision, it can be concluded that obtained correlations may be employed to get rough approximations for practical purposes.



Johann Penuela

## 17:25 - 17:45

## Slot Coating flow of particle suspensions Simone Araujo and Marcio Carvalho Dept. of Mechanical Engineering, PUC-Rio, Rio de Janeiro, Brazil

Slot coating process is commonly used in the manufacture of many different products such as flexible circuits, LCD and OLED displays, among others. The thickness of the coated liquid



Simone Bochner de Araujo

film depends on the flow rate and substrate velocity. The characteristics of the coated layer are directly related to the flow in the coating bead. Most of the available studies of slot coating flow consider the fluid as a Newtonian liquid. However, coating liquids are usually polymer solutions or particle suspensions. The effect of suspended particles in the coating liquid remains unknown. Local variation of particle concentration may lead to viscosity and surface tension gradients, which can change the flow pattern and consequently the process limits.

In this research, the particle suspension is a system composed by a Newtonian liquid as a continuous phase and rigid spherical particles as the dispersed phase. The particle transport equation takes into account diffusion due to viscosity and deformation rate gradients. The particle transport equation together with mass and momentum conservation equations are used to describe the two-dimensional free surface flow of a particle suspension in a slot coating bead. The system of differential equations is solved by the Galerkin/Finite element method.

The results show regions of high and low concentration of particles in the bead and the associated flow fields. The concentration profile along the depth of the coated layer, which may have a strong effect on the drying process and film performance, is a strong function of the process conditions. New development is under way to include the effect of surface tension variation (Marangoni effect).

## Friday - February, 21 - "Complex flows in micro channels and porous media"

8:00 - 9:30

## Introduction to Microfludics Patrick Tabeling MMN ESPCI-ParisTech, France



In this tutorial, I will present a number of notions useful to know for understanding the physics of miniaturization. The hydrodynamics of microfluidics will be introduced, along with a number of important effects to be aware of in order to understand the dynamics of droplets, the phenomena of mixing in microfluidic systems.



Prof. Patrick Tabeling

#### 10:00 - 11:30

## **Complex Fluids and Interfaces and Waterflooding Enhancement Connections (EOR)**

Vladimir Alvarado Department of Chemical and Petroleum Engineering University of Wyoming, Laramie, WY, USA

Enhanced-oil recovery relies on the traditional paradigms based on capillary number theory and viscous displacement in porous media. In these views, the mechanistic interfacial tension along with equilibrium contact line force balance on one hand, and the relative mobility of fluid phases, on the other hand, should be properly manipulated to enhance hydrocarbon production from the subsurface. These mechanisms are also recalled to explain other immiscible displacement results in environmental remediation in soils as well as other analogue systems. Complex fluids and interfaces offer additional EOR mechanisms, some of which are poorly understood. Examples of the latter arise in polymeric solutions, emulsions and foam flow. The most commonly used secondary recovery process in the oilfield is based



on injection of water, more traditionally called waterflooding, which is the starting point of many EOR processes, including the so-called chemical EOR. Injection of water with designed chemistry has been proposed as a novel enhanced-oil recovery (EOR) method in this family, often referred to as low salinity and smart waterflooding, among other names. The plethora of names encompasses a family of EOR methods relying on modifying water chemistry to increase oil recovery. Despite successful laboratory experiments and field trials, underlying EOR mechanisms remain controversial and poorly understood. The majority of hypotheses proposed rely on rock-fluid interactions. In this talk, we make connections interfacial properties between water-oil that require understanding dynamic properties of the interface, namely the interface visco-elastic properties. We will show how one must include additional mechanisms beyond capillary number theory such as buildup of viscoelastic interfaces at low-ionic



strength conditions. A crude oil from Wyoming is used to show the impact of dynamic interfacial viscoelasticity on recovery by measuring these properties using double-wall ring fixture. а dilational rheology as well as through direct visualization in microfluidic devices and coreflooding experiments in model rock. We close the talk by showing potential connections of this type of process with emulsion flow through porous media.

Prof. Vladimir Alvarado

## 11:30 - 11:50

## A Tale of Two Applications of Microfluidics: Kinetics Measurement and Alzheimer Diagnosis Azarmidokht Gholamipour-Shirazi

PUC-. Rio, Dept. of Mechanicl Engineeering, Brazil



Kinetics data by themselves can provide very useful information about the reaction. For fast and very fast reactions, special techniques have been developed to study them. However, the difficulties still remain. One is taking data at very short time intervals and the other one is controlling and changing the reaction temperature. Here we have developed a microfluidic based set up to measure the kinetics of fast reactions at very short time intervals and at different temperatures.

Western blotting is a common assay method for proteins. Despite being a highly selective method; it is a multistep method and it takes long time for one analysis. Here, a microchip-based Western blotting analysis system was developed, which consisted of a protein separation by microchip electrophoresis and successive aptamer reaction in a microchannel.

Dr. Azarmidokht Gholamipour-Shirazi

#### 14:00 - 14:45

## The flow of an aqueous foam through a two-dimensional porous medium

Yves Méheust, *Géosciences, Université Rennes 1, Rennes, France* 

Co-authors: S. A. Jones , B. Géraud , B. Dollet , J. Cox and I. Cantat (1) Institut de Physique, Université Rennes 1, Rennes, France

(2) Géosciences, Université Rennes 1, Rennes, France

(3) Institute of Mathematics and Physics, Aberystwyth University, Aberystwyth, U. K.

