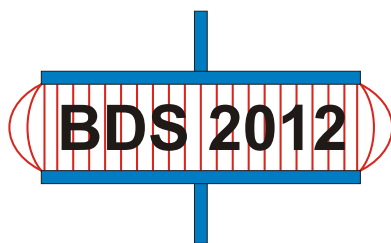


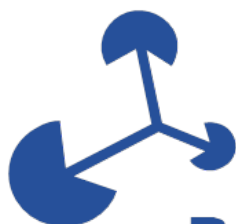
# Broadband Dielectric Spectroscopy and its Applications



**Leipzig - 2012**  
**3rd- 7th September**

**UNIVERSITÄT LEIPZIG**

The conference is a joint meeting of the 7th "Conference of the International Dielectric Society" and the 13th "Conference on Dielectric & Related Phenomena".



**BuildMoNa**

**INTER**phases  
&faces

*novento* Technologies 

 **IONIC LIQUIDS**  
DFG – SPP 1191

	Monday	Tuesday	Wednesday	Thursday	Friday
09:00	Tutorial I	Session 3	Session 7	Systems 11	Session 14
09:30		Biological Systems I	Terahertz Spectroscopy I	Confined systems I	Electrode Polarization
10:00					
10:30	Coffee	Coffee	Coffee	Coffee	Coffee
11:00	Tutorial II	Session 4	Session 8	Session 12	Session 15
11:30		Biological Systems II	Terahertz Spectroscopy II	Confined systems II	Industry forum
12:00					
12:30	Lunch	Lunch	Lunch	Lunch	Lunch
14:00	Opening	Session 5	Session 9	Session 13	Session 16
14:30	Session 1	Glassy Dynamics I	BDS and other techniques I	Charge transport	Conducting glasses Ionic Liquids
15:00	Theory of Dielectrics I				
15:30				Peter Debye Prize	
16:00	Coffee	Coffee	Coffee	Coffee	Closing
16:30	Session 2	Session 6	Session 10	City Tour	
17:00	Theory of Dielectrics II	Glassy Dynamics II	BDS and other techniques II		
17:30					
18:00	Welcome Party and Poster M				
18:30		Panel disc. Scaling of relaxiaion processes	Poster W		
19:00					
19:30					
20:00				Conference Dinner	
20:30	IDS Board Meeting	Piano Concert			
22:00					



**Monday, September 3th, 2012**

**Tutorial session I**

**9:00 to 10:30**

Röling	Bernhard	Marburg	Broadband electrochemical impedance spectroscopy	45 min
Sokolov	Alexei	Knoxville	Combining dielectric spectroscopy with scattering techniques	45 min

**Tutorial session II**

**11:00 to 12:30**

Kremer	Friedrich	Leipzig	The interplay between intra- and inter-molecular dynamics as studied by Broadband Dielectric- and Fourier-Transform Infrared -Spectroscopy	45 min
Feldman	Yuri	Jerusalem	Dielectric properties of biological materials; what we can learn from them?	45 min

**14:00 to 14:30 Opening of the conference**

**Session 1  
14:30 to 16:00 "Theory of Dielectrics I"**

Schröder	Christian	Vienna	Computational dielectric spectroscopy of polarizable ionic liquids	30 min.
Ngai	Kia	Pisa	Universal Relaxation and Diffusion in Interacting Complex Systems:	30 min.
Coffey	William	Dublin	High-Frequency resonance absorption as evidence for oscillation in a well before escape from a metastable in the kramers energy controlled diffusion	30 min.

<b>Session 2</b> <b>16:30 to 18:00</b>		<b>"Theory of Dielectrics II"</b>		
Dyre	Jeppe	Roskilde	Shear and dielectric responses of glass-forming liquids: What is the relation between the dielectric and mechanical relaxations?	30 min
Fragiadakis	Daniel	Washington	Molecular dynamics simulations of the Johari-Goldstein relaxation in a	20 min.
Nigmatullin	Raoul	Kazan	The derivation of the Cole-Cole and Cole-davidson functions and their	20 min.
Hilfer	Rudolf	Stuttgart	Time evolution of macroscopic dielectric phenomena	20 min.
<b>Tuesday, September 4th, 2012</b>				
<b>Session 3</b> <b>9:00 to 10:30</b>		<b>"Dielectric properties of Biological systems I"</b>		
Robitzki	Andrea	Leipzig	Microelectrode arrays for electrochemical immuno-sensing and cell	30 min.
Capaccioli	Simone	Pisa	Hydration Water Dynamics in Bioprotected Protein Glasses Studied by	30 min.
Mazzeo	Brian	Provo, Utah	From numerical simulation to measurement of protein dielectric relaxation	30 min.
<b>Session 4</b> <b>11:00 to 12:30</b>		<b>"Dielectric properties of Biological systems II"</b>		
Cerveny	Silvina	San Sebastian	Dielectric response on fully hydrated zwitterionic aminoacids	30 min.
Kyrtsis	Apostolos	Athens	Water and protein dynamics in protein-water mixtures	20 min.
Nakanishi	Masahiro	Tennessee	Dynamics of Hydrated Proteins	20 min.
Lyashchenko	Andrey	Moskau	From elementary dynamics to dielectric spectra and thermodynamic properties of water in electrolyte solutions.	20 min.

**Session 5**  
**14:00 to 16:00**  
**"Glassy dynamics and its scaling I"**

Loidl	Alois	Augsburg	Broadband nonlinear dielectric response of supercooled liquids	30 min.
Colmenero	Juan	San Sebastian	Chain dynamics in asymmetric polymer blends by broadband dielectric	30 min.
Massalska-Arodz	Maria	Krakow	Signatures of glass transition for partially ordered phases	20 min
Wibbenhorst	Michael	Leuven	Liquids with memory	20 min.
Böhmer	Roland	Dortmund	Dynamics in solid and supercooled liquid acid and base hydrates	20 min

**Session 6**  
**16:30 to 18:30**  
**"Glassy dynamics and its scaling II"**

Gainaru	Catalin	Dortmund	The Debye process in monoalcohols: a century-old puzzle and means to its	30 min.
Runt	James	Pennsylvania	Dynamics of Microphase Separated Polyurea and Polyurethane Copolymers	30 min.
Lunkenheimer	Peter	Augsburg	Fast dynamics of glassforming liquids probed by dielectric spectroscopy	30 min
Nozaki	Ryusuke	Hokkaido	Origin of boson peak in polyhydric alcohols	30 min.

**18:30 to 20:00**  
**Panel discussion: "The scaling of relaxation processes"**

**Wednesday, September 5th, 2012**

**Session 7**  
**9:00 to 10:30**  
**"Terahertz spectroscopy I"**

Havenith-Newen	Martina	Bochum	THz Spectroscopy: A Novel Experimental Tool to Study Water Network	30 min.
Feldman	Yuri	Jerusalem	Unexplored avenues of human skin: Reading personal stress in the Sub-THz	30 min.
Yamamoto	Naoki	Kobe City	Temperature and hydration dependence of functional proteins studied by	30 min.

<b>Session 8</b> <b>11:00 to 12:30</b>		<b>"Terahertz spectroscopy II"</b>	
Kawase	Kodo	Tokio	Tunable THz wave sources and real life applications
Ben Ishai	Paul	Nagoya	Water Revisited – Unifying a Myriad of Beliefs
Andachi	Tomoyo	Kobe City	Low-frequency dynamics of lipid studied by terahertz time-domain
Hayut	Itai	Jerusalem	The circular polarization of sub-THz signal reflected from the human skin
<b>Session 9</b> <b>14:00 to 16:00</b>		<b>"BDS and other techniques I"</b>	
Richert	Ranko	Tempe,	Heating Liquid Dielectrics by Time Dependent Fields
Bartos	Josef	Bratislava	Atomistic and molecular probe characterization of poly(isoprene)s by PALS
Ulanski	Jacek	Lodz	Impedance measurements and modelling of the persistent photoexcitation
Huth	Heiko	Rostock	AC-calorimetry as a complementary method to dielectric spectroscopy
Saad	Azima	Cairo	Studies of Particle Dispersion of Plasticized Poly (vinyl chloride) / Organically Modified Montmorillonite Nanocomposites
			30 min.
			30 min.
			20 min.
			20 min.
			20 min.



**Session 10**  
**16:30 to 18:30**  
**"BDS and other techniques II"**

Gerhard	Reimund	Potsdam	Physico-Chemical Modification of Polymer Dielectrics for Electromechanically Active Elastomers, for Piezoelectric Systems, and for Pyro- or Piezoelectric Time domain reflectometry technique for the Aqueous and Non-Aqueous	20 min.
Kumbharkhane Singh	Ashok Lokendra P.	Nanded Tempe,	Two-channel impedance spectroscopy for comparing the dynamics of 2-ethyl-	20 min.
Boucher	Virginie M	San Sebastian	Aging-time dependence of the segmental relaxation time of PVAc/SiO2 nanocomposites: a combined BDS and TSDC study	20 min.
Novikov Kisel	Gennady Renata	Chernogolovka Lodz	Comparative dielectric studies of Ag nanoparticles in matrix of polymers and Comparison of relaxation processes in poly(2-(2-methoxyethoxy)ethyl methacrylate) hydrogels differ on crosslinking density.	20 min.

**Thursday, September 6th, 2012**

**Session 11**  
**9.00 to 10:30**  
**"Confined systems of different dimensionality I"**

Fukao	Koji	Ritsumeikan	Heterogeneous and aging dynamics in single and stacked thin polymer films	30 min.
Alegria	Angel	San Sebastian	Dynamics of rouse chains under soft-confinement with different geometries	20 min.
Schönhalbs	Andreas	Berlin	Glassy dynamics of ultra-thin polymer films investigated by a combination of	20 min.
Dequidt	Alain	Aubiere	Mechanical Properties of Thin Confined Polymer Films Close to the Glass Transition in the Linear Regime of Deformation: Theory and Simulations	20 min.

<b>Session 12</b> <b>11:00 to 12:30</b>		<b>"Confined systems of different dimensionality II"</b>	
Floudas	George	Ioannina	Soft matter under Hard confinement
Kremer	Friedrich	Leipzig	Glassy Dynamics in one- and two-dimensional geometrical confinement
Prevosto	Daniele	Pisa	Influence of interfacial interactions and annealing on dielectric relaxation in
<b>Session 13</b> <b>14:00 to 15:30</b>		<b>"Charge transport and glassy dynamics"</b>	
Sokolov	Alexei	Tennessee	Ionic conductivity in glass-forming systems and polymers
Ezquerro	Tiberio	Madrid	On the dielectric relaxation of Natural Rubber and the effect of vulcanizing
Cangialosi	Daniele	San Sebastian	Are the thermal T <sub>g</sub> and the segmental dynamics in polymer thin films fully
Nogales	Aurora	Madrid	Dynamics on nanotubes of a potential ferroelectric polymer
<b>15:30 to 16:00</b>		<b>Peter Debye Prize - Award Ceremony and Lecture</b>	
<b>Friday, September 7th, 2012</b>			
<b>Session 14</b> <b>9:00 to 10:30</b>		<b>"Electrode &amp; Maxwell-Wagner Polarization"</b>	
Boiteux	Gisèle	Lyon	"Novel Polymeric Materials for Electrochemical Applications based on epoxy r
Sergei	Anatoli	Lyon	Interfacial polarization in dielectric spectra: theory and applications
Niklasson	Gunnar A.	Uppsala	Impedance spectroscopy on electrochromic tungsten and nickel oxide films
Abd-El-Messieh	Salwa L.	Dokki, Egypt	Dielectric relaxation of NBR/EPDM Blend loaded with various types of nano scaled carbon black. Applicability of some conductivity models.

<b>Session 15</b>		<b>Industry Forum with panel discussion</b>	
<b>11:00 to 12:30</b>			
Petzold	Albrecht	Goodyear	15 min.
Logakis	Emmanuel	ABB	15 min.
Reich	Marisa	Schott Mainz	15 min.
Svanberg	Christer	Borealis	15 min.
<b>Session 16</b>		<b>"Conducting glasses and ionic liquids"</b>	
<b>14:00 to 16:00</b>			
Rössler	Ernst	Bayreuth	30 min.
Paluch	Marian	Katowice	30 min.
Sangoro	Joshua	Oak Ridge	30 min.
Röling	Bernd	Berlin	30 min.
<b>Closing</b>			
<b>16:00</b>			



# Introduction

**BDS 2012** is a festival of Dielectrics. In 2012 there are many things to celebrate; (i) one hundred years ago P. Debye published (Phys. Zeitschrift 13, 97 (1912)) for the first time his famous formula, which is still the basis for analysing dielectric relaxation processes; (ii) the International Dielectric Society (IDS) has developed since its foundation in 2002 in a splendid manner. International conferences were organized in 2001 (Jerusalem), in 2002 (Leipzig), in 2004 (Delft), in 2006 (Poznan), in 2008 (Lyon) and in 2010 (Madrid) with increasing attendance; (iii) the “Peter Debye Prize for Young Investigators for Excellence in Dielectric Research” has been recognized as an extraordinary distinction in the field with Anatoli Serghei as prize winner in 2006, Periklis Papadopoulos and Daniele Prevosto in 2008 and Catalin Gainaru in 2010; (iv) the equipment has developed strongly covering typically 8-10 decades (or more) in frequency or time; (v) temperature- and pressure- dependent measurements can be carried out readily with commercially available systems; (vi) the amount of sample material required for dielectric measurements can be reduced down to the limit of monomolecular layers and of isolated polymer coils. The scope of the conferences has widened enormously covering nowadays hot topics like “Scaling of relaxation frequencies”, “Terahertz spectroscopy”, “Charge transport and glassy dynamics”, “The interrelationship between Impedance Spectroscopy, Electrochemical measurements and Broadband Dielectric Spectroscopy”, “Biological systems” to mention a few. Dielectric methods gain increasing interest in modern technology. One can be happy to witness and to be part of this exciting development.

Friedrich Kremer, Chairman of BDS 2012 and of IDS



# General Information

## Tutorial

The tutorial will be held in the large auditorium on Monday 3rd of September from 9:00 to 12:30 and covers basic concepts of BDS as well as advanced applications and complementary techniques. It is open for students of the Leipzig School of Natural Sciences “BuildMoNa” and all conference participants.

## Talks

The program will consist of talks of 20–30 minutes length (including discussion). To ensure that there is enough time for each speaker it is inevitable to stay in time. In the lecture hall a video projector with a native resolution of 1024x768 pixels is available, which accept VGA signals via a 15-pol. Sub-D-socket. Digital connections to the projector via DVI-D-socket are also possible. These adapters will be available on site. Others (such as Apple’s Mini DisplayPort, Mini DVI, or HDMI) are to be brought by the speakers themselves. Please make sure that your presentation works properly before the session starts.

## Posters

Poster sessions are held on Monday at 18:00 (3rd of September, poster with numbers 1–49) and on Wednesday at 18:30 (5th of September, posters with numbers greater than 49) in the reception hall of the chemistry department.

The posters can be pinned to the poster walls between Monday and Wednesday and will be present for the whole time. Please remove your poster before Thursday morning, as then the poster boards will be removed. Equipment to fix the posters to the boards will be available on site. We kindly ask the presenters to be at their poster(s) for discussions during the allocated time.

The poster boards at the University of Leipzig are dimensioned 1.2 m width  $\times$  1.45 m height. Therefore, please be aware that your poster has to be printed in the portrait orientation, i.e., width smaller than height.

## Conference Desk

The conference desk opens on Monday (3rd of September) and is located in the Aula of the Physics Department (see map on page 14). Please get registered there as soon as you arrive. You will receive your conference documents, name badge and meal vouchers.

**Opening hours: Mo: 8:30 to 18:00, Tue to Fri: 9:00 to 16:30**

## Wi-Fi access

During the conference you can access the event Wi-Fi of the University using the following settings. After you are connected to the network you need to accept the terms of service within your web browser. This needs to be done once per day. The following services will be provided: http(s), pop3(s), imap(s), vpn and ssh.

Network name: UniLeipzig-Event

Password (PSK): GIBeT-2012

Security: WPA2/AES

IP-address: automatic (DHCP)

DNS-server: automatic (DHCP)



## Lunch

Lunch will be offered between 12:30 and 14:00 at the Mensa Liebigstr., which is about 10 minutes walking distance from the institute (see map on page 14 or backsheet). In the dining-hall there will be an area reserved just for conference attendees. With the conference documents you get luncheon vouchers for each day of the conference which allow you to choose one out of three hot meals (the menu list of the week can be viewed at <http://www.studentenwerk-leipzig.de/mensen-und-cafeterien/speiseplan/>). Instead of a meal you may have a salad and a bun from the salad bar. Additionally, with the voucher you can take a 0.5-l-drink and a dessert which will be provided close to the reserved place. After your meal your conference ID allows you to take a coffee from the service area. Everything exceeding the aforementioned extent has to be paid by yourselves.

## Conference Dinner

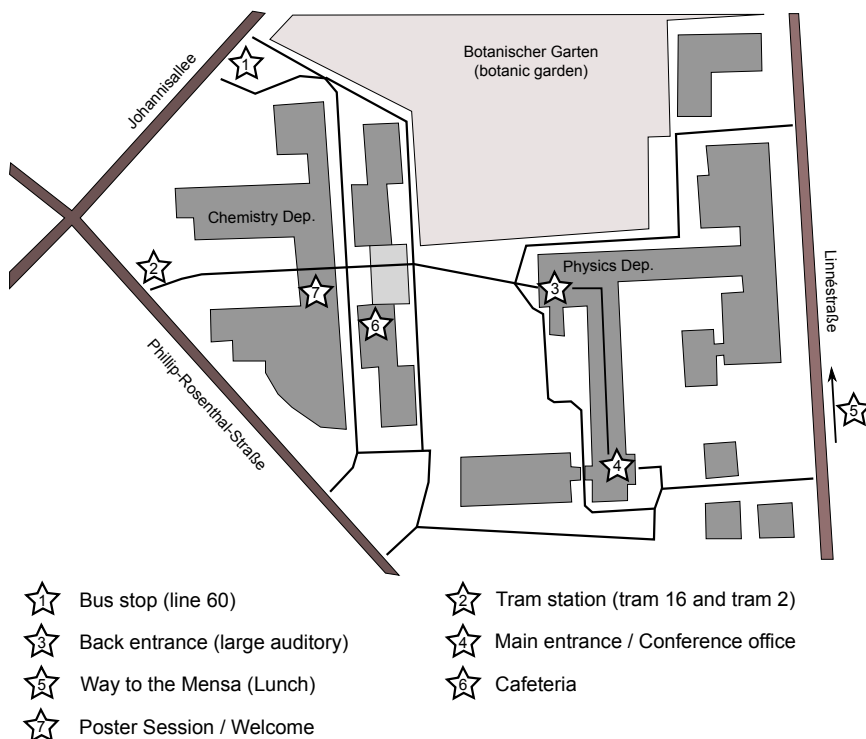
The Conference dinner takes place after at 20:00 on Thursday in Auerbachs Keller. It is one of the most famous restaurants of the world, as even Goethe's Faust had a glass or two there. The restaurant is situated within the Mädlar Passage in the city centre (see map on backsheet). If you participate in the city tour you will be guided there. The menu can be found within the Appendix on page 175.

## Public Transport

Your conference name badge is valid as a ticket for public transport between Monday and Friday (03.09–07.09) for all trams, trains and buses within the MDV (Mitteldeutscher Verkehrsverbund) zone 110. This covers the whole inner city of Leipzig and be sufficient for most of the trips you plan. The timetables of Johannisalle (station next to the Chemistry Department) and public transport network map, including zone boundaries, are provided at the end (page 176–180).

## Conference Venue

The conference takes place in the Faculty of Physics and Earth Sciences of the University of Leipzig situated in the south-east of Leipzig. The talks are held in the large lecture hall, whereas the poster session and the welcome party are located in the reception hall of the chemistry department. Be aware, that both departments are locked by the security service at 19:00 in the evening. We will ensure that the main entrances (as shown on the map below) remain open, but no side entrance can be used after that time.



# 1 Timetable

## 1.1 Programme Monday

### Tutorial I, Monday 9:30–10:30

- 09:00 **Broadband Electrochemical Impedance Spectroscopy** 45  
B. Roling *Department of Chemistry, University of Marburg, Hans-Meerwein-Straße, 35032 Marburg, Germany*
- 09:45 **Combining dielectric spectroscopy with scattering techniques** 47  
A.P. Sokolov *Department of Chemistry, University of Tennessee, Knoxville, TN 37996, USA*

### Tutorial II, Monday 11:00–12:30

- 11:00 **The interplay between intra- and inter-molecular dynamics as studied by Broadband Dielectric- and Fourier-Transform Infrared -Spectroscopy** 46  
F. Kremer<sup>1</sup>, W. Kossack<sup>1</sup>, P. Papadopoulos<sup>2</sup>, M. Jasiurkowska<sup>1</sup>, M. Treß<sup>1</sup>, E. U. Mapesa<sup>1</sup>, W. K. Kipnusu<sup>1</sup> and C. Iacob<sup>1</sup> <sup>1</sup> *Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany* <sup>2</sup> *Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany*
- 11:45 **Dielectric properties of biological materials; what we can learn from them?** 45  
Y. Feldman *Department of Applied Physics, The Hebrew University of Jerusalem, 91904, Israel*

## Session 1: Theory of Dielectrics I, Monday 14:30-16:00

- 14:30 **Computational dielectric spectroscopy of polarizable ionic liquids** 48  
C. Schröder *Institute for Computational Biological Chemistry, University of Vienna, Vienna, Austria*
- 15:00 **Universal Relaxation and Diffusion in Interacting Complex Systems: Fundamental Physics and Rich Applications** 49  
K.L. Ngai *Dipartimento di Fisica, Università di Pisa, Largo B. Pontecorvo 3, I-56127, Pisa, Italy*
- 15:30 **High-frequency resonance absorption as evidence for oscillation in a well before escape from a metastable state in the Kramers energy controlled diffusion model** 49  
W.T. Coffey<sup>1</sup>, Y.P. Kalmykov<sup>2</sup>, S.V. Titov<sup>3</sup> and D.S.F. Crothers<sup>4</sup>  
<sup>1</sup> *Department of Electronic and Electrical Engineering, Trinity College, Dublin 2, Ireland* <sup>2</sup> *Lab. Mathématiques et Physique, Université de Perpignan Via Domitia, 52, Avenue de Paul Alduy, 66860 Perpignan Cedex, France* <sup>3</sup> *Institute of Radio Engineering and Electronics, Russian Academy of Sciences, Vvedenskii Square 1, Fryazino, Moscow Region, 141190, Russian Federation* <sup>4</sup> *Dept. of Applied Mathematics and Theoretical Physics, Queen's University Belfast, Belfast, BT7 1NN, Northern Ireland*

## Session 2: Theory of Dielectrics II, Monday 16:30-18:00

- 16:30 **Shear and dielectric responses of glass-forming liquids: What is the relation between the dielectric and mechanical relaxations?** 50  
C. Gainaru<sup>1</sup>, T. Hecksher<sup>2</sup>, N.B. Olsen<sup>2</sup>, R. Böhmer<sup>1</sup> and J.C. Dyre<sup>2</sup>  
<sup>1</sup> *Fakultät für Physik, Technische Universität Dortmund, 44221 Dortmund, Germany* <sup>2</sup> *Roskilde Univ, DNRF Ctr Glass and Time, IM-FUFA, Dept Sci Syst and Models, DK-4000 Roskilde, Denmark*
- 17:00 **Molecular dynamics simulations of the Johari-Goldstein relaxation in a molecular liquid** 51  
D. Fragiadakis and C.M. Roland *Naval Research Laboratory, Chemistry Division (Code 6120), Washington DC, USA*

- 17:20 **The derivation of the Cole-Cole and Cole-davidson functions and their possible generalizations** 52  
A.F. Kamzin, I.I. Popov and R.R. Nigmatullin *Kazan (Volga region) Federal University, Institute of Physics, Theoretical Physics and Radioelectronics Departments, Kazan, Russian Federation*
- 17:40 **Time Evolution of Macroscopic Dielectric Phenomena** 52  
R. Hilfer *Insitut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Germany*

**18:00–20:00 Welcome Party and Poster M (poster no. 1–49)**

## 1.2 Programme Tuesday

### Session 3: Dielectric properties of biological systems I, Tuesday 9:00–10:30

- 09:00 **Microelectrode arrays for electrochemical immuno-sensing and cell monitoring** 53  
A.A. Robitzki, O. Pänke, A. Steude, S. Schmidt and H.G. Jahnke *University of Leipzig, Centre for Biotechnology and Biomedicine, Institute of Biochemistry, Division of Molecular biological-biochemical Processing Technology, Deutscher Platz 5, 04103 Leipzig, Germany*
- 09:30 **Hydration Water Dynamics in Bioprotected Protein Glasses Studied by Broadband Dielectric Spectroscopy** 54  
S. Capaccioli<sup>1,2</sup>, D. Prevosto<sup>2</sup>, P.A. Rolla<sup>1</sup>, A. Paciaroni<sup>3</sup> and K.L. Ngai<sup>1</sup> <sup>1</sup> *Dipartimento di Fisica, Università di Pisa, Largo Pontecorvo 3, 56127 Pisa, Italy* <sup>2</sup> *Istituto per i Processi Chimico Fisici (IPCF), CNR, Pisa, Italy* <sup>3</sup> *Dipartimento di Fisica, Università di Perugia, Via Pascoli, Perugia, Italy*
- 10:00 **From numerical simulation to measurement of protein dielectric relaxation in solution** 55  
B.A. Mazzeo<sup>1</sup>, B.L. Mellor<sup>1</sup> and D.D. Busath<sup>2</sup> <sup>1</sup> *Department of Electrical and Computer Engineering, Brigham Young University, Provo, UT 84602, USA* <sup>2</sup> *Department of Physiology and Developmental Biology, Brigham Young University, Provo, UT 84602, USA*

**Session 4: Dielectric properties of biological systems II, Tuesday 11:00–12:30**

- 11:00 **Dielectric response on fully hydrated zwitterionic aminoacids** 56  
S. Cervený<sup>1</sup>, I.R. Arteché<sup>1</sup>, A. Alegría<sup>2</sup>, J. Colmenero<sup>1-3</sup> <sup>1</sup> *Centro de Física de Materiales-Material Physics Centre (MPC), CSIC-Universidad del País Vasco (UPV/EHU), Paseo Manuel de Lardizabal 5 (20018), San Sebastian, Spain* <sup>2</sup> *Departamento de Física de Materiales, UPV/EHU, Facultad de Química, San Sebastián, Spain* <sup>3</sup> *Donostia International Physics Center, Paseo Manuel de Lardizabal 4, San Sebastián, Spain*
- 11:30 **Water and protein dynamics in protein-water mixtures** 57  
A. Kyritsis<sup>1</sup>, A. Panagopoulou<sup>1</sup> and N. Shinyashiki<sup>2</sup> <sup>1</sup> *National Technical Univ. of Athens, Department of Physics, 157 80 Athens, Greece* <sup>2</sup> *Department of Physics, Tokai University, Hiratsuka, Kanagawa, 259-1292 Japan*
- 11:50 **Dynamics of Hydrated Proteins** 57  
M. Nakanishi, A.L. Agapov and A.P. Sokolov *University of Tennessee, Oak Ridge National Laboratory, Department of Chemistry, 552 Buehler Hall, 1420 Circle Dr, 37996-1600, Knoxville, USA*
- 12:10 **From elementary dynamics to dielectric spectra and thermodynamic properties of water in electrolyte solutions** 58  
A. Lyashchenko<sup>1</sup>, A. Lileev<sup>1</sup>, I. Karataeva<sup>2</sup> and T. Novskova<sup>2</sup> <sup>1</sup> *Institute of General and Inorganic Chemistry RAS, Moscow* <sup>2</sup> *Moscow State University of Environmental Engineering, Moscow*

**Session 5: Glassy dynamics and its scaling I, Tuesday 14:00–16:00**

- 14:00 **Broadband nonlinear dielectric response of supercooled liquids** 58  
Th. Bauer, P. Lunkenheimer and A. Loidl *Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany*
- 14:30 **Chain dynamics in asymmetric polymer blends by broadband dielectric spectroscopy and MD-simulations** 60  
J. Colmenero *Centro de Física de Materiales, CFM, (CSIC-UPV/EHU) University of the Basque Country, San Sebastián, Spain*

- 15:00 **Signatures of glass transition for partially ordered phases** 60  
M. Massalska-Arodz , E. Juszynska , L. Kolek , J. Krawczyk , N. Osiecka and T. Rozwadowski *Institute of Nuclear Physics Polish Academy of Sciences Krakow, Poland*
- 15:20 **Liquids with memory** 61  
M. Wübbenhorst<sup>1</sup>, S. Capponi<sup>1</sup> and S. Napolitano<sup>1,2</sup> <sup>1</sup> *Department of Physics and Astronomy, Katholieke Universiteit Leuven, Celestijnenlaan 200D, Leuven, 3001, Belgium* <sup>2</sup> *Department of Physics, Université Libre de Bruxelles, Boulevard du Triomphe CP 223, Bâtiment NO, B-1050 Bruxelles, Belgium*
- 15:40 **Dynamics in solid and supercooled liquid acid and base hydrates** 63  
H. Didzoleit , M. Frey , C. Gainaru and R. Böhmer *Fakultät für Physik, Technische Universität Dortmund, 44221 Dortmund, Germany*
- Session 6: Glassy dynamics and its scaling II, Tuesday 16:30–18:30**
- 16:30 **The Debye process in monoalcohols: a century-old puzzle and means to its resolution** 62  
C. Gainaru and R. Böhmer *Fakultät für Physik, Technische Universität Dortmund, 44221 Dortmund, Germany*
- 17:00 **Dynamics of Microphase Separated Polyurea and Polyurethane Copolymers** 63  
J. Runt<sup>1</sup>, D. Fragiadakis<sup>2</sup> T. Choi<sup>1</sup> and C.M. Roland<sup>2</sup> <sup>1</sup> *Department of Materials Science and Engineering, Penn State University, University Park, PA 16802 USA* <sup>2</sup> *Naval Research Lab, Chemistry Division, Code 6120, Washington DC 20375 USA*
- 17:30 **Fast dynamics of glassforming liquids probed by dielectric spectroscopy** 64  
P. Lunkenheimer<sup>1</sup>, M. Köhler<sup>1,2</sup> and A. Loidl<sup>1</sup> <sup>1</sup> *Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany* <sup>2</sup> *present address: Osram AG, 86136 Augsburg*
- 18:00 **Origin of boson peak in polyhydric alcohols** 65  
R. Nozaki *Department of Physics, Faculty of Science, Hokkaido University, Sapporo, Japan*

**16:30–18:30 Panel Discussion: “The scaling of relaxation processes”**

**20:30–22:00 IDS Board meeting**

## 1.3 Programme Wednesday

### Session 7: Terahertz Spectroscopy I, Wednesday 9:00–10:30

- 09:00 **THz Spectroscopy: A Novel Experimental Tool to Study Water Network Dynamics** 66  
M. Havenith *Physical Chemistry II, Ruhr University Bochum, NC 7/74, 44780 Bochum, Germany*
- 09:30 **Unexplored avenues of human skin: Reading personal stress in the Sub-THz frequency range** 66  
Y. Feldman, A. Puzenko, P. Ben Ishai and E. Safrai *Department of Applied Physics, The Hebrew University of Jerusalem, Givat Ram, 91904, Jerusalem, Israel*
- 10:00 **Temperature and hydration dependence of functional proteins studied by terahertz time-domain spectroscopy** 67  
N. Yamamoto<sup>1</sup>, A. Tamura<sup>2</sup>, K. Tominaga<sup>1,2</sup> <sup>1</sup> *Molecular Photoscience Research Center, Kobe University, Japan* <sup>2</sup> *Graduate School of Science, Kobe University, Japan*

### Session 8: Terahertz Spectroscopy II, Wednesday 11:00–12:30

- 11:00 **Tunable THz wave sources and real life applications** 68  
K. Kawase<sup>1,2</sup>, S.R. Tripathi<sup>1,2</sup>, M. Yamaguchi<sup>1</sup> and S. Hayashi<sup>2</sup>  
<sup>1</sup> *Nagoya University, Ecotopia Science Institute, Furocho, Nagoya 464-8603, Japan* <sup>2</sup> *RIKEN, Advanced Science Institute, 519-1399 Aramaki-cho, Sendai 980-0845, Japan*



- 11:30 **Water Revisited – Unifying a Myriad of Beliefs** 68  
P. Ben Ishai<sup>1,2,4</sup>, E. Mamontov<sup>2</sup>, A.P. Sokolov<sup>2,3</sup>, J. Nickels<sup>2,3</sup>, K. Kawasa<sup>4</sup> and Y. Feldman<sup>1</sup> <sup>1</sup> *Department of Applied Physics, The Hebrew University of Jerusalem, Givat Ram Jerusalem 94901, Israel* <sup>2</sup> *Chemical and Engineering Materials Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA* <sup>3</sup> *Department of Chemistry and Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA* <sup>4</sup> *EcoTopia Science Institute, Nagoya University Furocho, Chikusa, Nagoya 464-8603, Japan*
- 11:50 **Low-frequency dynamics of lipid studied by terahertz time domain spectroscopy** 70  
T. Andachi<sup>1</sup>, N. Yamamoto<sup>2</sup>, A. Tamura<sup>1</sup> and K. Tominaga<sup>1,2</sup> <sup>1</sup> *Graduate School of Science, Kobe University, Kobe City, Japan* <sup>2</sup> *Molecular Photoscience Research Center, Kobe University, Kobe City, Japan*
- 12:10 **The circular polarization of sub-THz signal reflected from the human skin** 70  
I. Hayut, P. Ben Ishai, A. Puzenko, A.J. Agranat and Y. Feldman  
*Department of Applied Physics, The Hebrew University of Jerusalem, Israel*

### Session 9: BDS and other techniques I, Wednesday 14:00–16:00

- 14:00 **Heating Liquid Dielectrics by Time Dependent Fields** 71  
A. Khalife, U. Pathak and R. Richert *Department of Chemistry and Biochemistry, Arizona State University, Tempe, Arizona 85287-1604, USA*
- 14:30 **Atomistic and molecular probe characterization of poly(isoprene)s by PALS and ESR in relation to broadband dielectric spectroscopy** 71  
J. Bartoš<sup>1</sup>, H. Švajdlenková<sup>1</sup>, Y. Yu<sup>2</sup>, R. Krause-Rehberg<sup>2</sup>, S. Arrese-Igor<sup>3</sup> and A. Alegría<sup>3</sup> <sup>1</sup> *Polymer Institute of SAS, Dubravská cesta 9, 845 41 Bratislava, Slovakia* <sup>2</sup> *Institut für Physik, Martin Luther Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany* <sup>3</sup> *Centro de Física de Materiales, Centro Mixto CSIC-UPV/EHU, Edificio Korta, 20018 San Sebastián, Spain*

- 15:00 **Impedance measurements and modelling of the persistent photoexcitation effect in poly(3-hexylthiophene)** 90  
 K. Kisiel<sup>1</sup>, J. Jung<sup>1</sup>, C.H. Kim<sup>2</sup>, D. Tondelier<sup>2</sup>, B. Gffroy<sup>2,3</sup>, Y. Bonnassieux<sup>2</sup>, G. Horowitz<sup>2</sup> and J. Ulanski<sup>1</sup>  
<sup>1</sup> *Department of Molecular Physics and European Centre of Bio- and Nanotechnology, Technical University of Lodz, 90-924 Lodz, Poland* <sup>2</sup> *LPICM, Ecole Polytechnique, CNRS, 91128 Palaiseau, France* <sup>3</sup> *CEA Saclay, DSM/IRAMIS/SPCSI/LCSI, 91191 Gif-sur-Yvette, France*
- 15:30 **AC-calorimetry as a complementary method to dielectric spectroscopy** 72  
 H. Huth and C. Schick *Universität Rostock, Institut für Physik, Wismarsche Str. 43-45, 18051 Rostock, Germany*

**Session 10: BDS and other techniques II, Wednesday 16:30–18:30**

- 16:30 **Physico-Chemical Modification of Polymer Dielectrics for Electromechanically Active Elastomers, for Piezoelectret Systems, and for Pyro- or Piezoelectric Films** 74  
 R. Gerhard *Applied Condensed-Matter Physics, Institute of Physics and Astronomy, Faculty of Science, University of Potsdam, Germany*
- 16:50 **Time domain reflectometry technique for the Aqueous and Non-Aqueous solutions** 75  
 A.C. Kumbharkhane *School of Physical Sciences, Swami Ramanand Teerth Marathwada University, Nanded (India)*
- 17:10 **Two-channel impedance spectroscopy for comparing the dynamics of 2-ethyl-1-hexanol and its water mixture** 75  
 L.P. Singh and R. Richert *Department of chemistry and biochemistry Arizona State University, Tempe, Arizona, U. S. A.*
- 17:30 **Aging-time dependence of the segmental relaxation time of PVAc/SiO<sub>2</sub> nanocomposites: a combined BDS and TSDC study** 76  
 V.M. Boucher<sup>1</sup>, D. Cangialosi<sup>2</sup>, A. Alegría<sup>2,3</sup> and J. Colmenero<sup>1-3</sup>  
<sup>1</sup> *Centro de Física de Materiales Centro Mixto (CSIC-UPV/EHU), Apartado 1072, 20080 San Sebastián, Spain* <sup>2</sup> *Departamento de Física de Materiales, Universidad del País Vasco (UPV/EHU), Apartado 1072, 20080 San Sebastián, Spain* <sup>3</sup> *Donostia International Physics Center, Paseo Manuel de Lardizabal 4, 20018 San Sebastián, Spain*

- 17:50 **Comparative dielectric studies of Ag nanoparticles in matrix of polymers and monomers.** 77  
G.F. Novikov, E.V. Rabenok, L.M. Bogdanova and L.I. Kuzub *Institute of Problems of Chemical Physics, RAS.Semenov's pr., 1, Chernogolovka, Moscow region, Russia*
- 18:10 **Comparison of relaxation processes in poly(2-(2-methoxyethoxy)ethyl methacrylate) hydrogels differ on crosslinking density** 78  
R. Kisiel, K. Krysiak, L. Okrasa, M. Kozanecki and J. Ulanski  
*Department of Molecular Physics, Technical University of Lodz, Zeromskiego 116, 90-924 Lodz, Poland*

**18:30–20:00 Poster W (poster no. 50–91)**

**20:30–22:00 Piano concert**

## 1.4 Programme Thursday

**Session 11: Confined systems of different dimensionality I, Thursday 09:00–10:30**

- 09:00 **Heterogeneous and aging dynamics in single and stacked thin polymer films** 79  
K. Fukao, H. Takaki, T. Terasawa, K. Nakamura and D. Tahara  
*Department of Physics, Ritsumeikan University, Noji-Higashi 1-1-1, Kusatsu 525-8577, Japan*
- 09:30 **Dynamics of Rouse Chains Under Soft-Confinement with Different Geometries** 79  
A. Alegría<sup>1,2</sup>, R. Lund<sup>2,3</sup>, F. Barroso-Bujans<sup>1</sup>, A. Arbe<sup>1</sup>, L. Willner<sup>4</sup>, D. Richter<sup>4,5</sup> and J. Colmenero<sup>1-3</sup>  
<sup>1</sup> *Centro de Física de Materiales (CSIC-UPV/EHU), M. de Lardizabal 5, 20018 San Sebastián, Spain* <sup>2</sup> *Departamento de Física de Materiales (UPV/EHU), Facultad de Química, Apdo 1072. 20080 San Sebastián, Spain* <sup>3</sup> *Donostia International Physics Center, Paseo Manuel de Lardizabal 4, 20018 San Sebastián, Spain* <sup>4</sup> *Forschungszentrum Jülich GmbH, Institute of Solid State Research, 52425 Jülich, Germany* <sup>5</sup> *Jülich Center for Neutron Science (JCNS) at FRM-II, Lichtenbergstr. 1, 85747 Garching, Germany*