Flowing foams are used in many engineering and technical applications. A well-known application is oil recovery. Another one is the remediation of polluted soils: the foam is injected into the ground in order to mobilize pollutants present in the medium or deliver chemicals that are expected to react with the pollutants in situ. Apart from potential interesting physico-chemical and biochemical properties, foams have peculiar flow properties that applications might benefit of. In particular, viscous dissipation arises mostly from the contact zones between the soap films and the walls, which results in peculiar flows allowing the foam to invade narrow pores more efficiently than Newtonian fluids would.

We investigate the flow of a two-dimensional foam in three geometrical configurations. The flow velocity field and pressure field can both be reconstructed from the kinematics of the foam bubbles. We first consider a medium consisting of two parallel channels with different widths, at fixed medium porosity, that is, at fixed total combined width of the two channels. The flow behavior is highly dependent on the foam structure within the narrowest of the two channels [1]; consequently, the flux ratio between the two channels exhibits a non-monotonic dependence on the ratio of their widths. We then consider two parallel channels that are respectively convergent and divergent. The resulting flow kinematics imposes asymmetric bubble deformations in the two channels; these deformations strongly impact the foam/wall friction, and consequently the flux distribution between the two channels, causing flow irreversibility. We quantitatively predict the flux ratio as a function of the channel widths by



modeling pressure drops of both viscous and capillary origins [2], and compare it to what would be expected for a Newtonian fluid. This study reveals the crucial importance of boundary-induced bubble deformation on the mobility of a flowing foam. We then study how film-wall friction, capillary pressures and bubble deformation impact the flow of a foam in a two-dimensional porous medium consisting of randomly-positioned cylindrical grains. Irreversibility, intermittency and non-stationarity characterize the velocity field under permanently imposed inlet flow. In this grain geometry, flow channeling appears to be different from what would be expected for a Newtonian fluid, which allows a different part of the pore population to be visited. The influence of the ratio of the typical pore size to the bubble size is also addressed, and the evolution of the bubble size distribution as the foam penetrates inside the porous medium is measured.

[1] S. A. Jones, B. Dollet, Y. Méheust, S. J. Cox, I. Cantat, Structure-dependent mobility of a dry aqueous foam flowing along two parallel channels, *Phys. Fluids* **25**, 063101 (2013).

[2] B. Dollet, S. A. Jones, Y. Méheust, I. Cantat, Influence of the elastic deformation of a foam on its mobility in a model porous medium, submitted to *Phys. Rev. Lett.* (2013).

Prof. Yves Méheust

Abstracts from 3<sup>rd</sup> International Workshop on "Complex Physical Phenomena in Materials" Pontifícia Universidade Católica do Rio de Janeiro - PUC-Rio, Brazil, Feb. 17- 22, 2014

14:45 - 15:30

#### Flow of oil-water emulsion through porous media

V. Alvarado<sup>2</sup> and M. S. Carvalho<sup>1</sup> <sup>1</sup> Department of Mechanical Engineering, PUC-Rio, Rio de Janeiro, RJ, Brazil <sup>2</sup> Dept. of Chemical and Petroleum Engineering, University of Wyoming, Laramie, WY, USA



The flow properties of complex fluids through porous media give rise to multiphase flow displacement mechanisms that operate at different scales, from pore-level to Darcy scale. Experiments have shown that injection of oil-in-water emulsions can be used as an effective enhanced-oil recovery (EOR) method, leading to substantial increase in the volume of oil recovered. Pore-scale flow visualization as well as core flooding results available in the literature have demonstrated that the enhanced recovery factor is regulated by the capillary number of the flow. However, the mechanisms by which additional oil is displaced during emulsion injection are still not clear. In this work, we carried out two different experiments to evaluate the effect of emulsion flooding both at pore and macro scales. Visualization of the flow through sand packed between transparent plexiglass parallel plates shows that emulsion flooding improves the pore-level displacement efficiency, leading to lower residual oil saturation. Oil recovery results during emulsion flooding in tertiary mode (after waterflooding) in parallel sandstone cores with very different absolute permeability values prove that emulsion flooding also leads to enhancement of conformance or volumetric sweep efficiency. Combined, the results presented here show that injection of emulsion offers multi scale mechanisms resulting from capillary-driven mobility control.

Prof. Marcio S. Carvalho

Abstracts from 3<sup>rd</sup> International Workshop on "Complex Physical Phenomena in Materials" Pontifícia Universidade Católica do Rio de Janeiro - PUC-Rio, Brazil, Feb. 17- 22, 2014

#### 16:00 - 16:20

#### **Emulsion Flow Model Based on Mobility Control and Displacement Efficiency Effects**

Ranena V. Ponce Flores, Márcio S. Carvalho PUC-Rio, Department of Mechanical Engineering, Rio de Janeiro, RJ – Brazil poncerv@puc-rio.br, msc@puc-rio.br Vladimir Alvarado University of Wyoming, Department of Chemical and Petroleum Engineering, Laramie, U.S.A. valvarad@uwvo.edu



Emulsion flooding has a significant potential as an enhanced-oil recovery (EOR) strategy. Additionally, recovery mechanisms of several chemical EOR methods, including alkaline and alkaline-surfactant flooding applied to heavy oil, are consistent with the formation of in-situ emulsions. To enable emulsion flooding designs, EOR recovery mechanisms must be adequately represented in reservoir simulators to upscale porelevel effects to the continuum in porous media. In this work, we have incorporated two known effects of emulsion flooding, namely an increased porelevel displacement efficiency and second, a macroscopic mobility control. through а parametrization of the relative permeability curves as functions of the dispersed phase concentration. In the first mechanism, relative permeability endpoint saturation was parameterized with respect to the dispersed phase concentration to allow mobilization of residual oil after waterflooding.