- 09:50 **Glassy dynamics of ultra-thin polymer films investigated by a combination of complementary methods** 81  
H. Yin and A. Schönhalz *BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany*
- 10:10 **Mechanical Properties of Thin Confined Polymer Films Close to the Glass Transition in the Linear Regime of Deformation: Theory and Simulations** 81  
A. Dequidt, D.R. Long, P. Sotta and O. Sanséau *Institut de Chimie de Clermont-Ferrand, Laboratoire des Polymères et Matériaux Avancés, France*

**Session 12: Confined systems of different dimensionality II, Thursday 11:00–12:30**

- 11:00 **Soft matter under Hard confinement** 85  
G. Floudas<sup>1,2</sup>, H. Duran<sup>1</sup>, C. Grigoriadis<sup>2</sup>, M. Steinhart<sup>3</sup> and H.-J. Butt<sup>1</sup> <sup>1</sup> *Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany* <sup>2</sup> *University of Ioannina, Department of Physics, 451 10 Ioannina, Greece* <sup>3</sup> *Institut für Chemie, Universität Osnabrück, D-49069 Osnabrück, Germany*
- 11:30 **Molecular dynamics in 1- and 2-dimensional geometric confinement as studied by Broadband Dielectric Spectroscopy** 83  
F. Kremer, W. K. Kipnusu, M. Treß, M. Jasiurkowska, C. Iacob and W. Kossack *Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany*
- 12:00 **Influence of interfacial interactions and annealing on dielectric relaxation in ultrathin films** 84  
D. Prevosto<sup>1</sup>, H.K. Nguyen<sup>2</sup>, M. Labardi<sup>1</sup>, S. Capaccioli<sup>1,2</sup>, M. Lucchesi<sup>1,2</sup> and P.A. Rolla<sup>1,2</sup> <sup>1</sup> *CNR-IPCF, Consiglio Nazionale delle Ricerche, Istituto per i Processi Chimico-Fisici, c/o Dip. Fisica Largo Pontecorvo 3, 56127 Pisa, Italy* <sup>2</sup> *Dipartimento di Fisica "Enrico Fermi", Università di Pisa, Largo Pontecorvo 3, 56127 Pisa, Italy*

**Session 13: Charge transport and glassy dynamics, Thursday 14:00–16:00**

- 14:00 **Ionic conductivity in glass-forming systems and polymers** 93  
A.P. Sokolov *The University of Tennessee, Department of Chemistry, USA*

- 14:30 **On the dielectric relaxation of Natural Rubber and the effect of vulcanizing agents** 87  
M. Hernández<sup>1</sup>, T.A. Ezquerro<sup>2</sup>, R. Verdejo<sup>1</sup> and M.A. López-Manchado<sup>1</sup>  
<sup>1</sup> *Instituto de Ciencia y Tecnología de Polímeros, ICTP-CSIC, Juan de la Cierva 3, Madrid 28006, Spain* <sup>2</sup> *Instituto de Estructura de la Materia, IEM-CSIC, Serrano 119, Madrid 28006, Spain*
- 14:50 **Are the thermal  $T_g$  and the segmental dynamics in polymer thin films fully interdependent?** 88  
D. Cangialosi<sup>1</sup>, V.M. Boucher<sup>1</sup>, H. Yin<sup>2</sup>, A. Schönhals<sup>2</sup>, A. Alegría<sup>1,3</sup> and J. Colmenero<sup>1,3,4</sup>  
<sup>1</sup> *Centro de Física de Materiales (CSIC-UPV/EHU), Paseo Manuel de Lardizabal 5, 20018 San Sebastián, Spain* <sup>2</sup> *BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany* <sup>3</sup> *Departamento de Física de Materiales, Universidad del País Vasco (UPV/EHU), Apartado 1072, 20080 San Sebastián, Spain* <sup>4</sup> *Donostia International Physics Center, Paseo Manuel de Lardizabal 4, 20018 San Sebastián, Spain*
- 15:10 **Dynamics on nanotubes of ferroelectric polymer: Confinement and stress effects** 88  
A. Nogales, J. Martín, A. Sanz and T.A. Ezquerro *Instituto de Estructura de la Materia, CSIC, Física Macromolecular, Serrano 121, 28006, Madrid, Spain*
- 15:30–16:00 **Peter Debye Prize — Award Ceremony and Lecture**
- 16:30 **City Tour**
- 20:00 **Conference Dinner**

## 1.5 Programme Friday

Session 14: Electrode and Maxwell-Wagner Polarization, Friday  
09:00–10:30

- 09:00 **Novel Polymeric Materials for Electrochemical Applications Based on Epoxy Resins Hardened by Phosphotungstic Heteropolyacid** 83  
 G. Boiteux<sup>1</sup>, O. Matkovska<sup>2</sup>, Y. Mamunya<sup>2</sup>, A. Serghei<sup>1</sup>, M. Shandruk<sup>2</sup> and E. Lebedev<sup>2</sup> <sup>1</sup> *Université de Lyon, Université Lyon 1, Ingénierie des Matériaux Polymères, UMR CNRS 5223, 15 Boulevard Latarget, F-69622 Villeurbanne, France* <sup>2</sup> *Institute of Macromolecular Chemistry, 48 Kharkivske Chaussee, Kyiv 02160, Ukraine*
- 09:30 **Interfacial polarization in dielectric spectra: theory and applications** 89  
 A. Serghei *Université Lyon 1, CNRS UMR 5223, Ingénierie des Matériaux Polymères, 69622 Villeurbanne, France*
- 09:50 **Impedance spectroscopy on electrochromic tungsten and nickel oxide films as a function of applied potential** 91  
 E. Pehlivan<sup>1,2</sup>, C.G. Granqvist<sup>1</sup> and G.A. Niklasson<sup>1</sup> <sup>1</sup> *Department of Engineering Sciences, The Ångström Laboratory, Uppsala University, P.O. Box 534, SE-751 21, Uppsala, Sweden* <sup>2</sup> *ChromoGenics AB, Märstagatan 4, SE-753 23, Uppsala, Sweden*
- 10:10 **Dielectric relaxation of NBR/EPDM Blend loaded with various types of nano scaled carbon black: Applicability of some conductivity models** 73  
 S.L. Abd-El-Messieh<sup>1</sup>, D.E. El-Nashar<sup>2</sup>, A.F. Younan<sup>2</sup>, K.N. Abd-El-Nour<sup>1</sup> <sup>1</sup> *Microwave Physics and Dielectrics Department, National Research Centre, Dokki, Cairo, Egypt* <sup>2</sup> *Polymers and Pigments Department, National Research Centre, Dokki, Cairo, Egypt*

**Session 15: Industry forum with panel discussion, Friday 11:00–12:30**

- 11:00 **t.b.a**  
 Petzold, A. *Goodyear, Luxembourg*
- 11:15 **DC Conduction in Polymer Insulation: Applications of Dielectric Spectroscopy and Thermally Stimulated Current Techniques** 91  
 E. Logakis<sup>1</sup>, L. Herrmann<sup>1</sup>, L. Petersson<sup>2</sup> and T. Christen<sup>1</sup> <sup>1</sup> *ABB Corporate Research, Segelhofstrasse 1, CH-5405 Baden-Dättwil, Switzerland* <sup>2</sup> *ABB Corporate Research, Forskargränd, S-721 78, Västerås, Sweden*

- 11:30 **Signatures of glass transition for partially ordered phases** 95  
M. Reich, M. Schneider and W. Schmidbauer *Schott AG, Hattenbergstr. 10, 55122 Mainz, Germany*
- 11:45 **Dielectric characterisation of polyolefins for power cable applications: insulation and semiconductive materials** 92  
C. Svanberg<sup>1</sup>, G. Stalmann<sup>2,3</sup>, T. Gkourmpis<sup>1</sup>, J. Andersson<sup>1</sup>, Villgot Englund<sup>1</sup>, Ulf Nilsson<sup>1</sup>, Aleksandar Matic<sup>2</sup> and Per Jacobsson<sup>2</sup>  
<sup>1</sup> *Innovation & Technology, Borealis, Sweden* <sup>2</sup> *Applied Physics, Chalmers University of Technology, Göteborg, Sweden* <sup>3</sup> *Department of Physics, University of Marburg, Germany*

## 12:00–12:30 Panel Discussion: “Applications of BDS”

### Session 16: Conducting glasses and ionic liquids, Friday 14:00–16:00

- 14:00 **From boiling point to glass transition temperature: re-orientational correlation time in molecular liquids follow three-parameter scaling** 86  
B. Schmidtke, N. Petzold, R. Kahlau, M. Hofmann and E.A. Rössler  
*Universität Bayreuth, Experimentalphysik II, D-95440 Bayreuth, Germany*
- 14:30 **Electrical Conductivity Relaxation Studies of Supercooled Protic Ionic Liquids** 93  
M. Paluch<sup>1</sup>, Z. Wojnarowska<sup>1</sup>, C.M. Roland<sup>2</sup>, A. Swiety-Pospiech<sup>1</sup> and K. Grzybowska<sup>1</sup>  
<sup>1</sup> *Institute of Physics, Silesian University, ul. Uniwersytecka 4, 40-007 Katowice, Poland* <sup>2</sup> *Naval Research Laboratory, Chemistry Division, Code 6120, Washington, D.C. 20375 - 5342, USA*
- 15:00 **Glassy dynamics and charge transport in Ionic Liquids** 94  
J.R. Sangoro<sup>1,4</sup>, C. Iacob<sup>1</sup>, J. Kärger<sup>1</sup>, V. Strehmel<sup>2</sup>, R. Buchner<sup>3</sup>, A.P. Sokolov<sup>4</sup> and F. Kremer<sup>1</sup>  
<sup>1</sup> *Institute of Experimental Physics I, University of Leipzig, Leipzig, Germany* <sup>2</sup> *Institute of Polymer Chemistry, University of Potsdam, Potsdam, Germany* <sup>3</sup> *Institute of Physical and Theoretical Chemistry, University of Regensburg, Regensburg, Germany* <sup>4</sup> *Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA*

15:30 **Ion Transport across Grain Boundaries in Fast Lithium Ion Conducting Ceramics** 95

B. Roling<sup>1</sup>, M. Gellert<sup>1</sup>, F. Rosciano<sup>2</sup> and C. Yada<sup>3</sup> <sup>1</sup> *Department of Chemistry, University of Marburg, Hans-Meerwein-Straße, 35032 Marburg, Germany* <sup>2</sup> *Advanced Technology 1 Division, Toyota Motor Europe, Hoge Wei 33, B-1930 Zaventem, Belgium* <sup>3</sup> *Battery Research Division, Toyota Motor Corp., Higashifuji Technical Center 1200, Mishuku, Susono, Shizuoka 410-1193 Japan*

**Closing remarks**

## 1.6 Poster M

**Monday: 18:00–20:00 Chemistry Department**

**1: Rotational and Translational Diffusion of Ionic Liquids Confined in Nanoporous Silica** 97

C. Iacob<sup>1</sup>, J.R. Sangoro<sup>1,2</sup>, J. Kärgel<sup>1</sup> and F. Kremer<sup>1</sup> <sup>1</sup> *Institute of Experimental Physics I, University of Leipzig, Leipzig, Germany* <sup>2</sup> *Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830-6197, United States*

**2: Structure property relationship of nanocomposites based on Poly(lactide) and Layered Double Hydroxide** 97

P.J. Purohit and A. Schönhals *BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany*

**3: Characteristics of frequency response functions for ion motions in inhomogeneous free space between crystallites in several polymers** 98

Y. Anada *Department of Business and Information Systems, Hokkaido Information University, Ebetsu, Japan*

**4: Gradual Redehydration of a Dehydrated CaFe-Layered Double Hydroxide under Controlled Humidity Studied by Broadband Dielectric Relaxation Spectroscopy** 99

V. Bugris<sup>1</sup>, H. Haspel<sup>1</sup>, Á. Kukovecz<sup>1</sup>, Z. Kónya<sup>1</sup>, P. Sipos<sup>2</sup> and I. Pálinkó<sup>3</sup> <sup>1</sup> *Department of Applied and Environmental Chemistry, University of Szeged, Rerrich B. tér 1, Szeged, H-6720 Hungary* <sup>2</sup> *Department of Inorganic and Analytical Chemistry, University of Szeged, Dóm tér 7, Szeged, H-6720 Hungary* <sup>3</sup> *Department of Organic Chemistry, University of Szeged, Dóm tér 8, Szeged, H-6720 Hungary*



- 5: Dielectric Spectroscopy of Hydrogen Bonded Thermotropic Liquid Crystalline Polymer with Six Methylene Units in the Side Chain** 100  
H. Cinkaya, Y.H. Gürsel and F. Salehli *Physics Engineering Department , Faculty of Sciences and Arts, 34469, Istanbul Technical University, Maslak, 34469, Istanbul, Turkey*
- 6: Comparative Analysis of the Dielectric Relaxational Behaviour of Poly(methacrylates) Containing a Phenyl group in the Side Chain** 100  
B. Redondo-Foj<sup>1</sup> , M. Carsí<sup>1</sup> , P. Ortiz-Serna<sup>1</sup> , M.J. Sanchis<sup>1</sup> , R. Díaz-Calleja<sup>1</sup> , E. Riande<sup>2</sup> , L. Gargallo<sup>3</sup> and D. Radic<sup>3</sup> <sup>1</sup> *Instituto de Tecnología Eléctrica (ITE), Departamento de Termodinámica Aplicada, Universidad Politécnica de Valencia, Spain* <sup>2</sup> *Instituto de Ciencia y Tecnología de Polímeros (CSIC), Spain* <sup>3</sup> *Departamento de Química Física, Pontificia Universidad Católica de Chile*
- 7: Broadband Dielectric Spectroscopy to study the molecular dynamics in nanometer thin layers of poly (styrene-block-isoprene-1.4) diblock copolymer** 102  
M.M. Elmahdy<sup>1,2</sup> , M. Treß<sup>2</sup> , M. Fuchs<sup>2</sup> , E.U. Mapesa<sup>2</sup> and F. Kremer<sup>2</sup>  
<sup>1</sup> *Institute of Experimental Physics I, Leipzig University, Linnéstrasse 5, 04103, Leipzig, Germany* <sup>2</sup> *Department of Physics, Mansoura University, Mansoura 35516, Egypt*
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E. Ermilova, F.F. Bier and R. Hölzel *Fraunhofer Institute for Biomedical Engineering, Am Mühlenberg 13, 14476 Potsdam-Golm, Germany*
- 9: Dielectric Characterisation of Polymer Structures with an Inclusion of a Metal Center** 103  
V.T. Avanesyan and E.G. Vodkailo *Herzen Russian State Pedagogical University, nab. Reki Moiki 48, St. Petersburg, 191186 Russia*
- 10: Electrical Conduction and Dielectric Properties in Piezoelectric Fibre Composites** 104  
H. Hammami and A. Kallel *Faculty of sciences of sfax, Physics Department, Route de la Soukra km 3.5, B.P. no. 1171 - 3000 Sfax, Sfax, Tunisia*
- 11: Dielectrophoretic response of DNA determined by impedance measurements** 105  
A. Henning, F.F. Bier and R. Hölzel *Fraunhofer Institute for Biomedical Engineering, D-14476 Potsdam-Golm, Germany*

**12: Giant permittivity and low dielectric loss in new three phases: BaTiO<sub>3</sub>-carbon nanotube / polyvinylidene fluoride composite** 105

Z. Ghallabi, H. Rekik, M. Arous, A. Kallel, I. Royaud, G. Boiteux and G. Seytre *faculty of sciences of sfax, physics Department, Route de la Soukra km 3.5, B.P. no. 1171 - 3000 Sfax, Sfax, Tunisia*

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A. Ladhar, M. Arous, H. Kaddami, M. Raihane and A. Kallel *Faculty of sciences of sfax, Physics Department, Route de la Soukra km 3.5, B.P. no. 1171 - 3000 Sfax, Sfax, Tunisia*

**14: Modified Polymer Dynamics in PDMS Nanocomposites: Dielectric and Thermal Studies** 106

P. Klonos<sup>1</sup>, K. Kyriakos<sup>1</sup>, I. Vangelidis<sup>1</sup>, I. Sulym<sup>2</sup>, M. Borysenko<sup>2</sup>, V.M. Gun'ko<sup>2</sup>, A. Kyritsis<sup>1</sup> and P. Pissis<sup>1</sup> <sup>1</sup> *Department of Physics, National Technical University of Athens, Zografou Campus, 15780, Athens, Greece* <sup>2</sup> *Institute of Surface Chemistry, 17 Genetal Naumov Str., 03164, Kiev, Ukraine*

**15: Phase transitions and dynamics in semifluorinated side-chain poly(methacrylate) random copolymers studied by dielectric spectroscopy and other techniques** 107

K. Sotiria<sup>1</sup>, P. Christos<sup>1</sup>, K. Apostolos<sup>1</sup>, P. Doris<sup>1</sup>, J. Dieter<sup>2</sup> and P. Polycarpus<sup>1</sup> <sup>1</sup> *National Technical University of Athens, School of Applied Mathematical and Physical Science, Iroon Polythechneiou 9, 157 80, Athens, Greece* <sup>2</sup> *Leibniz- Institute of Polymer Research Dresden*

**16: Study of the dynamic heterogeneity in poly(ethylene-ran-vinyl acetate) co-polymer using nano-Dielectric Spectroscopy (nDS)** 108

M.M. Kummali<sup>1,2</sup>, L.A. Miccio<sup>2,3</sup>, G.A. Schwartz<sup>2</sup>, A. Alegría<sup>1,2</sup> and J. Colmenero<sup>1-3</sup> <sup>1</sup> *Departamento de Física de Materiales UPV/EHU, Fac. de Química, 20080 San Sebastián, Spain* <sup>2</sup> *Centro de Física de Materiales CSIC-UPV/EHU, Paseo Manuel de Lardizabal 5, 20018 San Sebastián, Spain* <sup>3</sup> *Donostia International Physics Center, Paseo Manuel de Lardizabal 4, 20018 San Sebastián, Spain*

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E. Levy, A. Puzenko and Y. Feldman *Department of Applied Physics, the Hebrew University of Jerusalem, Givat Ram, Jerusalem 91904, Israel*

- 18: Dielectric characterization of gold nanoparticles / antiferroelectric liquid crystal composites** 109  
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## 2 Abstracts

### 2.1 Tutorial

#### **Dielectric properties of biological materials; what we can learn from them?**

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Tut II: Mon 11:45, Lecture Hall

The investigation of dielectric properties of biological systems and their components is important not only for the fundamental scientific knowledge but also for its applications in medical physics, biophysics, and biotechnology. A comprehensive theoretical and experimental study of static and dynamic dielectric properties of different biological systems including globular [1,2,3] and membrane proteins [1,4], protein hydrated powders [5,6] and human erythrocytes [7,8] are presented in the tutorial paper.

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## Broadband Electrochemical Impedance Spectroscopy

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Tut I: Mon 09:00, Lecture Hall

Broadband impedance spectroscopy is a powerful and versatile tool for investigating charge transport phenomena in solid and liquid materials. For the application of broadband impedance spectroscopy to electrochemical systems, two important points have to be considered: (i) Electrochemical measurements are usually done in a three-electrode configuration. In this case, the potential of a working electrode, where the electrochemical process of interest takes place, can be controlled with respect to a reference electrode. (ii) For electrochemical impedance spectroscopy, the dc potential applied to the working electrode is superimposed by a small ac potential. In this tutorial lecture, I will start with some basics about electrochemical processes and electrochemical characterization techniques. Then I will give examples for the application of broadband electrochemical impedance spectroscopy, in particular for studying processes in supercapacitors and batteries.

## The interplay between intra- and inter-molecular dynamics as studied by Broadband Dielectric- and Fourier-Transform Infrared -Spectroscopy

F. Kremer<sup>1</sup>, W. Kossack<sup>1</sup>, P. Papadopoulos<sup>2</sup>, M. Jasiurkowska<sup>1</sup>, M. Treß<sup>1</sup>,  
E. U. Mapesa<sup>1</sup>, W. K. Kipnusu<sup>1</sup> and C. Iacob<sup>1</sup>

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Tut II: Mon 11:00, Lecture Hall

The inter- and intra-molecular interactions of low molecular weight and polymeric glass-forming model systems are studied by Broadband Dielectric (BDS) - and Fourier-Transform Infrared (FTIR) - Spectroscopy. Analyzing the temperature dependencies of specific IR absorption bands, reflecting the intramolecular potentials of dedicated molecular moieties, enables one to unravel on a submolecular scale the process of glass formation and to compare it with the dielectrically determined primarily intermolecular dynamics. By that a wealth of novel information is obtained proving that the different units of a glass former show specifically different temperature dependencies. This proves the fundamental importance of intramolecular mobility

giving refined insights into the underlying interactions beyond coarse-grained models treating the glassformer as rigid body.

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## Combining dielectric spectroscopy with scattering techniques

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Tut I: Mon 09:45, Lecture Hall

Dielectric spectroscopy provides fast and accurate measurements of the relaxation spectra in extremely broad frequency range. However, significant disadvantage of the dielectric spectroscopy is the absence of direct microscopic information on underlying molecular motions. In this talk we present an overview of scattering techniques (light, neutron and X-ray) and their comparison to dielectric spectroscopy. Scattering techniques provide not only characteristic time (frequency) of the molecular motions, but also their geometry due to additional measured variable-scattering wave-vector (scattering angle). We will briefly overview theory of scattering and emphasize specifically advantage of neutron scattering spectroscopy because of direct interactions of neutrons with atoms and the wavelength of neutrons comparable to interatomic distances. Several examples of scattering studies of dynamics of glass forming systems, polymers and biological macromolecules will be discussed. The results will be compared to dielectric spectroscopy studies of the same materials. Concluding part of the talk stresses the advantages of combining the dielectric and scattering measurements. Adding microscopic information from scattering techniques to the broad

frequency range accessible for the dielectric spectroscopy opens tremendous possibilities for studies of dynamics of complex materials.

## 2.2 Talks

### Computational dielectric spectroscopy of polarizable ionic liquids

C. Schröder

*Institute for Computational Biological Chemistry, University of Vienna, Vienna, Austria*

Theory I: Mon 14:30, Lecture Hall

Experimental dielectric spectra of ionic liquids usually display a very broad and complex peak structure. Here, computational dielectric theory may help to disentangle the peaks and assign characteristic motions of the involved species to those peaks [1,2]. In particular, the collective rotation and translation [3] of the ions as well as induced dipoles of both, cations and anions contribute to the dielectric spectrum [2]. Classical molecular dynamic simulations on molecular ionic liquids are based on pairwise additive Coulomb forces with fixed partial charges which cannot respond to the local field. In our polarizable equilibrium simulations virtual mobile Drude particles are added [4]. They carry a "Drude charge" and are bound by a harmonic spring to their reference atoms. This spring mimics an induced atomic dipole which is orientated by the local field. The emerging polarizable forces enhances the single-particle dynamics of ionic liquids, e.g. diffusion coefficients, by a factor of two and more without changing the structure significantly [4]. In addition, they affect the collective dynamics in a multiple way. The viscosity is lowered, peaks in the THz regime are enhanced and the dynamics of ion cages is changed [2,4].

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# Universal Relaxation and Diffusion in Interacting Complex Systems: Fundamental Physics and Rich Applications

K.L. Ngai

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Theory I: Mon 15:00, Lecture Hall

Relaxation and diffusion are fundamental processes in physics and chemistry that determine not only the physical properties of the condensed matter, but also its potential for applications. In most condensed matter of current interest, the basic units involved in the relaxation/diffusion process have mutual interaction/constraint. Hence this is necessarily a many-body problem, which has yet to be solved in theoretical chemistry and physics. One purpose of my talk is to make the audience aware of the universality of the dynamic properties of many-body relaxation/diffusion processes of different kinds manifested in experiments and simulations on condensed matter with diverse chemical compositions and physical structures [1]. This remarkable experimental fact indicates that many-body relaxation/diffusion is governed by some fundamental physics. I shall demonstrate the universality of dynamic properties of many-body relaxation/diffusion principally from the dynamic processes related to glass transition in glass-forming systems. This is reinforced by few examples of strikingly similar properties of different processes in other interacting systems having nothing to do with glass transition. Examples include pharmaceuticals, hydrated and solvated proteins, nano-structured materials, and energy storage materials that could be of interest to researchers attending the BDS 2012. The existence of universal dynamic properties is perhaps not surprising because many-body relaxation and diffusion stem from fundamental physics and the consequences should be general. The search for this fundamental physics that leads to solution of the problem is a challenging and important task. If successful, it is an important advance and it will benefit many research areas. It had been suggested that nonlinear Hamiltonian dynamics (i.e., classical chaos) is the fundamental physics giving rise to the universal dynamic properties. The Coupling Model of the author based on classical chaos indeed has predictions that are consistent with the experimental findings [1]. Although the Coupling Model is not yet a complete solution of the many-body relaxation, its precepts and predictions can be used as a stepping stone for others to construct rigorous theory to fully solve this fundamental problem with rich applications.

[1] Relaxation and Diffusion in Complex Systems, K.L. Ngai, Springer (New York, 2011).

## High-frequency resonance absorption as evidence for oscillation in a well before escape from a metastable state in the Kramers energy controlled diffusion model

W.T. Coffey<sup>1</sup>, Y.P. Kalmykov<sup>2</sup>, S.V. Titov<sup>3</sup> and D.S.F. Crothers<sup>4</sup>

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Theory I: Mon 15:30, Lecture Hall

A variety of disparate physical systems which are modeled in terms of their relaxation behavior by the Brownian motion of a dipolar particle in a potential and its extensions to anomalous diffusion exhibit slow over barrier relaxation accompanied by relatively fast relaxation due to exponential decays in the potential wells and high frequency resonance absorption due to small oscillations about the minima of the wells. It is argued that the high frequency resonant process provides abundant evidence for the Kramers concept of oscillations in a potential well of particles with energy equal to the separatrix energy before escape as both are simply limiting cases of the same family of librational dynamical processes in a well [1].

[1] W. T. Coffey and Yu. P. Kalmykov, *The Langevin Equation*, 3rd edition (World Scientific, Singapore, 2012).

## Shear and dielectric responses of glass-forming liquids: What is the relation between the dielectric and mechanical relaxations?

C. Gainaru<sup>1</sup>, T. Hecksher<sup>2</sup>, N.B. Olsen<sup>2</sup>, R. Böhmer<sup>1</sup> and J.C. Dyre<sup>2</sup>

<sup>1</sup> *Fakultät für Physik, Technische Universität Dortmund, 44221 Dortmund, Germany*

<sup>2</sup> *Roskilde Univ, DNRF Ctr Glass and Time, IMFUFA, Dept Sci Syst and Models, DK-4000 Roskilde, Denmark*  
Theory II: Mon 16:30, Lecture Hall

Propylene carbonate and a mixture of two secondary amides, N-methylformamide and N-ethylacetamide, were investigated by means of broadband dielectric and mechanical

shear spectroscopy. The similarities between the rheological and the dielectric responses of these liquids and of the previously investigated tripropylene glycol are discussed within a simple approach that employs an electrical circuit analog for describing the frequency-dependent behavior of viscous materials. The circuit is equivalent to the Gemant-DiMarzio-Bishop model, but allows for a negative capacitive element. The circuit can be used to calculate the dielectric from the mechanical response and vice versa. Using a single parameter for a given system, good agreement between model calculations and experimental data is achieved for the entire relaxation spectra, including secondary relaxations and the Debye-like dielectric peak in the secondary amides. In addition, the predictions of the shoving model are confirmed for the investigated liquids.

## **Molecular dynamics simulations of the Johari-Goldstein relaxation in a molecular liquid**

D. Fragiadakis and C.M. Roland

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Theory II: Mon 17:00, Lecture Hall

Molecular dynamics simulations (MDS) were carried out to investigate the reorientational motion of a rigid (fixed bond length), asymmetric diatomic molecule in the liquid and glassy states[1]. In the latter the molecule reorients via large-angle jumps, which we identify with the Johari-Goldstein (JG) dynamics. This relaxation process has a broad distribution of relaxation times, and at least deeply in the glassy state, the mobility of a given molecule remains fixed over time; that is, there is no dynamic exchange among molecules. Interestingly, the JG relaxation time for a molecule does not depend on the local density, although the non-ergodicity factor is weakly correlated with the packing efficiency of neighboring molecules. In the liquid state the frequency of the JG process increases significantly, eventually subsuming the slower alpha-relaxation. This evolution of the JG-motion into structural relaxation underlies the correlation of many properties of the JG- and alpha-dynamics.

[1] <http://arxiv.org/abs/1203.2127>

## The derivation of the Cole-Cole and Cole-davidson functions and their possible generalizations

A.F. Kamzin, I.I. Popov and R.R. Nigmatullin

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Theory II: Mon 17:20, Lecture Hall

A model of the self-similar process of relaxation and a method of derivation of kinetic equations for the total polarization based on ideas of the fractional kinetics is suggested. The derived kinetic equations contain integro-differential operators having non-integer order. They lead to the Cole-Cole and Cole-Davidson expressions for the complex dielectric permittivity. It is shown that the power-law exponent  $\alpha$  in the Cole-Cole expression coincides with the dimension of the mixed space-temporal fractal ensemble. The Cole-Davidson expression takes into account the influence of thermostat. If the discrete scale invariance for the temporal-space structure of the dielectric medium considered becomes important then the expression for the complex dielectric permittivity contains the log-periodic corrections (oscillations) and, hence, generalizes the conventional Cole-Cole and Cole-Davidson expressions, correspondingly. The corrections obtained in this model suggest another way of interpretation and analysis of dielectric spectra for different complex materials.

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## Time Evolution of Macroscopic Dielectric Phenomena

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Theory II: Mon 17:40, Lecture Hall

Analysis of excess wings in broadband dielectric spectroscopy data of glass forming materials [1] is found to provide evidence for anomalous time evolutions and fractional semigroups [2]. Solutions of fractional evolution equations in frequency space are used to fit dielectric spectroscopy data of glass forming materials with a range between 4 and 10 decades in frequency. With only three parameters (two relaxation times plus one exponent) excellent fits can be obtained for 5-methyl-2-hexanol and for methyl-m-toluate over up to 7 decades. The traditional Havriliak-Negami fit with three parameters (two exponents and one relaxation time) fits only 4-5 decades. Using a second exponent, as in Havriliak-Negami fits, the  $\alpha$ -peak and the excess wing



can be modeled perfectly for up to 10 decades for all materials at all temperatures considered in this work. Traditionally this can only be accomplished by combining two Havriliak-Negami functions with 6 parameters. The temperature dependent relaxation times are fitted with the Vogel-Tammann-Fulcher relation which provides the corresponding Vogel-Fulcher temperatures. The relaxation times turn out to obey almost perfectly the Vogel-Tammann-Fulcher law. Finally, new and computable expressions of time dependent relaxation functions corresponding to the frequency dependent dielectric susceptibilities are reported that are helpful to compare theory and experiment.

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- [2] R. Hilfer, FOUNDATIONS OF FRACTIONAL DYNAMICS: A SHORT ACCOUNT  
In: Fractional Dynamics: Recent Advances , edited by: J. Klafter and S. Lim and R. Metzler, World Scientific, pages 207-227, 2011.

## **Microelectrode arrays for electrochemical immuno-sensing and cell monitoring**

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Biological systems I: Tue 09:00, Lecture Hall

The demand on electrochemical biosensors represents a fast and sensitive analyte detection. Therefore, immunosensors are useful for a specificity and affinity of antigen recognition by the appropriate associated antibody. This report addresses a novel microelectrode array qualified and validated for parallel analysis in a higher sample throughput. The microarray consists of nine independent chambers, each of these contains a circular gold working electrode with a diameter of 1.9 mm surrounded by a ring-shaped auxiliary electrode with a platinum surface. A corresponding Ag/AgCl reference electrode of the second art is embedded in a sealing lid of each of the measurement chambers. The array is ready for running a full range of electrochemical real-time detection methods. Concerning these detection techniques, impedance spectroscopy is an attractive measurement tool for recording fast and label-free interfacial changes at the electrode surface. The proof of principle of the novel electrode array could be verified detecting the glioblastoma marker tenascin C. Tenascin C is a glycoprotein of the extracellular matrix and occurs in higher concentrations in transformed e.g. neuronal tissues, in solid tumours like glioma. For monitoring this tumour marker microelectrodes are covered with specific antibodies directed to tenascin C positive samples [1].

[1] Steude A, Schmidt S, Robitzki A A, Pänke O. Lab Chip (2011) 11: 2884–2892.

## Hydration Water Dynamics in Bioprotected Protein Glasses Studied by Broadband Dielectric Spectroscopy

S. Capaccioli<sup>1,2</sup>, D. Prevosto<sup>2</sup>, P.A. Rolla<sup>1</sup>, A. Paciaroni<sup>3</sup> and K.L. Ngai<sup>1</sup>

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Biological systems I: Tue 09:30, Lecture Hall

In biopreservation, bio-macromolecules are often made more stable against aggregation or chemical degradation at low and high temperatures by embedding them in polyols- or sugar-based glass forming matrices [1]. The stabilizing effect of sugar-glass matrix for freeze-drying proteins or nucleic acids has been ascribed to the interaction of the matrix molecules with the protein surface groups via direct hydrogen bond [2] and to the arrested dynamics imposed by the surrounding glassy matrix [3,4]. Actually, the nature of dynamical processes in solvated bio-macromolecules is more complex [5], as demonstrated by optimal biopreservation through antiplasticization [6]. Indeed, both fast and slow protein dynamics seem to be slaved to the structural and secondary relaxation of the environment [7]. Protein stability in sugar-glass matrices has been found to be directly linked to  $\beta$ -relaxations as revealed by Broadband Dielectric Spectroscopy (BDS) and even to fast cage motions observed by neutron scattering (NS) [6,8]. Degradation rate of the proteins in sugar-glasses is correlated to  $\beta$ -relaxation time, and then to local molecular mobility promoting diffusion of small molecules [8], even when efficient sugar excipients with high glass transition temperature  $T_g$  are able to slow down protein conformations and to protect against thermal denaturation. A key role seems to be played by hydration water, in particular by its local  $\beta$ -relaxation [9]. In this study, we have analyzed the dynamic behavior of lysozyme embedded in different sugar matrices above and below  $T_g$ , with different hydration levels. We performed BDS measurements (over the range 2 mHz-20 GHz), calorimetric analysis and elastic incoherent NS experiments [10]. Our BDS and NS results reinforce the idea of a strong coupling between dynamics of solvent and bio-macromolecules over a wide timescale range. Two main dynamic processes were identified: while the slowest process, with features of structural  $\alpha$ -relaxation, is due to cooperative motion of the solvent physically coupled to the bio-macromolecule, the fastest process, related to protein surface motions, is identical to the secondary relaxation of water in the aqueous solvent and determines the mobility and stability in the glassy state.

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## From numerical simulation to measurement of protein dielectric relaxation in solution

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Biological systems I: Tue 10:00, Lecture Hall

Protein dielectric relaxation measurements have been studied extensively under a variety of conditions throughout the past century. These measurements have advanced both the theory and practice of liquid impedance measurements. A process to take molecular structures from the Protein Data Bank and subsequently estimate the dielectric relaxation properties of the proteins in solution is presented. This process enables screening of target compounds for analysis by dielectric spectroscopy as well as better interpretation of protein relaxation data. For charge estimation, the shifted pKa values for amino acid residues are calculated using Poisson-Boltzmann solutions of the protein electrostatics over varying pH conditions. The estimated internal permittivity [1] and estimated dipole moments through shifted pKa values [2] are then calculated. Molecular dynamics simulations are additionally used to refine and approximate the solution-state conformation of the proteins. These calculations and simulations are then verified with laboratory experiments over a large pH and frequency range (1 kHz-100 MHz) [3] with reduced electrode polarization through electrode surface preparation [4]. Further extensions to molecular dynamics simulations of the protein responses will refine the accuracy of this technique and improve the predictive capability.

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## Dielectric response on fully hydrated zwitterionic aminoacids

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Biological systems II: Tue 11:00, Lecture Hall

The complex dielectric permittivity of eight different amino acids in water solutions was determined in the frequency range from 0.2 to 20 GHz at room temperature. Two relaxations were observed, which can be mainly assigned to the rotation of amino acids in the aqueous environment, and the reorientational motion of water molecules, respectively. Although the amino acids have a charged (zwitterionic) nature with huge dipole moments, the tendency to dipolar alignment seems to be very weak over the investigated concentration ranges. For these small bio-molecules, water screens solute-solute interactions and amino acids remain typically as isolated hydrated monomers. The comparison between the amino acid relaxation times made possible to discuss the relationship between rotational dynamics and the structure and hydrodynamic coupling of the amino acid studied. Finally, these results will be discussed and compared with the dynamic of hydrated proteins.

## Water and protein dynamics in protein-water mixtures

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Biological systems II: Tue 11:30, Lecture Hall

Water and protein dynamics in two globular protein-water systems, water-lysozyme and water-BSA (bovine serum albumine), were studied by dielectric relaxation spectroscopy (DRS) and thermally stimulated depolarization currents (TSDC) techniques. Water equilibrium sorption isotherms (ESI) measurements were also recorded at room temperature. Differential Scanning Calorimetry, DSC, measurements were employed to investigate crystallization and melting events of water and to estimate the amount of uncrystallized water. The samples covered a wide range of composition, from practically dry solid pellets (2wt% of water) to dilute solutions (82wt% of water). The evolution of dynamics with hydration level was followed for various dielectric relaxation processes, the emphasis being given to relaxation processes of polar groups on the surface of the proteins and of uncrystallized water molecules. A relationship between the formation of a conductive percolating water cluster and the saturation of the so-called water  $\nu$  process was found. Contributions originating from water molecules in excess (uncrystallized water or ice), follow separate relaxation modes slower than the  $\nu$  relaxation.

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## Dynamics of Hydrated Proteins

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Biological systems II: Tue 11:50, Lecture Hall

Dynamics of biological macromolecules and their dependence on hydration water remain poorly understood. Previously, three processes (slow, main and fast) have been reported in dielectric spectra of hydrated protein powders, and their relations to processes in protein solution have been discussed [1,2]. In this presentation, we report detailed dielectric relaxation studies of several hydrated proteins. By carefully evaluating the contribution from electrode polarization, we extended the low frequency range

and find new relaxation process at frequency lower than the slow process. This process reaches  $\sim 100$ s around glass transition temperature which reported for hydrated proteins from a variety of measurements, such as Brillouin scattering and calorimetry [3]. Moreover, main process changes the temperature dependence around this glass transition temperature, as is often observed in glass transition. The relation between other aqueous systems and this main process will be also discussed.