The second mechanism was modeled through changes of the end-point value of the water relative permeability. Experimental results of water and emulsion flooding of viscous oil were historymatched. A parametric analysis of a 1/4 of a 5-spot geometry shows that the main contribution to incremental oil recovery observed experimentally corresponds to increase in the displacement efficiency. However, if viscous fingering is allowed to occurred, a benefit of mobility control is observed in the case of more unfavorable mobility ratio. Attention must be paid to details of the relative permeability curves and not only to oil viscosity. The results indicate that properly designed emulsions should produce significant recovery benefits.

Dr. Ranena Ponce Flores

## 16:20 - 16:40

## Multiscale modeling of clay surfaces and interaction with SiO2 nanoparticles for EOR applications

Raphael S. Alvim\*, Lucas S. De Lara, Aline O. Pereira and Caetano R. Miranda Centro de Ciências Naturais e Humanas, F ABC, Santo André, SP, Brazil \* raphael.alvim@ufabc.edu.br



Dr. Raphael S. Alvim

The adsorption of functionalized silica nanoparticles (NPs) onto representative clays and at the brine/oil/clay interfaces and their effect on enhanced oil recovery process were studied through a combined multiscale molecular modeling. Clay swelling is widely considered to be a major cause for the formation of damage in hydrocarbon reservoirs and can greatly reduce nanoparticle mobility in porous media. Initially, clay models (Montmorillonite and Muscovite) were investigated with properly van der Waals (vdW) correction, using density functional theory (DFT) with the generalized gradient approximation (GGA) and Gauge-Including Projector Augmented Wave (GIPAW) method implemented in the Quantum Espresso (QE) package. The clay surfaces sites were fully characterized by determining accurate forces models through simulated AFM and the surface sites studied by X-ray photoelectron spectroscopy (XPS) and state nuclear magnetic resonance (SS-NMR) spectroscopy simulations. Additionally, fully atomistic molecular dynamics (MD) were performed to simulate functionalized SiO2 nanoparticles adsorbed in clays and brine/oil/clay interfaces. By our MD results, a rationalized model for the effects of NPs in clay swelling was obtained based on the ion distribution and the double layers interactions formed on the clay and NP's surfaces. The surface tension, viscosity and diffusion were obtained for different functionalized SiO2 NPs under different salt concentration. Based on the MD results, Boltzmann Lattice calculations were performed to estimate the amount of oil displaced by injecting nanoparticles dispersed in aqueous solution.

#### 16:40 - 17:00

## Molecular confinement of fluids on amorphous sílica nanopores.

James M.de Almeida.\*, Yuri M. Celaschi and Caetano R. Miranda NanoPetro, Centro de Ciências Naturais e Humanas, UFABC Santo André, SP, Brazil caetano.miranda@ufabc.edu.br, james.almeida@ufabc.edu.br

In order to improve the mechanical properties, control degradation and obtain more protected and durable concrete, it becomes fundamental to understand the thermodynamics, kinetics and dynamics of the interaction of absorbed molecules (CO2, chlorine, nitrates) into cement at various conditions (temperature, pressure and salinity). Although the cement has been widely used for a long time, very little is known regarding the atomistic mechanism behind its functionality. Particularly, the dynamics of molecular systems at confined nanoporous and water hydration is largely unknown. In this work, we have focused on two problems on the Concrete Science using First Principles Methods. Firstly, the thermodynamic properties of ettringitite ( $(CaO)_3(Al_2O_3)(CaSO_4)_3 \cdot 32H_2O$ ) were determined and its relation with cement

degradation. Also, the structural, electronic and dynamic properties of confined H<sub>2</sub>O on lavered Tobermorite have been characterized by Car-Parrinelo molecular dynamics with without van der Waals and (vdW) interactions, at room temperature. In order to achieve the cement description at larger scales, we need to employ a combined molecular modeling approach. Firstly, a benchmark, comparing to ab initio results of two different force fields were performed. The first is the Clay Force Field, developed for clays, but widely used for cement. The second one is the REAX Force Field, which is a reactive force field, so it can describe bond breaks and forming. By settling a methodology for higher scale simulations, will be able to assess longer simulation times and larger systems, like, larger pore diameters. The obtained properties such as thermal decomposition reactions, vibrational spectra, diffusion coefficient and molecular ordering are important to understand the degradation effect, the hydration on cement as a whole and could be used to predict concrete properties at larger scale.



Dr. James M.de Almeida

## 17:00 - 17:20

## An overview of core flooding experiments investigating the application of hydrophilic silica nanofluids for enhanced oil recovery (EOR)

Katherine Aurand, Luky Hendraningrat, Shidong Li, and Ole Torsæter Norwegian University of Science and Technology (NTNU), Trondheim, Norway

As fewer new oil fields are being discovered, attention has turned to focusing on new ways to extract more oil from existing reservoirs through enhanced oil recovery (EOR). Nanofluids show promise as a new technology for better mobilizing the remaining oil.