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## **From elementary dynamics to dielectric spectra and thermodynamic properties of water in electrolyte solutions**

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Biological systems II: Tue 12:10, Lecture Hall

This is difficult to establish the correspondence between short scale dynamics of water molecules to long scale and thermodynamic properties of electrolyte solutions. Dielectric spectroscopy allows to solve this problem because of low frequency limit of spectra is the static dielectric permittivity. It is calculated for 40 systems in temperature range 288-308K. The systematization was developed. Water dynamics is considered on the basis of confined rotator theoretical model, experimental dielectric (7-120 GHz) and absorption (up to 800 cm<sup>-1</sup>) data. The model of ion hydration shell is suggested. New scheme of dielectric polarization is proposed, where bulk water and partly "frozen" molecules are present. For 1:1 electrolytes the dielectric saturation and electrostriction are absent. The correlation of changes of water activity ( $a$ ) and static dielectric constants ( $\epsilon$ ) of the salt solutions in a wide range of concentrations was investigated. Linear character of dependence  $a$  of  $1/\epsilon$  is dependence is observed was established. (concentrations, where ionic-water clusters are realized). The obtained dependences were used for calculation and the analysis of osmotic coefficients and other properties of the concentrated solutions. The common principles of the structure-kinetic and thermodynamic theory of hydration are established at the level of the molecular orientation processes.

## Broadband nonlinear dielectric response of supercooled liquids

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Glassy dynamics I: Tue 14:00, Lecture Hall

Broadband dielectric spectroscopy is an invaluable method for investigating the slowing down of molecular motion at the glass transition. In these experiments, the linear response to an applied external field is detected, which allows covering an unsurpassed frequency range of 20 decades [1]. However, theory and experiments on spin [2] and orientational glasses [3,4] have taught that the linear response is blind to hidden order and that nonlinear susceptibilities may reveal critical dynamics. Hence, the investigation of the nonlinear dielectric response of glass forming matter is attracting increasing interest (see, e.g., [5,6,7]). Nonlinear dielectric spectroscopy can be performed in different ways: Hole burning experiments can be considered as early nonlinear experiments in supercooled liquids [8]. Nowadays nonlinearity is measured by comparing and quantifying the difference of high- and low-field permittivity or by the application of a high ac voltage and determination of the higher harmonics. In the present work, we provide results on the nonlinear behavior following the latter two methods in a broad range of frequencies covering the structural relaxation and the so-called excess wing. We present nonlinear dielectric susceptibilities of glycerol and propylene carbonate for almost 8 decades in frequency. We find distinct differences in the nonlinear behavior of the excess wing as compared to the alpha process, with far-reaching implications on microscopic modeling.

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## Chain dynamics in asymmetric polymer blends by broadband dielectric spectroscopy and MD-simulations

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Glassy dynamics I: Tue 14:30, Lecture Hall

Miscible polymer blends are systems of wide technological interest whose dynamical and rheological properties can be tuned by varying the mixture composition. They are also very interesting systems from a basic scientific point of view. Even being miscible, these systems are dynamically heterogeneous: starting from two homopolymers with different mobility (different glass transition temperatures  $T_g$ ) two separated segmental ( $\alpha$ ) relaxations are still observed in the miscible blend state. When the difference in segmental mobility ( $T_g$ ) of the two-homopolymer components is not too high, they exhibit qualitative similar dynamic features in the blend. However, a rather different scenario emerges for low concentration of the fast component, if the two homopolymers display very different  $T_g$ 's. In this case, the two components in the blend exhibit strong dynamic immiscibility, with a large separation (dynamic asymmetry) in their respective  $\alpha$ -relaxation times. In such conditions the motion of the fast component seems to be strongly restricted ("confined") by the slowly relaxing matrix formed by the slow component. Recently, we have extended the investigations of dynamic properties of asymmetric polymer blends to the large-scale dynamics (chain dynamics) mainly by dielectric spectroscopy [1] and molecular dynamics simulations [2]. We found that the anomalous dynamic features induced by the slow matrix on the fast component also extend to this regime. The dynamic asymmetry induces strong non-exponentiality of the Rouse modes for the fast component. Moreover, we observe a striking crossover, by increasing the dynamic asymmetry in the blend, to a regime resembling scaling features characteristic of entangled-like chain dynamics, despite the used chain length being much shorter than the critical value for entanglement. We associate these features to strong memory effects that are induced by the slow nature of the confining matrix and thereby implying strong correlations between the external forces acting on the tagged chain. Theoretical methods based on generalized Langevin equations seem to be the suitable framework to describe chain dynamics in asymmetric polymer blends [3].

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## Signatures of glass transition for partially ordered phases

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Glassy dynamics I: Tue 15:00, Lecture Hall

Studies of compounds exhibiting liquid-like and crystal-like liquid crystalline phases and ODIC and CONDIS crystals were performed using DRS and other complementary experimental techniques. In cases when tendency to glass formation rather than to crystallization were detected results in the vicinity of  $T_g$  are shown. Special interest is focused on evidence of glass transition observed by polarizing microscopy and inelastic neutron scattering as well as by adiabatic calorimetry. Some hypotheses on dynamical and structural features of phases of partially ordered organic molecules are presented.

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## Liquids with memory

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Glassy dynamics I: Tue 15:20, Lecture Hall

Opposed to crystals, glasses are considered as the disordered solid state of condensed matter that is usually formed upon cooling of a supercooled liquids below their glass transition temperature,  $T_g$ . Owing to their "quenched disorder", glasses are in a non-equilibrium state which explains many of the specific properties of glasses: i) the glass transition temperature depends on the cooling rate and thermal history, ii) glasses show slow relaxation processes below  $T_g$  known as physical aging that manifest themselves as volume relaxation and creep. While the dynamics of glass forming liquids above  $T_g$  has been subject of a great deal of recent work, bringing understanding in the fast dynamics from the cooperative-relaxation via the Johari-Goldstein mode up to collective vibrational states (Boson peak), one might speculate about what happens if we could prepare glasses with a highly improved packing (ultradense glasses [1]) that maintain thermal equilibrium to a temperature far below the "conventional"  $T_g$ ? Would one encounter qualitative modifications in the glassy dynamics and structure including changes in local order parameters? We have investigated thin

films of glycerol and related polyols (threitol, xylitol and sorbitol) that were produced by molecular beam deposition (OMBD) onto a glass substrate patterned with an interdigitated comb electrode to allow for the real-time study of the dielectric relaxations upon continuous variation of the film thickness or sample temperature [2]. The experiments revealed a strong enhancement in the dielectric strength with respect to the ordinary supercooled liquid for devitrified films, which were deposited directly into the glassy state, suggesting the existence of a metastable liquid phase with enhanced orientation correlation. Upon variation of the deposition conditions and of the molecular size, we could tune the kinetic stability towards conversion into the ordinary liquid phase, up to timescales limited by the experiment [3]. This approach opens a possible route to achieve hidden liquid phases with appealing materials properties.

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## The Debye process in monoalcohols: a century-old puzzle and means to its resolution

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Glassy dynamics II: Tue 16:30, Lecture Hall

It is by now well established that monohydroxy alcohols, at variance with other supercooled molecular liquids, exhibit in their dielectric spectra a dominant Debye-like absorption peak at frequencies lower than those characterizing structural rearrangements. In spite of being detected almost one century ago [1], the origin of the slow dielectric feature in monoalcohols, which carries no significant signature in the response of most other experimental techniques [2,3] remained subject of stimulating controversy. Aiming for a microscopic description of the Debye process, several studies proposed a direct connection between its characteristic time scale and the lifetime of the hydrogen bonds [4] that support the formation of supramolecular structures in these associating liquids. In this work we will address this point and, in addition, we will discuss several other important aspects regarding the origin of the Debye peak by presenting experimental results that we recently obtained for neat, diluted, and solvated monoalcohols.

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## Dynamics in solid and supercooled liquid acid and base hydrates

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Glassy dynamics I: Tue 15:40, Lecture Hall

Various acid and base hydrates are relevant for chemical reactions taking place in the upper atmosphere or they play an essential role in the context of the cryo-volcanism on some icy satellites in our solar system [1]. Often, but not exclusively, the crystalline modifications of the hydrates, e.g., of ammonia, sulfuric acid, or nitric acid are important in these environments. Furthermore, these systems can easily be vitrified in appropriate compositional ranges [2]. From previous studies it is known that sulfuric acid trihydrate is a glass former [3] with a particularly large fragility index [4]. But overall, laboratory studies of these substances, which in view of their highly dissociated nature may be viewed as inorganic ionic liquids, are scarce. For the present work we studied several ammonia hydrates, sulfuric acid hydrates, and nitric acid hydrates using temperature and frequency dependent dielectric and conductivity spectroscopy and with other techniques. Comparison of these results is made with those obtained for other aqueous systems [5,6] as well as for lightly doped ice [7].

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## Dynamics of Microphase Separated Polyurea and Polyurethane Copolymers

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Glassy dynamics II: Tue 17:00, Lecture Hall

This presentation will provide an overview of our recent research on the dynamics of microphase separated polyureas and polyurethanes using dielectric spectroscopy. Polyureas are attractive for various applications due to their outstanding mechanical properties, which can be tuned by varying component chemistry, molecular weight, and reaction stoichiometry. In particular, polyureas synthesized from a modified methylene diphenyl diisocyanate and polytetramethylene oxide-di-p-aminobenzoate are being widely investigated for energy absorbing applications such as impact mitigation and ballistic protection. In order to develop a more complete understanding of their mechanical response, we explored the influence of uniaxial strain on the phase separated microstructure (using small-angle X-ray scattering) and molecular dynamics[1]. In the neo-Hookean region there is no permanent effect of strain, whereas deformation beyond the yield stress gives rise to unrecovered strain and orientation of the domains, along with disruption of the hard domains with consequent reduction in the degree of phase segregation. These morphological changes, in turn, result in significant slowing down of the segmental dynamics, broadening of its distribution of relaxation times, and a large increase in apparent activation energy (fragility). The extent of these changes varies continuously over the course of the deformation. The second part of the presentation will focus on the dynamics of segmented polyurethane copolymers having the same hard segment chemistry and content, but with various soft segment chemistries: oligomeric tetramethylene oxide,[2] hexamethylene oxide, aliphatic carbonate and dimethylsiloxane. All soft segments have MW ~ 1000 g/mol. The polyurethanes under investigation exhibit rich relaxation behavior: up to two relaxations in the glassy state, a segmental  $\alpha$  relaxation, and three slower relaxations. The slowest process arises from interfacial (MWS) polarization and its strength decreases gradually with increasing temperature (over a few tens of degrees), and disappears at a temperature similar to that where the small-angle X-ray scattering from the phase separated microstructure disappears. We would like to express our appreciation to the NSF Polymers Program and the Office of Naval Research for support of this work.

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## Fast dynamics of glassforming liquids probed by dielectric spectroscopy

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Glassy dynamics II: Tue 17:30, Lecture Hall

In broadband dielectric loss spectra of glass forming materials extending from  $\mu\text{Hz}$  to THz, a number of spectral features like peaks, power laws, or minima is revealed [1,2,3]. Except for the so-called alpha peak mirroring the structural relaxation processes, their microscopic origin is still controversially discussed. Understanding the underlying processes seems to be a prerequisite for achieving a deeper insight into the glass transition. Especially, it seems clear nowadays that the different spectral features are closely interrelated and cannot be described independently. In the present talk, I provide broadband spectra of a variety of glass formers extending up to the boson peak. Of special interest are the results on glycerol, whose dielectric response is systematically modified by the addition of ions. Dissolving salts in glycerol leads to strong shifts of the alpha peaks [4,5]. However, almost nothing is known about the behavior of the faster processes like excess wing, fast beta process, and boson peak, which all are observed in pure glycerol [2,6]. For example, according to mode-coupling theory, which describes various dynamic properties of pure glycerol [7,8,9,10], the temperature dependences of such different quantities as the alpha-relaxation rate (in the mHz to GHz range) and the frequency of the loss minimum (10-100 GHz), are predicted to be closely correlated. These correlations are discussed in detail, also including results on other glass formers.

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## Origin of boson peak in polyhydric alcohols

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Glassy dynamics II: Tue 18:00, Lecture Hall

We are going to discuss about origin of THz dielectric loss peak observed in polyhydric alcohols by using our experimental data of dielectric loss for many different alcohols between 10MHz and 2.5THz [1].

- [1] Y. Yomogida et.al., Journal of Molecular Structure 970 (2010) 171-176.

## THz Spectroscopy: A Novel Experimental Tool to Study Water Network Dynamics

M. Havenith

*Physical Chemistry II, Ruhr University Bochum, NC 7/74, 44780 Bochum, Germany*  
Terahertz Spectroscopy I: Wed 09:00, Lecture Hall

In recent years a new frequency window has been opened: The THz range. We could demonstrate that precise THz absorption measurements is a new tool to directly study the solvation dynamics of biomolecules [1]. THz absorption spectroscopy probes sensitively the fast (sub-psec) collective network dynamics of bulk water. Accompanying ab initio MD simulation unravel the underlying molecular motions: In contrast to the mid infrared regime — where the absorption peaks can be assigned to intramolecular motions — in the frequency regime below 1000 cm<sup>-1</sup> intermolecular motions with concerted particle motions dictate the spectrum [2]. Precise measurements of absorption coefficients of solvated solutes in the THz regime allow now a detailed view on the role of the water for biological function [3–5].

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## Unexplored avenues of human skin: Reading personal stress in the Sub-THz frequency range

Y. Feldman, A. Puzenko, P. Ben Ishai and E. Safrai

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Terahertz Spectroscopy I: Wed 09:30, Lecture Hall

The coiled structure of the tips of the sweat ducts embedded in the epidermis of human skin has given rise to the supposition that at sub-THz frequencies the response of the ducts should be similar to low Q helical antennas [1,2]. As such, this response should reflect the activity of the perspiration system, governed by the Sympathetic Nerve System [3]. We show that indeed the temporal behavior of the reflection coefficient at sub THz frequencies is highly correlated to the temporal behavior of the blood pressure, the pulse rate and other physiological parameters in response to physical, mental and emotional stresses imposed on the subject.

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## Temperature and hydration dependence of functional proteins studied by terahertz time-domain spectroscopy

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Terahertz Spectroscopy I: Wed 10:00, Lecture Hall

Because of recent dramatic progress in generation and detection of terahertz wave, spectroscopic studies in the far-infrared region have been extensively promoted on condensed phases like proteins and DNA [1,2]. Because their functions are expressed in thermal fluctuation of solvent, It can be considered that solvent thermal fluctuation is an important factor for their functional expressions. Terahertz time-domain spectroscopy is a powerful tool to monitor such fluctuation [3,4]. In this study we investigated temperature and hydration dependence of a functional protein, amylase. We used several kinds of the protein that derive from different bacterial species. It was revealed that in every protein we observed sudden increase in absorption coefficients at around 220 K only when the samples are hydrated. This phenomenon is

known to a protein dynamical transition, which is believed to strongly correlated with protein functional expression [5,6]. Furthermore, we also found that when the samples are hydrated absorption coefficients decrease compared to dried samples in spectral regions lower than around  $25\text{ cm}^{-1}$ . These observations indicate that hydration plays a role to make proteins stiff. The results suggest diversity of the effects of hydration water.

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- [6] S. Kawaguchi, et al., Physical Chemistry Chemical Physics, vol. 12, pp. 10255-10262, 2010.

## Tunable THz wave sources and real life applications

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Terahertz Spectroscopy II: Wed 11:00, Lecture Hall

Among our research activities for THz sources, we can mention: THz-wave parametric oscillator/generator (TPO/TPG); Injection-seeded THz-wave parametric generator (is-TPG); Compact TPG using top-hat Nd:YAG laser; is-TPG pumped by microchip Nd:YAG laser; Cherenkov type difference frequency generation (DFG), etc. THz wave generation based on nonlinear frequency conversion is promising way for realizing a widely tunable monochromatic bright THz-wave source. Such a development of THz-wave source depends on brilliant nonlinear crystals. Unfortunately, many nonlinear crystals have strong absorption at THz region. Recently, we showed that Cherenkov radiation with waveguide structure is an effective strategy for achieving efficient and extremely wide tunable THz-wave source. Among our research activities for applications, we can mention: Time of flight THz reflection tomography for multi layered thin coatings; THz spectroscopic imaging for the detection of illicit drugs in the envelopes; THz computed tomography for the inspection of soot distribution in a ceramic filter; a possible sweat-duct helical antenna in the THz region on human skin; etc. Although still at the beginning of a long road, the applications of THz waves have started to make visible progress and the results shown here represent a part of our contribution to the field.



## Water Revisited – Unifying a Myriad of Beliefs

P. Ben Ishai<sup>1,2,4</sup>, E. Mamontov<sup>2</sup>, A.P. Sokolov<sup>2,3</sup>, J. Nickels<sup>2,3</sup>, K. Kawasa<sup>4</sup>  
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Terahertz Spectroscopy II: Wed 11:30, Lecture Hall

Diverse communities have diverse views on what constitute the true behavior of water. When considering the THz behavior of water it is common to consider the behavior as a superposition of fundamental Debye relaxations. Yet the view held by many in the Soft Condensed Matter community is that water is a glass former and that a simple Debye laws will not adequately describe its dynamic behavior. This is partly because the role of the cluster structure, reorientation and its relationship to the H-bond network has not been fully explored up to the higher frequencies. We attempt to marry THz spectroscopy and traditional dielectric spectroscopy to provide a complete picture of the dynamics of water and also of aqueous salt solutions, in the frequency range covering all reorientation and transport phenomena. Additional microscopic information is gained from neutron scattering. Consequently we hope to span two sometimes opposing world views and lead to a unified discussion on what water really does in the higher frequency spectrum of THz. The talk will present dielectric measurements carried out in the Hebrew University of Jerusalem and THz results measured in the University of Nagoya. The microscopic picture will be further probed by considering Neutron Scattering on aqueous salt solutions, carried out in Oak Ridge National Laboratory.

## Low-frequency dynamics of lipid studied by terahertz time domain spectroscopy

T. Andachi<sup>1</sup>, N. Yamamoto<sup>2</sup>, A. Tamura<sup>1</sup> and K. Tominaga<sup>1,2</sup>

<sup>1</sup> Graduate School of Science, Kobe University, Kobe City, Japan

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Terahertz Spectroscopy II: Wed 11:50, Lecture Hall

Lipids are a main component of cell, which form lipid bilayers by self-assembling. Lipid molecules continuously fluctuate in the thermal environment surrounded by water. In the terahertz (THz;  $1 \text{ THz} \approx 33 \text{ cm}^{-1}$ ) frequency region, the fluctuation derives from delocalized vibrational motions and hydrogen bond forming and deforming with water molecules. Therefore terahertz time-domain spectroscopy (THz-TDS) is a powerful tool to investigate lipid molecule dynamics. In this study, we focused on dependence of the lipid low-frequency dynamics on hydration, temperature, and lipid structure by using THz-TDS. As a sample, we selected 1,2-Dimyristoyl-sn-glycero-3-phosphoglycerol (DMPG), which is known to form several different structures like crystalline or gel phase states. We measured the temperature dependence of the low-frequency spectra of the lipid under different hydration degrees and structures. The absorption coefficients of each sample were obtained in the frequency region from  $10 \text{ cm}^{-1}$  to  $50 \text{ cm}^{-1}$ . We discuss about the lipid dynamics from the changes of the absorption coefficients.

## The circular polarization of sub-THz signal reflected from the human skin

I. Hayut, P. Ben Ishai, A. Puzenko, A.J. Agranat and Y. Feldman

Department of Applied Physics, The Hebrew University of Jerusalem, Israel

Terahertz Spectroscopy II: Wed 12:10, Lecture Hall

The helical structure of the human eccrine sweat ducts, combined with the dielectric properties of their surrounding tissue, suggested that the electromagnetic (EM) reflection from the multi-layered structure of the skin organ can exhibit properties similar to those of an array of helical antennas operating at extremely high frequencies ( $0.1 \text{ THz}$ - $0.7 \text{ THz}$ ). We henceforth propose to explore the validity of this suggestion by exploiting the fact that the chirality of the ducts has a preferred direction, implying circular dichroism of the reflected electromagnetic field in the vicinity of the expected axial (end-fire) mode. In order to examine the implications of this presumption, a simulation model of the human skin with embedded sweat ducts was designed and

numerical simulations in the frequency range of 100 GHz to 450 GHz, were conducted using CST studio software. A polarization measuring system was constructed based on an AB-mm frequency-domain vector network analyzer, and the polarization of the EM field reflected from the skin was measured. In this work we show that: 1) Circular dichroism is apparent in the simulation model, 2) Preliminary results of the circularly polarized nature of the signal reflected from the skin are presented. The implications of such discovery will be discussed.

## Heating Liquid Dielectrics by Time Dependent Fields

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BDS and other techniques I: Wed 14:00, Lecture Hall

Steady state and time-resolved dielectric relaxation experiments are performed at high fields on viscous glycerol and the effects of energy absorption from the electric field are studied. Time resolution is obtained by a sinusoidal field whose amplitude is switched from a low to a high level and by recording voltage and current traces with an oscilloscope during this transition. Based on their distinct time and frequency dependences, three sources of modifying the dynamics and dielectric loss via an increase in the effective temperature can be distinguished: electrode temperature, real sample temperature, and configurational temperatures of the modes that absorbed the energy. Isothermal conditions that are desired for focusing on the configurational temperature changes (as in dielectric hole burning and related techniques) are maintained only for very thin samples and for moderate power levels. For high frequencies, say  $f > 1$  MHz, changes of the real temperature will exceed the effects of configurational temperatures in the case of macroscopic samples. Regarding microwave chemistry, heating via cell phone use, and related situations in which materials are subject to fields involving frequencies beyond the MHz regime, we conclude that changes in the configurational (or fictive) temperatures remain negligible compared with the increase of the real temperature. This simplifies the assessment of how time dependent electric fields modify the properties of materials.

## **Atomistic and molecular probe characterization of poly(isoprene)s by PALS and ESR in relation to broadband dielectric spectroscopy**

J. Bartoš<sup>1</sup>, H. Švajdlénková<sup>1</sup>, Y. Yu<sup>2</sup>, R. Krause-Rehberg<sup>2</sup>, S. Arrese-Igor<sup>3</sup>  
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BDS and other techniques I: Wed 14:30, Lecture Hall

Structure and dynamics of glass-forming systems can be studied by two main classes of experimental techniques. In addition to the traditional structural diffraction methods and dynamic ones such as dielectric spectroscopy and neutron scattering based on various internal probes, external probes are of a great interest such as atomic-sized ortho-positronium (o-Ps) and the so-called molecular spin probes as investigated by positron annihilation lifetime spectroscopy (PALS) or electron spin resonance (ESR), respectively. To reveal the possibilities of these indirect probing techniques at the structural-dynamic characterization of glass-forming systems we have carried out the detailed study of a series of oligomer and polymer 1,4-poly(isoprene)s (PIP) by means of PALS and ESR measurements. The corresponding PALS and ESR responses have been compared with the dynamic information about a variety of the relaxation processes in 1,4-PIP as obtained by the detailed broadband dielectric spectroscopy (BDS). The findings and conclusions about the potential of the PALS and ESR methods stemming from this mutual comparative and complementary studies with BDS will be presented.

## **AC-calorimetry as a complementary method to dielectric spectroscopy**

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BDS and other techniques I: Wed 15:30, Lecture Hall

Calorimetry has proven to provide useful information about glass transition and material properties in general, because it establishes a direct link to energetic characterization. Due to MEMS technology in recent years new calorimetric devices were

developed for heating/cooling rates respectively frequency ranges not easy or not at all accessible earlier. In several cases now a direct comparison with results from other dynamic methods like dielectric spectroscopy in a broader range is possible. While in dielectric spectroscopy all processes including dipole fluctuations are detected in calorimetry the local modes as side group rotations and similar processes are not seen. Due to this, in several examples the combination of the different methods gives further insights in molecular processes [1,2].

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## **Dielectric relaxation of NBR/EPDM Blend loaded with various types of nano scaled carbon black: Applicability of some conductivity models**

S.L. Abd-El-Messieh<sup>1</sup>, D.E. El-Nashar<sup>2</sup>, A.F. Younan<sup>2</sup>, K.N. Abd-El-Nour<sup>1</sup>

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Electrode and Maxwell-Wagner Polarization: Fri 10:10, Lecture Hall

The permittivity  $\epsilon'$  and dielectric loss  $\epsilon''$  were measured for NBR/EPDM blends (50/50) at room temperature and different frequencies. Three types of carbon black which were analyzed by TEM and found to be in the nano scale were added with various content to this blend. The analyses of the data revealed relaxation mechanisms ascribed the main chain and its related motions. At certain concentration, sharp increase in the dielectric parameters and electrical conductivity was noticed which reflect the net work formation (percolation phenomena). This was confirmed by using SEM and the applicability of various conductivity models were studied and compared with the experimental results. The mechanical properties of all composites were also studied.

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## **Physico-Chemical Modification of Polymer Dielectrics for Electromechanically Active Elastomers, for Piezoelectret Systems, and for Pyro- or Piezoelectric Films**

R. Gerhard

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BDS and other techniques II: Wed 16:30, Lecture Hall

The performance of dielectric elastomers ("electro-electrets") for actuator and sensor applications relies on high relative permittivity and low elastic modulus. Recent advances in the chemical modification of silicone elastomers allow for the stable attachment of molecular dipoles to the elastomer network, which leads to an overall improvement by a factor of 6 through an increase of the permittivity and a decrease of the modulus [1]. Space-charge electret films and ferroelectret systems depend on the thermal and long-term stability of trapped charges within the respective polymer materials. Recently, chemical surface treatments resulted in much higher charge stabilities even on standard polymers such as polyethylene, but also on fluoropolymers that already exhibited rather good charge stabilities [2]. Ferroelectric polymers from the polyvinylidenefluoride (PVDF) family show useful piezo- and pyroelectric properties if they are prepared in the relevant all-trans conformation that leads to parallel packing of the molecular dipoles in the crystalline  $\beta$ -phase. Recent experiments with the addition of ionic liquids to a PVDF solution yielded  $\beta$ -phase crystallites without further processing and thus allow for the preparation of pyro- and piezoelectric polymer films from solution even on substrates [3]. The unexpected and highly significant progress in three areas of dielectric polymers with electret properties will be discussed in view of open fundamental questions and of applications-relevant processing issues.

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- [3] F. Wang et al. *Appl. Phys.Lett.* 100, 062903 (2012).

## Time domain reflectometry technique for the Aqueous and Non-Aqueous solutions

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BDS and other techniques II: Wed 16:50, Lecture Hall

We have developed and established the TDR technique in laboratory provides information regarding dielectric permittivity in the frequency range 10 MHz to 30 GHz. There is a great interest to study the dielectric relaxation behaviour in liquid systems to understand the role of hydrogen bond in liquid system. The dynamics of hydrogen bonded liquids have been studied by dielectric spectroscopy technique. Alcohols are compounds in which hydroxyl (-OH) group is attached to saturated hydrogen atom. The hydroxyl group is a functional group of alcohols. Their general formula is R-OH and these are classified as monohydric, dihydric, trihydric and polyhydric alcohols. Polyhydric alcohol is one of the hydrogen bonding liquids, where each molecule has two or more -OH groups. In general, polyhydric alcohols exhibit the glass transition at temperature ( $T_g$ ) relatively higher than those of usual molecular liquids with similar molecular size. The dielectric constant for the mixtures can be explained using hydrogen bonded model by assuming the formation of hydrogen bonds between alcohol-alcohol and alcohol-dioxane pairs. The orientation correlation between neighbouring molecules due to hydrogen bonding interactions are determined in terms of Kirkwood factors. The number of hydrogen bonds of alcohol-alcohol and alcohol-dioxane molecules are computed. The theoretical model to explain the experimental results has been discussed.

## Two-channel impedance spectroscopy for comparing the dynamics of 2-ethyl-1-hexanol and its water mixture

L.P. Singh and R. Richert

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BDS and other techniques II: Wed 17:10, Lecture Hall

For many supercooled liquids, the high sensitivity of the dielectric relaxation behavior on temperature prevents a meaningful comparison of nearly identical dynamics on the basis of two separate measurements. In order to resolve this issue, we have devised a dielectric dual-channel spectrometer setup [1], which exploits that the SI-1260 gain/phase analyzer can operate three channels in parallel, where two are used to

analyze the currents through each capacitor, and one is used to measure the voltage applied to both capacitors that share a common center electrode. Here we used two-channel impedance spectroscopy [1] for the simultaneous measurements of 2-ethyl-1-hexanol and its water solutions. Based on dual-channel method, we found that the addition of small amount of water ( $x_m=0.01, 0.02$ ) in 2-ethyl-1-hexanol the strength of Debye process decreases while  $\alpha$ -process increases. Also the temperature dependence of relaxation times of Debye process becomes faster while  $\alpha$ -process becomes slower. The present result is more or less agreed with the application of pressure to 2-ethyl-1-hexanol.

[1] L. P. Singh and R. Richert, Rev. Sci. Instrum. 83, 033903 (2012).

## **Aging-time dependence of the segmental relaxation time of PVAc/SiO<sub>2</sub> nanocomposites: a combined BDS and TSDC study**

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BDS and other techniques II: Wed 17:30, Lecture Hall

The last 15 years have seen an increasing interest in polymer nanocomposites, particularly attractive for many applications (automobile, aerospace, microelectronic, drug delivery, etc) due to the combination, and sometimes the synergy, of the properties relative to both components [1]. However, little has been reported on the polymer nanocomposites long-term performances, which can be dramatically affected by chemical aging, and/or physical aging [2], a temperature and time dependent process. In particular, the physical aging of glassy polymers was shown to get faster with increasing the weight fraction of inorganic fillers [3,4], in glassy polymer nanocomposites whose segmental dynamics was unchanged related to the bulk polymer. Based on these observations, an intriguing scenario recently inferred that the densification occurring during physical aging may not be one-to-one related to the intrinsic segmental mobility of the glass; a result at odds with the conventional view on physical aging. In such systems, other parameters such as the amount of nanofillers in the glassy polymer, seem to play a role in the determination of the physical aging rate, whose characteristic time can thus be written as:  $\tau_{PA} = \tau \cdot f(A/V)$ , where  $\tau$  is the segmental relaxation time, and  $f(A/V)$  is a function related to the area of filler to volume of polymer ratio,  $A/V$ . However, no information on the aging time evolution



of the segmental relaxation time was provided. On this basis, the idea of monitoring the time evolution of the segmental relaxation time in a bulk glassy polymer and its nanocomposites by techniques such as Broadband Dielectric Spectroscopy (BDS) and Thermally-Stimulated Depolarization Current (TSDC) appeared as a mean to check this relation between  $\tau_{PA}$  and  $\tau$  via  $f(A/V)$  on one hand, and to provide direct evidence on the achievement of a similar equilibrium state below  $T_g$  for the bulk and its nanocomposites on the other. Such study has been carried out on poly(vinyl acetate) (PVAc)/silica ( $\text{SiO}_2$ ) nanocomposites displaying similar segmental dynamics (BDS) and accelerated aging related to bulk PVAc (Differential Scanning Calorimetry (DSC)). The monitoring of time dependence of the segmental relaxation time of PVAc in the bulk and in nanocomposites by TSDC and BDS supports the previously proposed scenario, showing that the instantaneous segmental relaxation time in PVAc/ $\text{SiO}_2$  nanocomposites is larger than in bulk PVAc, despite the faster evolution toward equilibrium in the former systems. This striking result provides evidence that, beyond molecular mobility, the physical aging rate also depends on the amount of interfaces in nanostructured glasses.

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- [3] D. Cangialosi, V. M. Boucher, A. Alegría, J. Colmenero, *Polymer* 53 (2012) 1362–1372.
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## Comparative dielectric studies of Ag nanoparticles in matrix of polymers and monomers.

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BDS and other techniques II: Wed 17:50, Lecture Hall

In this work the results of BDS study ( $10^{-3}$ – $10^5$  Hz, 140–180°C) of Ag nanoparticles (NPs) synthesized in different matrix (polymers and monomers) are presented. The frequency dependence of specific AC conductivity and complex electric modulus was used to estimate the temperature-frequency intervals of charge transfer by long and short distances, respectively. With increasing the concentration of Ag NPs, specific AC conductivity increases. In low frequency region, the AC conductivity dependence transformed into plateau, that corresponded to DC conductivity. The temperature dependence of specific DC conductivity show considerable deviation from Arrhenius dependence, that points to the significant contribution of cooperative effects in the charge carriers transport mechanism. In the sols and films of Ag NPs the considerable

increase of Vogel temperature and glass-transition temperature,  $T_g$ , in sols in comparison with pure solvent was found. Although the dielectric characteristics of sols generally controlled by the conductivity relaxation, the dielectric response was observed in the high-frequency range ( $1-10^3$  Hz) at low temperature ( $-50 - +10^\circ\text{C}$ ). This response was resulting from the presence of NPs in the solution. It was supposed that the relaxation was caused by motion of ion impurities on the Ag NPs surface within the carboxylate ligands shell. In contrast to the sols and films of Ag NPs in the epoxide and Ag NPs nanocomposites the  $T_g$  was varied from 90 to  $96^\circ\text{C}$ .

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## **Comparison of relaxation processes in poly(2-(2-methoxyethoxy)ethyl methacrylate) hydrogels differ on crosslinking density**

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BDS and other techniques II: Wed 18:10, Lecture Hall

Hydrogels are widely investigated materials due to their promising applications. Their main advantage is to change their properties in response by modification of the environmental conditions. The thermoresponsive hydrogels are characterized by Volume Phase Transition (VPT) but too slow response to stimuli is one of the most important problem to be solved [1]. The kinetics of VPT depends among other on dynamic of polymer chain. Influence of chemical structure of the polymer network, temperature and crosslinking density on the dynamic of thermo-responsive hydrogels synthesized from 2-(2-methoxyethoxy)ethyl methacrylate (MEO<sub>2</sub>MA) was investigated. The molecular dynamics was investigated in wide range of temperature and frequency. Comparison of dry uncrosslinked poly(MEO<sub>2</sub>MA) and crosslinked hydrogels synthesized by ATRP and FRP was done. The studies have shown presence of two relaxation regions. One, at low temperatures, is due to local motions present in glass state. The second one, visible at higher temperature range, is mainly due to segmental dynamics above  $T_g$  as was indicated by DSC measurement. The segmental dynamics seems to be independent of the polymerization process kind and crosslinking density. At similar temperature range but at lower frequencies additional process is observed. Dynamics of this process is different for each materials and depends on crosslinking density, what can indicate that this process is corresponding to some network dynamics.

Acknowledgements: This project was supported by Polish Ministry of Science and Higher Education (grants no. NN209200738 and N N209 413839).

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## **Heterogeneous and aging dynamics in single and stacked thin polymer films**

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Confined systems I: Thu 09:00, Lecture Hall

The glass transition and the alpha-process above the glass transition temperature,  $T_g$ , and the aging dynamics below  $T_g$  were investigated for single and stacked thin polymer films. First, the glass transition dynamics of stacked thin films of polystyrene (PS) and poly(2-chlorostyrene) (P2CS) were measured using DSC and dielectric relaxation spectroscopy. The  $T_g$  for as-stacked thin PS films has a strong depression from that of the bulk samples. However, after annealing at high temperatures, the stacked thin films exhibit glass transition at a temperature almost equal to the  $T_g$  of the bulk system. The alpha-process dynamics of stacked thin films of P2CS show a very slow time evolution from single thin film-like dynamics to bulk-like dynamics during the isothermal annealing process. The temperature dependence of the relaxation time for the alpha-process changes from Arrhenius-like to VFT-dependence with increase of the annealing time. Secondly, the aging dynamics of P2CS ultrathin films with thicknesses less than 10 nm were investigated using dielectric relaxation spectroscopy. The imaginary part of the dielectric susceptibility,  $\epsilon''$ , for P2CS ultrathin films with a thickness of 3.7 nm increases with an increase in isothermal aging time, while this is not the case for P2CS thin films thicker than 9.0 nm. This anomalous increase in  $\epsilon''$  for the ultrathin films is strongly correlated with the presence of a mobile liquid-like layer within the thin films [1,2].

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## Dynamics of Rouse Chains Under Soft-Confinement with Different Geometries

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Confined systems I: Thu 09:30, Lecture Hall

In this work we present results obtained by broad-band dielectric spectroscopy (BDS) on the dynamics of a polymer Rouse chain confined in lamellar (1D confinement), cylindrical (2D) and spherical (3D) domains of block copolymer melts. Particularly, we selected a fixed polyisoprene (PI) block (with 4 kg/mol molecular mass, un-entangled chain) with polydimethylsiloxane (PDMS) blocks of varying size. Since PI is a type A polymer we were able to follow the dynamics of the PI end-to-end vector, in addition to the segmental one. On the other hand, the ordered mesophases of these di-block copolymers were investigated by small-angle X-ray scattering (SAXS), confirming the presence of lamellar (1D confinement), cylindrical (2D) and spherical (3D) PI domains. In all cases the PI polymer is confined by a highly mobile phase (PDMS), i.e. "soft-confinement", which results in an accelerated segmental dynamics when compared with the corresponding PI melt. However, we observe that the behavior of the end-to-end dipole vector depends on the confined phase geometry. These results are interpreted as originated by the combination of internal chain modes with the motion of the PI-PDMS junction point.

## **Glassy dynamics of ultra-thin polymer films investigated by a combination of complementary methods**

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Confined systems I: Thu 09:50, Lecture Hall

The molecular dynamics especially the dynamic glass transition of ultra-thin polymeric films with thicknesses down to few nm was investigated by combining bulk methods with surface analytics. As bulk-like methods capacitive dilatometry, broadband dielectric and specific heat spectroscopy are employed. Surface analytics is carried out by using X-ray photoelectron spectroscopy (XPS) and contact angle measurements. From the latter experiments the interaction energy between the polymer and the substrate is estimated quantitatively where XPS gives the composition on the surface as function of the layer thickness. As homopolymer systems polystyrene [1], the main chain polymers polysulfone [2] and polycarbonate [3,4] are considered. Also measurements on the blend system polystyrene/poly(vinyl methyl ether) which is miscible in the bulk state are presented. It is discussed in detail which factors influences the glassy dynamics of ultra-thin polymer films.

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## **Mechanical Properties of Thin Confined Polymer Films Close to the Glass Transition in the Linear Regime of Deformation: Theory and Simulations**

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Confined systems I: Thu 10:10, Lecture Hall

Over the past twenty years, experiments performed on thin polymer films deposited on substrates have shown that the glass transition temperature can either decrease or increase depending on the strength of the interactions. Over the same period, experiments have also demonstrated that the dynamics in liquids close to the glass transition temperature is strongly heterogeneous, on the scale of a few nanometers. A model for the dynamics of non-polar polymers, based on percolation of slow subunits, has been

proposed and developed over the past ten years. It proposes a unified mechanism regarding these two features. By extending this model, we have developed a 3D model, solved by numerical simulations, in order to describe and calculate the mechanical properties of polymers close to the glass transition in the linear regime of deformation, with a spatial resolution corresponding to the subunit size. We calculate the evolution of the elastic modulus as a function of temperature, for different film thicknesses and polymer-substrate interactions. In particular, we show that for strong interactions and small thickness, glass transition is not only shifted (by up to 20 K) but also broadened and accompanied by huge fluctuations of the storage modulus. This effect due to the low percolation threshold across thin films conjugated to the huge difference between high and low frequency moduli, should be more apparent in mechanical experiments than in dielectric spectroscopy or calorimetry.