More than 70 core flooding experiments were conducted to investigate the effects of hydrophilic silica nanoparticles for enhanced oil recovery. The nanofluids used in this study were composed of synthetic brine (3 wt % NaCl) and 0.01 to 1.0 wt % LHP silica nanoparticles. Primary particle diameter was 7 nm. The water-wet Berea sandstone cores had permeability values ranging from 5 to greater than 400 mD.



Interfacial tension (IFT) between the aqueous solution and the oil droplet decreased when nanoparticle concentration was increased. Increasing the amount of nanoparticles in the solution caused the contact angle between the oil droplet and the rock surface to decrease, resulting in increased water-wetness on the rock surface. These mechanisms, among others, resulted in increased oil recovery of around 5% of the original oil in place (OOIP) for water-wet cores. Intermediate-wet core samples produced up to 10% of the OOIP and oil-wet core samples produced up to 9% of the OOIP.

The optimal nanoparticle concentration in the aqueous solution without the addition of a stabilizer was 0.05 wt %. The displacement efficiency of various nanofluids concentrations (nanoparticles ranging from 0.01 to 1.0 wt %) showed that oil recovery increases with increasing nanofluids concentration until 0.05 wt %. After 0.05 wt %, oil recovery decreases until no additional recovery is achieved at 1.0 wt %. The 1.0 wt % silica nanofluid resulted in nanoparticles blocking pore channels, decreasing the cores' porosity and permeability values.

Primary nanoparticle diameters of 14 and 40 nm were compared to the 7 nm results. Oil recovery decreased as the nanoparticle diameter increased. Increasing the temperature from 25 to 50 to 80 degrees C resulted in an increase in oil recovery. The permeability values did not show a proportional relationship to incremental oil recovery, so this EOR method is potentially applicable in reservoirs ranging from low to high permeability.

Katherine Aurand

## 17:20 - 17:40

## Pressure-driven drainage of fluid from a quasi-two-dimensional porous medium

M. N. Moura<sup>1</sup>, K. J. Måløy<sup>1</sup> and R. Toussaint<sup>2</sup> <sup>1</sup>Department of Physics, University of Oslo, Norway <sup>2</sup>Institut de Physique du Globe de Strasbourg, CNRS, Strasbourg Cedex, France marcel.moura@fys.uio.no



We present results of ongoing experiments regarding two-phase flow in a quasi-two-dimensional porous medium. The porous matrix is formed by a single layer of glass beads (diameter approx. 1mm) that are randomly distributed in the interior of a modified Hele-Shaw cell. At the beginning of the experiment a mixture of glycerol (80% weight) and water (20%) completely saturates the pores of the system. By decreasing the pressure in the outlet (liquid phase), air starts to invade the porous network from the inlet, displacing the glycerol-water mixture as it moves. We employed a feedback algorithm in order to carefully control the pressure in the liquid phase and guarantee a slow drainage. Due to the fact that the system is transparent, the evolution of the flow can be tracked visually and by measuring the pressure near the outlet of the model we have computed a pressure-saturation curve for this system.

Marcel Moura

## Tuesday - February, 18 1600-1800 Poster Session

### Poster

## EXAFS and XRD studies of water intercalation in synthetic nanosilicate Ni-Fluorohectorite

Luciano Ribeiro<sup>1,\*</sup>, Leander Michels<sup>2</sup>, Maria Suely Pedrosa Mundim<sup>3</sup>, Marcelo Henrique Sousa<sup>4</sup>, Roosevelt Droppa Jr.<sup>5</sup>, J.O. Fossum<sup>2</sup>, Geraldo José da Silva<sup>3</sup>, Kleber Carlos Mundim<sup>6</sup> <sup>1</sup>Unidade Universitária de Ciências Exatas e Tecnológicas, Universidade Estadual de Goiás, Anápolis– GO, Brazil

<sup>2</sup>Dept. of Physics, Norwegian University of Science and Technology – Trondheim, Norway
 <sup>3</sup>Instituto de Física, Universidade de Brasília, Brasília – DF, Brazil
 <sup>4</sup>Faculdade de Ceilândia, Universidade de Brasília, Brasília – DF, Brazil
 <sup>5</sup>Universidade Federal do ABC, Santo André – SP, Brazil
 <sup>6</sup>Instituto de Química, Universidade de Brasília, Brasília – DF, Brazil

X-ray diffraction (XRD) is a well suited technique for studying processes of water intercalation and diffusion in smectite clay minerals. However this technique does not give any details about solvation of the interlayer cation, and therefore extended X-ray absorption fine structure (EXAFS) measurements in conjunction with XRD were performed in order to obtain complete information about this process as function of temperature. We study the synthetic smectite clay fluorohectorite with nickel as the interlayer cation, we show that the nickel ion and water form a structure similar to Ni(OH)<sub>2</sub>(Brucite-like structure), and that this is a pH dependent process.