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[3] S. Merabia and D.R. Long, Macromolecules 41 (2008) p.3284.

## **Can the dielectric strength rationalize the deviation from bulk behavior in ultrathin polymer films?**

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Confined systems: Thu, Lecture Hall

The proximity of solid interfaces and free surfaces tremendously alters the behavior of small molecules and polymers. After almost three decades of intensive investigations, it seems possible to explain the deviation from bulk behavior in ultrathin polymer films in terms of a mere combination of the film thickness and interfacial interactions. However, a large number of experimental works highlighted how properties of ultrathin polymer films depend on the annealing conditions used during their preparation, for a review see [1]. We show clear evidence that also the adsorption degree should be taken into account to describe the behavior of polymers at the nanoscale [2]. To validate our hypothesis we developed an experimental approach that permitted us to quantify the free volume available at the polymer/metal interface, via dielectric spectroscopy. An increase in free volume, caused for example by packing frustration, results in an acceleration of the segmental dynamics and thus justify a reduction of  $T_g$  even in the presence of slower dynamics associated to chain adsorption. Our picture is confirmed and extended by further investigations of supported films by means of ellipsometry and neutron reflectivity. Finally, we discuss on the thickness, temperature and annealing time dependence of the dielectric strength, highlighting the possibility

to extract interfacial mobility profiles [3,4], and mass transport coefficients [5] from dielectric spectra.

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- [2] Napolitano and Wübbenhorst, Nature Communications, 2011, 2, 260.
- [3] Rotella, Wübbenhorst and Napolitano, Soft Matter, 2011, 7, 5260.
- [4] Yin, Napolitano and Schönhals, Macromolecules, 2012, 45, 1652.
- [5] Napolitano, Rotella and Wübbenhorst, Macromolecular Rapid Communications, 2011, 32, 844.

## **Novel Polymeric Materials for Electrochemical Applications Based on Epoxy Resins Hardened by Phosphotungstic Heteropolyacid**

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Electrode and Maxwell-Wagner Polarization: Fri 09:00, Lecture Hall

The polymeric systems with high level of ionic conductivity are perspective materials for application in autonomous current sources, sensors, supercapacitors and other electrochemical devices. The elaboration of such polymer materials is the actual task. The crosslinked flexible amorphous polymers with high content of ether oxygen in their chain structure have been synthesized with using (of) aliphatic epoxy resins DEG (diethyleneglycol diglycidyl ether) and LO (polyoxypropylenetriol triglycidyl ether). Aromatic epoxy resin ER (bisphenol A diglycidyl ether) without oxygen was also used. The water solution of the phosphotungstic heteropolyacid (PTA) have been used as a hardener for epoxy oligomers. The PTA provides the presence of the ionic conductivity, high thermal and chemical stability of the polymers. The dielectric characteristics in wide range of frequencies and temperatures have been investigated. It is shown the dielectric behavior dependence of the epoxy polymers on chemical structure of the resin. In the case of the resin mixture the average characteristics are between those of polymers based on aliphatic and aromatic resins. The conductivity of the polymers based on DEG or LO is higher than that in ER. The level and the character of the polymer conductivity  $\sigma$  depend on the solvent content in the reactive mixture: there are two plateaus on the  $\sigma'$ -f curves, which turn into one with increasing water content in the reactive mixture.

## Molecular dynamics in 1- and 2-dimensional geometric confinement as studied by Broadband Dielectric Spectroscopy

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Confined systems II: Thu 11:30, Lecture Hall

The question of how the *dimensionality of geometrical confinement* influences the molecular dynamics is up to now unexplored; 1-dimensional (1-D) confinement is realized in nanometer thin layers or films, while 2-D constraints take place for molecules contained in nanopores. Experimental results of poly-cis-1,4-isoprene (PI) in thin layers down to 6 nm thickness prepared as part of a nanostructured capacitor arrangement and when deposited in unidirectional nanopores having pore diameters down to 4 nm will be presented. Due to the fact that PI is a type – A polymer having two dielectrically active relaxation processes; one corresponding to the fluctuations of 2-3 polymer segments and the other being assigned to that of the end-to-end vector of the chain, it is possible to sense the dynamics at two well separated length scales. First results will be presented and compared to studies on the dynamics of low molecular weight glass formers and liquid-crystals confined in 2-D constraints of nanopores.

## Influence of interfacial interactions and annealing on dielectric relaxation in ultrathin films

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Confined systems II: Thu 12:00, Lecture Hall

The presence of long-living metastable states in ultrathin polymer films has been recently observed [1] after their prediction much longer ago [2]. In fact, relaxation dynamics depends on annealing over time scales much longer than any characteristic time scale of the bulk. In polystyrene the evolution of such metastable states



was related with the growth of an irreversibly adsorbed polymer layer at the substrate interface [3,4]. In this report I will present new results of dielectric relaxation in ultrathin poly(vinyl acetate) film, as obtained by Local Dielectric Spectroscopy measurements [5]. We evidenced that confinement in ultrathin supported films of PVAc on weakly interacting substrates (gold, aluminum) produces an increase of dielectric relaxation frequencies when film thickness decreases below 2-3 times the gyration radius, or equivalently a decrease of the glass transition temperature (about 2 K), whereas on Si substrates (with native oxide on top), having the highest interfacial energy, such confinement effect is not present [6,7]. Moreover, dielectric relaxation dynamics changes on annealing over time scales of several days [7]. Such evolution is accompanied by the growth of an irreversibly adsorbed layer at as for polystyrene. The influence of the substrate on the formation of such layer has been investigated, evidencing a reduction of the growth rate on substrates with more favorable interfacial energy.

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- [2] G. Reiter, P. G. de Gennes *Eur. Phys. J. E* 6, 25 (2001).
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- [7] H. K. Nguyen, D. Prevosto et al. *Macromol.* 45, 2138 (2012).

## Soft matter under Hard confinement

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Confined systems II: Thu 11:00, Lecture Hall

Soft matter under confinement is a growing, interdisciplinary research field with yet unknown basic principles. Nanoporous hard templates provide a two-dimensionally confined space in which self-organization processes such as crystallization, protein secondary structure formation, mesophase formation and phase separation can be manipulated giving rise to unprecedented confinement-induced morphologies with new and exciting properties. A principal focus of the current work is finding the basic underlying principles that give rise to directed self-organization and controlled phase state in a range of soft materials under confinement. It structural, thermodynamic and dynamical characterization (with BDS) in a number of soft materials with different types of interactions. These include crystallizable polymers [1], rod-like and

disk-like liquid crystals [2] and biopolymers [3] with important potential applications.

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- [2] C. Grigoriadis, H. Duran, M. Steinhart, M. Kappl, H.-J. Butt, G. Floudas ACS Nano 11, 9208, 2011.
- [3] H. Duran, A. Gitsas, G. Floudas, M. Mondeshki, M. Steinhart, W. Knoll Macromolecules (Commun.) 42, 2881, 2009.

## From boiling point to glass transition temperature: reorientational correlation time in molecular liquids follow three-parameter scaling

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Conducting glasses and ionic liquids: Fri 14:00, Lecture Hall

The most prominent feature of the glass transition phenomenon, the super-Arrhenius temperature dependence of the correlation time  $\tau_\alpha$  remains a challenge to be described over the full temperature range. Although extensively studied close to the glass transition temperature  $T_g$  molecular glass formers are not sufficiently well investigated in the high-temperature regime well above  $T_m$ , i.e., up to the boiling point. For a series of molecular glass formers, we have combined  $\tau_\alpha(T)$  from dielectric spectroscopy and dynamic light scattering (Fabry-Perot interferometry and photon correlation spectroscopy data) covering the range  $10^{-12} \text{ s} < \tau_\alpha < 10^2 \text{ s}$ . Describing the dynamics in terms of an activation energy  $E(T)$ , we distinguish a high-temperature regime characterized by an Arrhenius law with a constant activation energy  $E_\infty$  and a low-temperature regime for which  $E_{\text{coop}}(T) \equiv E(T) - E_\infty$  increases while cooling. A two-parameter scaling is introduced, specifically  $E_{\text{coop}}(T)/E_\infty \propto \exp(\lambda(T/T_A - 1))$ , where  $\lambda$  is a generalized fragility parameter, and  $T_A$  a reference temperature proportional to  $E_\infty$ . In order to describe  $\tau_\alpha(T)$  still the attempt time  $\tau_\infty$  has to be specified. Thus, a single interaction parameter  $E_\infty$  describing the high-temperature regime of molecular liquid together with  $\lambda$  controls the temperature dependence of low-temperature cooperative dynamics.

## On the dielectric relaxation of Natural Rubber and the effect of vulcanizing agents

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Charge transport and glassy dynamics: Thu 14:30, Lecture Hall

Natural Rubber (NR) holds a unique place in rubber technology. For most applications, it is necessary to convert the rubbery linear polymer into a three-dimensional network in order to assure a complete recovery after deformation. Such a network is the result of cross-linking, covalent bonding among some chain segments, by means of temperature and pressure in which an essentially fluid material is transformed into a fully elastic one. This process is commonly known as vulcanization. The influence of the addition of vulcanizing additives on the molecular dynamics of unvulcanized NR as studied by broadband dielectric spectroscopy reveals a slowdown of the segmental dynamics of NR, restricting the motion of the chains tightly bounded to the additive surfaces. In general, when zinc oxide is present a second dynamic process is detected, ascribed to strong interfacial interactions between the zinc ionic clusters and the NR polymer segments. The study of such interactions prior to vulcanization is a very useful strategy to control the vulcanization process, maximizing its benefits and, hence, improving the final products. Broadband dielectric spectroscopy is a good experimental alternative in order to obtain a deeper insight into the vulcanization mechanisms [1].

- [1] M. Hernández, T. A. Ezquerro, R. Verdejo, M. A. López-Manchado . *Macromolecules*, 45, 1070 (2012).

## Are the thermal $T_g$ and the segmental dynamics in polymer thin films fully interdependent?

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Charge transport and glassy dynamics: Thu 14:50, Lecture Hall

The present contribution aims to elucidate the glass transition behavior in thin polymer films. Special attention is dedicated to the kind of information delivered by different techniques, in particular those probing the molecular mobility in the linear regime as opposed to those providing the thermal glass transition temperature ( $T_g$ ) as a discontinuity in a second order thermodynamic magnitude. To do so, we investigate the segmental dynamics and glass transition temperature ( $T_g$ ) of thin polystyrene (PS) films. The former is investigated by alternating current (AC) calorimetry and broadband dielectric spectroscopy (BDS). The  $T_g$ , underlying the equilibrium to out-of-equilibrium crossover from the supercooled liquid to the glass, is obtained by differential scanning calorimetry (DSC) and capacitive dilatometry (CD). We show that the intrinsic molecular mobility of PS is independent of the film thickness both for freestanding and supported films, whereas  $T_g$  decreases with film thickness from several microns down to 15 nm [1]. This result is found for complementary methods and in a simultaneous measurement in BDS and CD. The most important implication of these results is that the widespread notion that segmental mobility and the equilibrium to out-of-equilibrium transition are, under any experimental conditions, fully interrelated must be questioned in confinement. In nanostructured systems, it appears that the molecular mobility and  $T_g$  are affected differently by geometric factors [2-4].

[1] V. M. Boucher, D. Cangialosi, H. Yin, Andreas Schönhals, A. Alegría, and J. Colmenero, *Soft Matter* 8, 5119 (2012).

[2] V. M. Boucher, D. Cangialosi, A. Alegría and J. Colmenero, *Macromolecules* 43, 7594 (2010).

[3] V. M. Boucher, D. Cangialosi, A. Alegría, J. Colmenero, I. Pastoriza-Santos and L. M. Liz-Marzan, *Soft Matter* 7, 3607 (2011).

[4] D. Cangialosi, V. M. Boucher, A. Alegría and J. Colmenero, *Polymer* 53, 1362 (2012).

## **Dynamics on nanotubes of ferroelectric polymer: Confinement and stress effects**

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Charge transport and glassy dynamics: Thu 15:10, Lecture Hall

Polymer nanostructures organized in nanoarrays exhibit interesting properties that make them very good candidates for electronics, photovoltaics and memory application. However, a crucial step in the design of these systems towards a particular application is to understand the behavior of systems at the nanometer scale. In the case of polymer physics, the confinement of molecules to dimensions that are in the range of their molecular sizes implies severe changes of the physical behavior. In recent time, electrochemically fabricated porous materials have been used as confining systems with very well-defined geometry for polymer crystallization studies. High surface energy solids such as metal oxides are wettable by almost all low surface energy systems like polymer melts. When a polymer melt is deposited on top of a porous anodic aluminum oxide (AAO) template, the polymer wets the pores. Depending on several parameters nanorods or nanotubes inside the pores (nanorods or nanotubes) have been observed. PVDF is a semicrystalline polymer which can be infiltrated in AAO templates producing either nanotubes or nanorods depending on the pore size and on the conditions of the infiltration. We present how confinement affects the relaxational behaviour and the ferroelectric to paraelectric transition in nanorods of PVDF and PVDF based ferroelectric copolymers. Results pointing towards the possibility of a transition between normal ferroelectricity and relaxor ferroelectricity will be presented.

## **Interfacial polarization in dielectric spectra: theory and applications**

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Electrode and Maxwell-Wagner Polarization: Fri 09:30, Lecture Hall

The phenomenon of interfacial polarization leads to significant changes in the dielectric spectra of the materials under investigation. The corresponding spectral features

do not directly reflect molecular physical parameters but originate from spatial variations in the local permittivity function at the interface between two regions having different dielectric properties. This contribution aims to analyze in detail the dielectric signature of the interfacial polarization effects. Two distinct aspects will be considered: (a) the phenomenon of the electrode polarization, taking place at the interface between a conductive sample and the metal electrodes employed for the measurement; (b) internal interfacial polarization arising in multi-phase systems which exhibit a non-uniform distribution of the local permittivity. As a practical application of this phenomenon, it will be shown how interfacial polarization can be used to create polymeric systems with giant permittivities.

## **Impedance measurements and modelling of the persistent photoexcitation effect in poly(3-hexylthiophene)**

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BDS and other techniques I: Wed 15:00, Lecture Hall

Impedance spectroscopy measurements were performed to follow the relaxation behaviour of an optically-excited thick poly(3-hexylthiophene) (P3HT) film. The sandwich-type metal/P3HT/metal devices with Au electrodes showed a nearly perfect ohmic behaviour, in contrast to the samples with blocking Al electrodes. The impedance data were obtained in the dark or upon light exposure. The samples were illuminated by white light or monochromatic light emitting diodes under ambient conditions. Impedance measurements of the illuminated P3HT device showed a dramatic change of the impedance modulus. The dependence of the photoexcitation effect on wavelength of the exciting light coincides with absorption spectrum of P3HT film in the visible range. Under illumination, the sample responded quickly and came to the state in which the overall impedance is reduced compared to the dark state. After turning off the light the relaxation took several hours. Impedance-frequency data obtained during the relaxation could not be explained by a simple parallel resistance-capacitance circuit but it could be best fitted by incorporating a constant-phase element instead of a normal capacitance. Impedance modelling allowed us to simplify the slow relaxation behaviour to an exponential decay of the photoconductivity with an extended time constant. By observing the variation of the circuit parameters, it was found that the relaxation process is dominated by slow detrapping of photogenerated carriers.

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## **Impedance spectroscopy on electrochromic tungsten and nickel oxide films as a function of applied potential**

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Electrode and Maxwell-Wagner Polarization: Fri 09:50, Lecture Hall

Electrochemical impedance spectroscopy measurements of hydrated cathodic electrochromic tungsten oxide films and anodic electrochromic nickel vanadium oxide films were carried out in the frequency range 0.01 Hz to 100 kHz, using a three-electrode setup. The applied potential between the sample and the reference electrode was varied in a wide range where the optical transmittance switches from bleached to fully colored state. The impedance spectra were fitted by an equivalent circuit including anomalous diffusion effects. The dependence of the chemical capacitance as well as the effective diffusion coefficient of the inserted ions was obtained from the equivalent circuit analysis. The chemical capacitance is proportional to the number of ions and charge compensating electrons inserted per unit of potential change. We interpret its voltage dependence in terms of the electron density of states of the oxide films.

## **DC Conduction in Polymer Insulation: Applications of Dielectric Spectroscopy and Thermally Stimulated Current Techniques**

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Industry forum: Fri 11:15, Lecture Hall

Progress in electric DC transmission technology, the continuous replacement of outdated electric insulation materials, like oil impregnated paper or porcelain, by modern

polymer materials and the aggressive up-scaling to higher and higher voltages necessitates an enhanced understanding of the underlying electric conduction in polymer insulation. In contrast to AC, where the electric field distribution is controlled by the displacement current, for DC the field distribution is governed by the conduction current that is naturally very small and exhibits large sensitivities with respect to various parameters and thus large relative fluctuations. This leads to field distributions which are not robust and thus impedes optimized design of insulation systems.

An appropriate understanding of DC properties involves the identification of the carrier species, the polarization mechanisms, as well as their origin and dynamic behaviour at low frequencies. In this contribution we focus on the separation between polarization current and free carrier current, the latter being relevant for the final DC field distribution, whereas the former decays to zero. Out of a large number of possible experiments for investigating electrical behaviour, we restrict our discussion here to measurements of isothermal polarization/depolarization current (PDC), broadband dielectric spectroscopy (BDS), and thermally stimulated depolarization currents (TSDC). The material under study is a non-stabilized low density polyethylene (LDPE) film.

Typical examples of isothermal polarization/depolarization currents as a function of time for various temperatures and electric fields, as well as BDS investigations at several temperatures from very low frequencies will be discussed.

## **Dielectric characterisation of polyolefins for power cable applications: insulation and semiconductive materials**

C. Svanberg<sup>1</sup>, G. Stalmann<sup>2,3</sup>, T. Gkourmpis<sup>1</sup>, J. Andersson<sup>1</sup>, Villgot Englund<sup>1</sup>, Ulf Nilsson<sup>1</sup>, Aleksandar Matic<sup>2</sup> and Per Jacobsson<sup>2</sup>

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Industry forum: Fri 11:45, Lecture Hall

The insulating properties of polyolefins make them ideal for electric power cable applications, and are today used commercially up to very high voltages in both AC and DC. Exposing materials to extreme electrical stresses over wide temperature ranges impose very tough design requirements including the need for long-term reliability. Electrical characterisation is therefore essential for the cable industry and dielectric loss measurements have been used for decades to secure high level of the cable insulation quality. Here we show that broadband dielectric spectroscopy can provide valuable information on the electrical properties for example in the development phase of novel compositions. We present dielectric data on polyethylene-based materials, ranging from highly insulating to semiconductive, using special experimental protocols. The



links between the fundamental materials properties via the dielectric properties to the performance of commercial power cables are discussed.

## **Ionic conductivity in glass-forming systems and polymers**

A.P. Sokolov

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Charge transport and glassy dynamics: Thu 14:00, Lecture Hall

Ionic conductivity in a liquid is defined by ionic diffusion coefficient  $D$  and concentration of free ions  $N_f$ . According to classical theories,  $D$  depends on structural relaxation time of the liquid  $\tau$ ,  $D \sim 1/\tau$ . However, it is known that diffusion in glass-forming liquids is often decoupled from structural relaxation and the degree of decoupling usually correlates with the steepness of the temperature dependence of  $\tau$  (fragility). Thus similar decoupling might be observed between ionic conductivity and structural relaxation. In this talk we present an overview of ionic conductivity in various glass-forming liquids and polymers. Ionic liquids, such as CKN indeed show the expected decoupling between conductivity and structural relaxation. However, room temperature ionic liquids show rather weak decoupling. Possible reasons for the difference in the behavior are discussed. Next, we overview studies of ionic conductivity in polymers. We demonstrate that ionic conductivity can be strongly decoupled from structural (segmental) relaxation in polymers. The decoupling increases with increase in polymer fragility. This observation suggests a new approach to design of polymer electrolytes with high ionic conductivity.