#### Poster

### **Cation Exchange in a Synthetic Clay Mineral**

G. Grassi<sup>1,2</sup>, L. Michels<sup>2</sup>, Z. Rozynek<sup>2</sup>, R. Droppa Jr.<sup>3</sup>, A. Gholamipour-Shirazi<sup>4,5</sup>, J. O. Fossum<sup>2</sup>, and G.J. da Silva<sup>1</sup> <sup>1</sup>Instituto de Física, Universidade de Brasília, Brasília – DF, Brazil <sup>2</sup>Dept. of Physics, Norwegian University of Science and Technology, Trondheim, Norway 4UFABC, Santo André – SP, Brazil <sup>4</sup>Department of Mechanical Engineering, PUC-Rio, Brazil <sup>5</sup>Centro de Componentes Semicondutores, UNICAMP Campinas – SP, Brazil

In this work we use XRD and EDS to investigate the cation exchange process in a saline (NiCl<sub>2</sub>) aqueous suspension of confined ions in a synthetic clay mineral Lithium-fluorohectorite, and the dynamics of the Lithium-fluorohectorite to Nickel-fluorohectorite transition. From investigations of water uptake in the nanoporous space of Nickel-fluorohectorite, we found this transition dynamics to be faster than 1 minute. The results are compared to the traditional cation exchange procedures in which the exchange process is typically performed on the time-scale of weeks. The Debye-Scherrer method was also used to estimate and compare the number of platelets within the clay mineral particle stacks for the standard and the present cation exchange procedures.

#### Multi-scale simulations of cement based materials.

Sylvia M. Mutisya\*, James M.de Almeida.\*, Veronica M. Sanchez and Caetano R. Miranda NanoPetro, Centro de Ciências Naturais e Humanas, Universidade Federal do ABC Santo André, SP, Brazil

caetano.miranda@ufabc.edu.br; james.almeida@ufabc.edu.br

In order to improve the mechanical properties, control degradation and obtain more protected and durable concrete, it becomes fundamental to understand the thermodynamics, kinetics and dynamics of the interaction of absorbed molecules (CO2, chlorine, nitrates) into cement at various conditions (temperature, pressure and salinity). Although the cement has been widely used for a long time, very little is known regarding the atomistic mechanism behind its functionality. Particularly, the dynamics of molecular systems at confined nanoporous and water hydration is largely unknown. In this work, we have focused on two problems on the Concrete Science using First Principles Methods. Firstly, we have determined the free energy formation of ettringitite ((CaO)<sub>3</sub>(Al<sub>2</sub>O<sub>3</sub>)(CaSO<sub>4</sub>)<sub>3</sub>:32H<sub>2</sub>O) and its relation with cement degradation. Also, the structural, electronic and dynamic properties of confined H<sub>2</sub>O on layered Tobermorite have been characterized by Car-Parrinelo molecular dynamics with and without van der Waals (vdW) interactions, at room temperature. The obtained properties such as thermal decomposition reactions, vibrational spectra, diffusion coefficient and molecular ordering are important to understand the degradation effect, the hydration on cement as a whole and could be used to predict concrete properties at larger scale. In order to achieve the cement description at larger scales, we need to employ computationally cheaper methodologies. We perform a benchmark, comparing to ab initio results of two kinds of classical molecular dynamics force fields. The first is the Clay Force Field, developed for clays, but widely used for cement. The second one is the REAX Force Field, which is a reactive force field, so it can describe bond breaks and forming. By settling a methodology for higher scale simulations, will be able to assess longer simulation times and larger systems, like, bigger pore diameters. In that sense, our work can get closer to the engineering science needs.

## Poster

## Negative Differential Resistance in Ludwigite Fe3O2BO3

E. Carvalho<sup>1</sup>, I. Fier<sup>1</sup>, M. A. Continentino<sup>2</sup>, J. C. Fernandes<sup>3</sup>, L. Walmsley<sup>1</sup> 1Dept. de Física, IGCE - Universidade Estadual Paulista – UNESP –Rio Claro - SP, Brazil. 2Centro Brasileiro de Pesquisas Físicas, , Rio de Janeiro, RJ – Brazil. 3Instituto de Física, Universidade Federal Fluminense, Niterói – RJ, Brazil.

Negative differential resistance (NDR) has been observed in single crystals of Fe3O2BO3 parallel and perpendicular to the c axis direction in the range 220K-320K. For the range in the V-I curves showing NDR, low frequency self-sustained oscillations could be observed using a simple RC circuit, with the voltage needed to drive the oscillations decreasing with the increase of temperature, being about 3V at 300 K. Pulsed measurements at room temperature revealed the dependence of the NDR curves with the pulse width.

## Electrohydrodynamic controlled assembly and fracturing of thin colloidal particle films confined at drop interfaces

Zbigniew Rozynek<sup>1,2</sup>, P. Dommersnes<sup>3</sup>, A. Mikkelsen<sup>1</sup>, L. Michels<sup>1</sup>, J.O- Fossum<sup>1\*</sup> <sup>1</sup>Dept. of Physics, Norwegian University of Science and Technology, Trondheim, Norway <sup>2</sup>Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland <sup>3</sup>Matière et Systèmes Complexes, Université Paris 7 Diderot, Paris, France <sup>\*</sup>Correspondence and requests for materials should be addressed to jon.fossum@ntnu.no

Small particles can adsorb strongly at liquid interfaces due to capillary forces, which in practice can confine the particles to the interface. Here we investigate the electrohydrodynamic flow driven packing and deformation of colloidal particle layers confined at the surface of liquid drops. The electrohydrodynamic flow has a stagnation point at the drop equator, leading to assembly of particles in a ribbon shaped film. The flow is entirely controlled by the electric field, and we demonstrate that AC fields can be used to induce hydrodynamic "shaking" of the colloidal particle film. We find that the mechanical properties of the film is highly dependent on the particles: monodisperse polystyrene beads form packed granular monolayers which "liquefies" upon shaking, whereas clay form cohesive films that fracture upon shaking. The results are expected to be relevant for understanding the mechanics and rheology of particle stabilized emulsions.



Sample cell with electrodes (left panel), oil drop covered with polyethylene particles assembles into a ribbon-like structure due to electrohydrodynamic liquid flows (middle panel), and fracturing (in horizontal or vertical direction) of a thin clay mineral film caused by electro-stretching of a drop.

<sup>1</sup>A. van Blaaderen, M. Dijkstra, R. van Roij, A. Imhof, M. Kamp, B. Kwaadgras, T. Vissers, and B. Liu, Eur. Phys. J.- ST 222 (11), 2895 (2013). Review on self-assembly by means of E-fields.
 <sup>2</sup>P. Dommersnes, Z. Rozynek, A. Mikkelsen, R. Castberg, K. Kjerstad, K. Hersvik, and J. O. Fossum, Nat. Commun. 4, 2066 (2013). Electrohydrodynamic driven assembly of particle on drop surfaces.
 <sup>3</sup>G. Taylor, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 291 (1425), 159 (1966) Electrohydrodynamics.

<sup>4</sup>D. A. Saville, Annu. Rev. Fluid Mech. 29, 27 (1997). Electrohydrodynamics

## Janus colloidal shells by microfluidics: Preliminary results on shell fabrication and sintering

Marzena Prus<sup>1</sup>, Anna Kalicka<sup>1</sup>, Tomasz Szymborski<sup>1</sup>, Zbigniew Rozynek<sup>1,2\*</sup> Alexander Mikkelsen<sup>1</sup>, Paul Dommersnes<sup>3</sup>, Jon Otto Fossum<sup>1</sup> <sup>1</sup>Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland <sup>2</sup>Dept.of Physics, Norwegian University of Science and Technology, Trondheim, Norway <sup>3</sup>Matière et Systèmes Complexes, Université Paris 7 Diderot, Paris, France <sup>\*</sup>Correspondence and requests for materials should be addressed to: zrozynek@ichf.edu.pl

We have recently introduced a route for forming heterogeneous capsules by producing highly ordered jammed colloidal shells of various shapes with domains of controlled size and composition. These structures combine the functionalities offered by patchy particles and those given by permeable shells such as colloidosomes. The simple assembly route involves the synergetic action of electro-hydrodynamic flow and electro-coalescence: Two leaky-dielectric drops partly covered by particles are subject to a DC electric field, which first induces structuring of particles on each drop; subsequently, the drops attract and electro-coalesce, producing Janus shells.

The next natural step was to employ microfluidic methods to better control and increase the throughput of the fabrication of shells. This would lead us to facilitate foundation for many more advanced applications. We also decided to make our first steps to produce patchy particles, rather than patchy shells, by core solidification at the end of the route.





Before coalescence Janus shells

After Coalescence Capillary assisted fabrication of Solid capsule after sintering at 130 °C

 <sup>1</sup>P. Dommersnes, Z. Rozynek, A. Mikkelsen, R. Castberg, K. Kjerstad, K. Hersvik, and J. O. Fossum, Nat. Commun. 4, 2066 (2013). Electrohydrodynamic driven assembly of particle on drop surfaces.
 <sup>2</sup>Z. Rozynek, A. Mikkelsen, P. Dommersnes and J. O. Fossum, Nat. Commun. (revision submitted in Feb 2014). Electroformation of patchy colloidal capsules.

<sup>3</sup>Z. Rozynek, P. Dommersnes, A. Mikkelsen, L Michels and J. O. Fossum, Eur. Phys. J. - ST (submitted in Feb 2014).Electrohydrodynamic assembly and fracturing of collidal films.

## Unraveling the behavior of a single superconducting weak-link using magneto-optical imaging

M. Valerio<sup>1</sup>, M. Motta<sup>1</sup>, F. Colauto<sup>1</sup>, A. A. M de Oliveira<sup>2</sup>, A. M. H. de Andrade<sup>3</sup>, T. H. Johansen<sup>4</sup>, and W. A. Ortiz<sup>1</sup>

<sup>1</sup>Departamento de Física, Universidade Federal de São Carlos, SP, Brasil

<sup>2</sup> Instituto Federal de Educação, Ciência e Tecnologia de São Paulo, Matão, SP, Brazil

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There have been numerous studies of granularity in type-II superconductors, which are often in the form of bulk samples. The magnetic properties and, thus, the critical current of these materials, are usually separated into intra- and intergranular contributions. The intragranular component is related to the essence of the grains, governed by the inherent properties of the material while, on the other hand, the intergranular part is associated with grain boundaries coupling neighboring grains - the so-called weak-links (WLs). Most of the real systems contain a number of different kinds of WLs, such as secondary phases, twin plans, as well as other structural defects. In this work we have aimed our investigation to a more controllable type of WL, which consists of a system composed by two grains and a joint between them. Several Nb thin film with rectangular shape (0.8 x 2.5 mm<sup>2</sup>) and thickness of 200 nm, were deposited by magnetron sputtering in a UHV system. Focused Ion Beam (FIB) was then used to make a groove in the center of each film, along its width, creating thus two identical grains. The groove depth, which acts as a single WL, was varied from sample to sample by controlling the FIB dose. As such, WLs of different strength were created, linking the twin grains of each film. Using DC magnetization and AC magnetic susceptibility measurements, the magnetic behavior of such WLs was traced. In addition, Magneto-optical imaging (MOI) experiments were conducted on the two-grain films, revealing the actual flux distribution within the samples. Proper combination of MOI experiments and magnetic measurements allowed us to discriminate the characteristic contribution of the single WL, unraveling it from the overall response.

## Combined GISAX and modeling studies on the wettability phenomena in Oil-Rock-Brine interface for Enhanced Oil Recovery applications

C. I. Silva Filho (PG), J. F. Q. Rey (PQ), C. R. Miranda (PQ), S. Brochsztain (PQ) *PGNMA*, *NanoPetro-Universidade Federal do ABC*, *Santo André-SP*, *Brazil* 

With the increasing of global energy demands and the limitation of oil reserves, it become imperative to develop new methodologies and approaches in the Oil & Gas industry from upstream to downstream. The primary and secondary production of oil from a petroleum reservoir may recover less than half of the oil originally in place. To recover additional oil, it is necessary to apply enhanced oil recovery (EOR) techniques such as miscible gas displacement. Even so, more than 50% of the oil remains in the ground due to cappilarity forces and adsorption of the oil within mineral surfaces.

In order to improve this technique, breakthroughs on the way that we think and know about oil on porous rock systems are needed. In this scenario, understanding the wettability phenomena at molecular level of oil-water-rock interface is crucial. It may allow us in a cost/effective way to propose new methodologies to not only be able to extract more efficiently oil and methane from the ground by determining the favorable thermodynamic and chemical conditions for Enhanced Oil recovery, but also to improve the efficiency of processing of their products by tailoring catalysts for specific functions such as separation and filtering of molecules or cracking of hydrocarbon.

In this project, we combine experimental and molecular modeling tools to determine and predict the wettability phenomena in the oil-brine-rock system. By better understanding a) the molecular structure arrangement on the interface b) oil-water-rock interface interactions at molecular level, c) the absorption and desorption of hydrocarbon molecules on surfaces of rocks and d) their diffusivity under different conditions (ambient and reservoir), it is possible to explore and evaluate new directions to improve Enhanced Oil recovery (EOR).

One of the most effective EOR technologies is to modify the physical-chemistry properties of the oil in-situ under reservoir conditions. Some recent experiments involved EOR were performed in collaboration between University of Texas-Austin and Universidade Federal do ABC (UFABC). It has been found from these experiments that by adding bare and functionalized SiO2 nanoparticles, oil-wet calcite surface in water can become water-wet.

Functionalization means the modification of nanoparticles surface to perform a given function. This modification can be done by attaching different functional groups on the nanoparticle surface either hydrophobic and hydrophilic. These studies suggests that SiO2 nanoparticles can modify the wettability of calcite surface and improve the mobility of the oil absorbed to the calcite, which opens the possibility to be applied as an EOR technique.

## **Poster presentations:**



Cicero Inacio da Silva



Sylvia M. Mutisya

Leander Michels Marzena Prus





Everton Carvalho dos Santos Marlon Ivan Valerio Cuadros



Giovanni Grassi

## **Poster session:**

















## 51 Participants and their institutions:

## Brazil (35):

Alexandra Alicke (PUC- Rio de Janeiro) Simone Bochner de Araujo (PUC- Rio de Janeiro) Bruno Azevedo (PUC- Rio de Janeiro) Pedro Azevedo (PUC- Rio de Janeiro) Talita Botti (PUC- Rio de Janeiro) Marcio Carvalho (PUC- Rio de Janeiro) Kelly Colmenares (PUC- Rio de Janeiro) Ricardo Dias (PUC- Rio de Janeiro) Azarmidokht Gholamipour-Shirazi (PUC- Rio de Janeiro) Frederico Carvalho Gomes (PUC- Rio de Janeiro) Danmer Maza (PUC- Rio de Janeiro) Paulo Roberto de Souza Mendes (PUC- Rio de Janeiro) Giovane Nogueira (PUC- Rio de Janeiro) Ranena Ponce (PUC- Rio de Janeiro) Johann Penuela (PUC- Rio de Janeiro) Mildre Sallas (PUC- Rio de Janeiro) James Moraes de Almeida (UFABC, São Paulo) Raphael da Silva Alvim (UFABC, São Paulo) Roosevelt Droppa Jr. (UFABC, São Paulo) Sylvia Mueni Mutisya (UFABC, São Paulo) Cicero Inacio da Silva (UFABC, São Paulo) Wilson Barros (UFPE, Recife) Marlon Ivan Valerio Cuadros (UFSCar, São Carlos, SP) Maycon Motta (UFSCar, São Carlos, SP) Wilson Ortiz (UFSCar, São Carlos, SP) Giovanni Grassi (UnB, Brasilia) Geraldo José da Silva (UnB, Brasilia) Everton Carvalho dos Santos (UNESP, São Paulo) Antonio M. Figueiredo Neto (USP, São Paulo) Bernardo Engelke (Schlumberger-Brasil) Flavio da Costa Ferreira (Schlumberger-Brasil) Maria Moura (IBM Research Brasil) Mathias Steiner (IBM Research Brasil) Flavio Marchesini (Halliburton Brasil) Bernardo Coutinho Camilo dos Santos (Petrobras Brasil)

## Denmark (1)

Heloisa Bordallo (Niles Bohr Inst. - Univ. Copenhagen)

## France (4):

Oliver Chao (Sanofi – Paris) Paul Dommersnes (Univ. Paris 7) Yves Meheust (Univ. Rennes 1, Geosciences) Patrick Tabeling (ESPCI-ParisTech)

## Netherlands (1):

Daniel Bonn (Univ. Amsterdam)

Abstracts from 3<sup>rd</sup> International Workshop on "Complex Physical Phenomena in Materials" Pontifícia Universidade Católica do Rio de Janeiro - PUC-Rio, Brazil, Feb. 17- 22, 2014

## Norway (9):

Jon Otto Fossum (NTNU-Trondheim) Giovanni Grassi (NTNU-Trondheim on exchange fom UnB, Brazil) Leander Michels (NTNU-Trondheim) Alexander Mikkelsen (NTNU-Trondheim) Katie Aurand (NTNU-Trondheim) Kenneth D. Knudsen (IFE – Kjeller) Reidar Lund (Univ. Oslo) Pavlo Mikheenko (Univ. Oslo) Marcel Moura (Univ. Oslo)

## Poland (2):

Zbigniew Rozynek (Polish Acad, Science – Warsaw) Marzen Barbara Prus (Polish Acad, Science – Warsaw)

## USA (2):

Vladimir Alvarado (Univ. Wyoming) Irep Gozen (Harvard Univ.)

## Happy hour (Academia de Cachaca):



## Lunches (Garota de Gavea):



## Workshop Dinner (Palace Churrascaria):



Maps:



The Google map shows Hotel Debret (A) located on Copacabana beach and PUC-Rio (B). Distance is about 6 km if driving along Ipnanema beach as shown in the map.

# CAMPUS 32 MAP

#### DAR - Admissions and Registrars Office

Oversees PUC-Rio's administrative affairs including university admissions, transcripts, course registration and student IDs.

## Leme Building

This 12-story building houses the Humanities (Psychology, Philosophy, Theology), Biology and Sciences departments as well as Engineering classes.

2

3

6

7

12

13

#### <u>RDC Computer</u> Center

A state-of-the-art computer lab and graphics center, offering internet, printers and scanners. Wi-fi access can also be requested here.

## Soccer Fields

To promote an active and healthy lifestyle as well as facilitate postitive student interaction, the soccer fields offer a place to practice and play sports with friends.

## <u>Gênesis Institute</u>

Coordinates PUC-Rio's entrepreneurial program, providing support and resources for the successful development of new enterprises.

## Amizade Building

Kennedy Wing (K): Vice-Rectory, admin. offices for academic affairs, undergraduate and graduate programs. Frings Wing (F): cafeteria, library, banks

## ) <u>Church of the</u> <u>Sacred Heart</u>

The campus church covers an area of 700 square meters and seats 400 people. Daily mass is given.

## 14 <u>School of Business</u> Administration (IAG)

Offers undergraduate and graduate business courses. More than 50,000 professionals have graduated from the IAG business school.

## **PUC-Rio Bus Terminal**

The bus terminal facilitates transportation to/from campus with connections to many city bus lines and to metro-connectors to the Sigueira Campos and Botafogo stations.

## <u>Main Gate Entrance:</u> <u>Av. Padre Leonel Franca</u>

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Located near the main entrance of the campus, students have access to the taxi terminal, bike lot, newsstand, and many food stands.



### Pontifícia Universidade Católica do Rio de Janeiro



The rear gate serves as a pedestrian-only entrance to the lush PUC-Rio campus.

## Gymnasium

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In addition to offering physical education classes and basketball/volleyball courts, cultural events, film festivals and community events are hosted here.

## Parking Lot

Parking is available to faculty, students and visitors for a daily rate. Parking fees are paid for in the Frings Wing (F) of the Amizade Building.

## <u>Tent for Dept. of</u> <u>Art/Design classes</u>

This open-air tent structure is reserved for Art and Design courses and offers students a serene place to express their creativity.

## 26) <u>Solar Grandjean de</u> <u>Montigny</u>

The former residence of a French architect, this neoclassical building today hosts year-round cultural events and art exhibitions.

## 25 <u>Classrooms for</u> <u>Dept. of Art/Design</u>

Provides classroom space specifically for for courses taught by the Department of Art and Design.

## 24 Dept. of Art / Design

Offers programs in product design, graphic design, fashion design, audio visual design, multimedia and art history, among others.

#### **16** Previously the living quarters of PUC's priests, this 12-story building houses the International Programs Central Coordination Office (8th floor) and the departments of Letters and Social Services, among others.

## <u>Departmental Offices</u> (Vila dos Directórios)

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This colorful street of houses is home to departmental Office and a student-managed copy center and major-specific associations.