## **Electrical Conductivity Relaxation Studies of Supercooled Protic Ionic Liquids**

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Conducting glasses and ionic liquids: Fri 14:30, Lecture Hall

Broadband dielectric spectroscopy was employed to study the conductivity relaxation process in supercooled protic ionic liquids as a function both of temperature and of pressure. Both temperature and pressure dependence of the conductivity relaxation

times exhibit anomalous behavior in vicinity of the glass transition temperature, manifested by abrupt changes in activation energy and activation volume, respectively. This anomalous behavior of the conductivity relaxation is due to huge decoupling between electrical conductivity and structural relaxation. In addition, we also examined changes in the conductivity relaxation process during physical aging. As a result we observed a narrowing of the relaxation dispersion that is a consequence of the heterogeneous dynamics of deeply supercooled materials.

- [1] Z. Wojnarowska, C. M. Roland, A. Swiety-Pospiech, K. Grzybowska, and M. Paluch, *Phys. Rev.Lett.* 108, 015701 (2012).

## Glassy dynamics and charge transport in Ionic Liquids

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Conducting glasses and ionic liquids: Fri 15:00, Lecture Hall

Broadband dielectric spectroscopy, pulsed field gradient nuclear magnetic resonance, calorimetry, rheology, and dynamic light scattering are combined to investigate glassy dynamics and charge transport in glass-forming ionic liquids over wide frequency, temperature and pressure ranges. Using a combination of Einstein, Einstein-Smoluchowski, and Langevin relations, the observed universal scaling of charge transport in ionic liquids is traced back to the dominant role of Brownian dynamics. A novel approach is applied to extract diffusion coefficients from BDS spectra in quantitative agreement with PFG NMR values but in a much broader range. It becomes possible to separately determine the effective number density and the mobility of the charge carriers as well as the type of their thermal activation from the measured dielectric spectra. It is shown that the observed Vogel-Fulcher-Tammann (VFT) dependence of the dc conductivity can be traced back to a similar temperature dependence of the mobility while for the number density an Arrhenius-type thermal activation is found. Details of the underlying mechanisms of ion transport in neat and polymerized ionic liquids will be discussed.

- [1] Sangoro, J.R. and Kremer, F. (2012). *Accounts of Chemical Research* 45 (4) 525-532; J. R. Sangoro, C. Iacob, A. Serghei, C. Friedrich, F. Kremer, *Phys. Chem. Chem. Phys.* 11, 913, (2009); Sangoro, J.R., Mierzwa, M., Iacob, C., Paluch, M., and Kremer, F. (2012). *RSC Advances* 2, 5047-5050.

- [2] J. R. Sangoro, A. Serghei, S. Naumov, P. Galvosas, J. Kärger, C. Wespe, F. Bordusa, and F. Kremer, *Phys. Rev. E* 77, 051202 (2008); J. R. Sangoro et al, *J. Chem. Phys.* 128, 214509 (2008); Sangoro, J. R., Iacob, C., Naumov, S., Hunger, J., Rexhausen, H., Valluilin, R., Strehmel, V., Buchner, R., Kärger, J., and Kremer, F. (2011). *Soft Matter* 7 (5), 1678-1681.
- [3] J.R. Sangoro, G. Turky, M. Abdel Rehim, S. Naumov, A. Ghoneim, J. Kärger, and F. Kremer, *Macromolecules*, 42(5) 1648-1651 (2009); C. Krause, J.R. Sangoro, C. Iacob and F. Kremer *J. Phys. Chem. B*, 114, 382-386 (2010).

## **Ion Transport across Grain Boundaries in Fast Lithium Ion Conducting Ceramics**

B. Roling<sup>1</sup>, M. Gellert<sup>1</sup>, F. Rosciano<sup>2</sup> and C. Yada<sup>3</sup>

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Conducting glasses and ionic liquids: Fri 15:30, Lecture Hall

Fast lithium ion conducting ceramics are promising solid electrolyte materials for all-solid-state lithium batteries and for lithium/air batteries [1]. In polycrystalline materials with NASICON, garnet or perovskite structure, the grains exhibit lithium ion conductivities up to  $10^{-3}$  S/cm. However, grain boundary resistances often limit the total conductivity of the materials. Up to now, quite little is known about the nature of the grain boundary resistances. By combining broadband electrochemical impedance spectroscopy with high-resolution TEM, we show that there are materials in which the grain boundary resistance is caused by purely geometrical current constriction due to small grain contact areas, while in other materials, the grain boundary transport is characterized by a higher activation energy than the grain transport [2,3]. In order to learn more about the nature of the activation barrier in the latter materials, we carried out nonlinear impedance measurements on the grain boundaries using high ac electric fields. Ac fields considerably exceeding the dc breakdown strength could be applied without deterioration of the samples. We compare our results to nonlinear current-voltage measurements on the grain boundaries of oxide ion conductors [4].

[1] R. Padbury, X. Zhang, *J. Power Sources* 196 (2011) 4436.

[2] C. R. Mariappan, C. Yada, F. Rosciano, B. Roling, *J. Power Sources* 196 (2011) 6456.

[3] C. R. Mariappan, M. Gellert, C. Yada, F. Rosciano, B. Roling, *Electrochem. Comm.* 14 (2012) 25.

[4] R. Meyer, X. Guo, R. Waser, *Electrochem. Solid-State Lett.* 8 (2005) E67.

## Signatures of glass transition for partially ordered phases

M. Reich, M. Schneider and W. Schmidbauer

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Industry forum: Fri 11:30, Lecture Hall

Increasing capacity and improving the safety of Lithium batteries are key challenges for battery application in electric vehicles. As a possible solution to the insufficient storage capacity of current batteries a Li-air battery has been proposed due to its potentially much higher energy storage density compared to other battery chemistries. With the aim of developing an innovative membrane for Li-air battery a joint industry and university project funded by BMBF has been initiated in 2011. The project members consist of battery research centre MEET (Münster) as well as partners from industry, namely Rockwood Lithium (previously Chemetall GmbH), VARTA Microbatteries, Volkswagen AG and SCHOTT AG.

As a technology based corporate group developing and manufacturing special glass and specialty materials SCHOTT AG is developing Li-ion conducting materials as an integral part of membranes for Li-air cells. Based on a fast Li-ion conducting glass-ceramic synthesized from the lithium-aluminum-germanium-phosphate system [1], a germanium free Li-ion conducting glass ceramic has been recently developed. The conductivity of the materials is characterised using impedance spectroscopy, which typically shows two contributions to sample resistance originating from grain-core and grain-boundary conduction respectively. It can be seen that the size of these contributions is influenced by the ceramization process which is mirrored in the microscopic morphology of the materials. Impedance spectroscopy not only plays an important role in determining the conductivity but also in characterising the chemical stability and interfacial resistivity, which will be briefly described.

[1] Kumar, B et.al., J. Electrochem. Soc. 156, 7 (2009), A506–A5013

## 2.3 Posters

### 1: Rotational and Translational Diffusion of Ionic Liquids Confined in Nanoporous Silica

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<sup>1</sup> *Institute of Experimental Physics I, University of Leipzig, Leipzig, Germany*

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Poster M: Mon 18:00, Chem

Charge transport and glassy dynamics of several classes of ionic liquids confined in uni-directional nanoporous silica membranes are investigated in a wide frequency and temperature range by a combination of Broadband Dielectric Spectroscopy (BDS), Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR) and Fourier Transform Infrared spectroscopy (FTIR). Two opposite effects are observed: (i) surface effects-resulting from strong interactions between the host system (nanoporous silica membrane) and the guest molecules (ILs) lead to slower dynamics-which are significantly reduced upon pore surface modification through silanization of the pores, and (ii) confinement effects-arising from spatial restriction of the molecules in nanometric length-scales-leading to enhancement of molecular dynamics. More than 10-fold systematic decrease in the effective diffusion coefficient (for HMIM<sup>+</sup>-based ionic liquids with  $\text{I}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$  anions) from the bulk value is observed in the silica nanopores. A model assuming a reduced mobility of the adsorbed layer at the pore wall/IL interface is shown to provide a quantitative explanation for the remarkable decrease of effective transport quantities (such as diffusion coefficient, dc conductivity and consequently, the dielectric loss) of the ILs in non-silanized porous silica membranes. For a second category of ILs including  $\text{BF}_4^-$  and  $\text{NTf}_2^-$ -based ionic liquids, it is experimentally demonstrated that the ionic mobility at lower temperatures is enhanced by more than two decades under nano-confinement in comparison to the bulk value. The effect becomes more pronounced with decreasing mean pore diameters. This is attributed to changes in ion packing under two-dimensional geometrical confinement, a view supported by recent atomistic simulations. In summary, the resultant macroscopic transport properties of glass-forming ionic liquids in confining space are determined by a subtle interplay between surface- and confinement-effects [11-3].

- [1] Iacob, C., Sangoro, J. R., Serghei, A., Korth, Y., Naumov, S., Friedrich, C., Kärger, J. and Kremer, F. (2008) *J. Chem. Phys.*, 129 (23) 234511.
- [2] Iacob, C., Sangoro, J. R., Papadopoulos, P., Schubert, T., Naumov, S., Valluillin, R., Kärger, J. and Kremer, F. (2010) *Phys. Chem. Chem. Phys.*, 12, 13798–13803.
- [3] Iacob, C., Sangoro, J. R., Kipnusu, W. K., Valluillin, R., Kärger, J. and Kremer, F. (2011) *Soft Matter*, 8, 289–293.

## **2: Structure property relationship of nanocomposites based on Polylactide and Layered Double Hydroxide**

P.J. Purohit and A. Schönhals

*BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany*

Poster M: Mon 18:00, Chem

Nanocomposites based on Polylactide (PLA) and organically modified MgAl Layered Double Hydroxide (MgAl-LDH) were prepared and investigated by a combination of differential scanning calorimetry (DSC), Small and Wide angle X-ray scattering (SAXS and WAXS) and Dielectric Relaxation Spectroscopy (DRS). DSC and WAXS show that the degree of crystallinity is influenced by the content of LDH. The dielectric response of the nanocomposites shows several relaxation processes. The intensity of the dynamic glass transition increases with the concentration of LDH. This is attributed to the increasing concentration of the exchanged anion sodium dodecylbenzene sulfonate (SDBS), which are adsorbed at the LDH layers. Two processes are identified at lower and higher temperatures both having a signature of the dynamic glass transition. The process at lower temperature originates from polymer segments close to the LDH whereas the one at higher temperature (bulk like) from the molecules at a farther distance from the LDH. Other than these two processes,  $\beta$  relaxation is identified which is related to localized fluctuations in the polymer chain.

## **3: Characteristics of frequency response functions for ion motions in inhomogeneous free space between crystallites in several polymers**

Y. Anada

*Department of Business and Information Systems, Hokkaido Information University, Ebetsu, Japan*

Poster M: Mon 18:00, Chem

In the melt-crystallized polymers, there are inhomogeneous free spaces in the non-crystalline parts between lamellae and in boundary regions between spherulites. These free spaces compose a hierarchical structure of inhomogeneous ion path. As a matter of fact, plural kinds of motion of impurity ions observed in the frequency dispersion of electric modulus for the low density polyethylene crystallized from melt[1]. Furthermore, similar result was also observed for the polyvinyl chloride-polybutadiene blends[2] although it has a different kind of inhomogeneity. In order to investigate

the ion motion in the inhomogeneous microstructure in detail, the permittivity, conductivity and electric modulus were obtained as a function of frequency at various temperatures by means of BDS for isotactic poly(propylene)(iPP), poly(ethylene terephthalate)(PET), poly(chlorotrifluoroethylene)(PCTFE) and plasticized poly(vinyl chloride) with dioctyl phthalate (p-PVC) . The p-PVC with non-crystalline structure shows only dc conduction with single conductivity relaxation time. However, for the iPP, an ion motion was found beside the dc conduction. This motion is caused by the inhomogeneous structure in non-crystalline parts between crystallites. On the other hands, as to the PET and the PCTFE, only dc conduction with a single conductivity relaxation time was observed although these polymers have the non-crystalline parts between lamellae.

[1] Y. Anada, *Macromol. Symp.* 2006, 245, 245-246.

[2] Y. Anada *J. Polym. Sci. Part B Polym. Phys.* 2002, 40, 226.

#### 4: Gradual Redehydration of a Dehydrated CaFe-Layered Double Hydroxide under Controlled Humidity Studied by Broadband Dielectric Relaxation Spectroscopy

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<sup>2</sup> *Department of Inorganic and Analytical Chemistry, University of Szeged, Dóm tér 7, Szeged, H-6720 Hungary*

<sup>3</sup> *Department of Organic Chemistry, University of Szeged, Dóm tér 8, Szeged, H-6720 Hungary*

Poster M: Mon 18:00, Chem

It is known that layered double hydroxides (LDHs) lose their layered structure on heating. However, the heat-treated LDHs regain their original structure in an environment saturated with water vapour. This is the so-called memory effect. While the steps of the dehydration are known, those of the rehydration are not. Information may be gathered about this process applying a technique sensitive to subtle structural changes, such as broadband dielectric relaxation spectroscopy (DRS). During rehydration water molecules entering into various positions help to reconstitute the original structure, easily followed by DRS. The LDH was prepared with co-precipitation and was characterised with various methods (X-ray diffractometry, scanning electron microscopy, FT-IR spectroscopy, etc.) Heat treatment was followed by thermogravimetry and was found that the layered structure collapsed above 750 K. For studying the rehydration procedure dehydrated samples were placed in environments with 12 preset vapour contents in the 6-97% relative humidity range. The equilibrated samples were fast

frozen with liquid N<sub>2</sub> and the DRS spectra were registered in the 5 mHz-10 MHz regime between 100 K and room temperature allowing the warm-up of the sample. Processes occurring during rehydration were identified and from the DRS spectra and the activation energies were determined at the preset humidity. The mechanism of the water uptake and the forms of bound water were deduced.

## **5: Dielectric Spectroscopy of Hydrogen Bonded Thermotropic Liquid Crystalline Polymer with Six Methylene Units in the Side Chain**

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Poster M: Mon 18:00, Chem

The aim of the present study is the investigation of the relaxation processes and successive mesophase transitions of poly(4-vinyl pyridine) based hydrogen bonded SCPLC (PLC6). Dielectric measurements are performed in the 133-423 K temperature range and the 10 mHz-10 MHz frequency range by the BDS technique. In addition, DSC and polarization microscopy are used. At low temperatures, local gamma and beta processes have been observed. In the vicinity of the glass transition temperature  $T_g$ , the deviation from linear dependence of relaxation times in the Arrhenius plot and Johari-Goldstein behavior are detected. The alpha- process is well fitted by the VFT relation and the glass transition temperature is found as 238 K which was confirmed by DSC measurements. In contrast to covalent bonded systems, in H-bonded PLC6 the temperature dependence of delta-relaxation times is described by Arrhenius formula and not converging with alpha-process in the vicinity of glass transition. The smectic A-nematic phase transition, in the region of 12 K, the coexisting of relaxation modes of both mesophases have been observed in the delta-process. At the smectic A-nematic phase transition, the deviation from VFT trace is observed for alpha-relaxation times. Moreover, a drastic increase of DC conductivity occurs in the nematic phase. It means that the nematic order of interdigitated layer structure is accompanied by partially melt of polymeric backbone prior to isotropic phase transition.



## 6: Comparative Analysis of the Dielectric Relaxational Behaviour of Poly(methacrylates) Containing a Phenyl group in the Side Chain

B. Redondo-Foj<sup>1</sup>, M. Carsí<sup>1</sup>, P. Ortiz-Serna<sup>1</sup>, M.J. Sanchis<sup>1</sup>,  
R. Díaz-Calleja<sup>1</sup>, E. Riande<sup>2</sup>, L. Gargallo<sup>3</sup> and D. Radic<sup>3</sup>

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<sup>2</sup> *Instituto de Ciencia y Tecnología de Polímeros (CSIC), Spain*

<sup>3</sup> *Departamento de Química Física, Pontificia Universidad Católica de Chile*

Poster M: Mon 18:00, Chem

In order to gain a better understanding on the influence of the chemical structure on relaxation dynamics, developed in the glassy state and in the neighborhood of the glass rubber transition, we have carried out a comparative analysis of the dielectric activity obtained for five structurally related poly(methacrylates) by means of Broadband Dielectric Spectroscopy (BDS) and Differential Scanning Calorimetry (DSC). BDS studies were performed in a frequency range of  $10^{-1}$  Hz to  $10^8$  Hz at temperatures ranging from 133 to 423K and the DSC measurements were performed between 203K and 418K.

By DSC measurements, significant differences were found in the glass transition temperature depending on the position of the aromatic ring in the side chain. Even when the aromatic group is located in the side chain end, the spectrum shows two glass transition temperatures, a phenomenon also observed in some poly-methacrylates and poly-itaconates with long side chains. Moreover, the BDS spectra exhibit several relaxations according to the chemical structure of the polymers and strong conductive processes are shown at low frequencies and high temperatures.

In order to characterize the relaxation processes present for the structural isomers analyzed, different empirical model have been used. Correlations between different parameters and the chemical structure have been carried out.

## 7: Broadband Dielectric Spectroscopy to study the molecular dynamics in nanometer thin layers of poly (styrene-block-isoprene-1.4) diblock copolymer

M.M. Elmahdy<sup>1,2</sup>, M. Treß<sup>2</sup>, M. Fuchs<sup>2</sup>, E.U. Mapesa<sup>2</sup> and F. Kremer<sup>2</sup>

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Poster M: Mon 18:00, Chem

Broadband dielectric spectroscopy (BDS) using nano-structured electrode arrangement is employed to investigate the molecular dynamics in nanometer thin layers ( $> 5$  nm) of poly(styrene-block-isoprene-1.4) (PS-b-PI) diblock copolymers with different PI volume fraction ( $f_{PI}$ ) and identical molecular weight of the PS blocks. Three relaxation processes are observed, which can be assigned to the two segmental modes of the styrene and isoprene blocks and a relaxation process related to the normal mode of the PI chain. The dynamic glass transition related to the segmental mode of the styrene and isoprene blocks is independent of the layer thickness, while the normal mode of the PI chains is changed similarly as observed in thin homopolymer layers [1-3]. The ordered state morphology, studied by AFM, revealed the formation of PI cylinders ( $f_{PI}=0.81$ ) and a lamellar structure ( $0.29 < f_{PI} < 0.53$ ) in good agreement with the literature [4].

[1] E.U. Mapesa et al. in preparation.

[2] M. Tress et al. *Macromolecules* 43, 9937 (2010).

[3] E.U. Mapesa et al. *EPJ-ST* 189, 173 (2010).

[4] A. K. Khandpur et al. *Macromolecules* 28, 8796 (1995).

## 8: Measurement system for dielectric spectroscopy of DNA up to 110 GHz

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Poster M: Mon 18:00, Chem

Recent technical advances in the generation and detection of coherent radiation in the upper GHz and lower THz range have opened novel opportunities for the application of these fields, especially in medicine and biosensing. Still, there are only few data on the properties of biomolecules like proteins or DNA in this frequency

range. Knowledge of the interaction mechanisms between electromagnetic radiation and DNA molecules surrounded by different kinds of ions can be exploited for medical diagnostics, for the improvement of biosensors presented nowadays on the market as well as for the development of novel sensors. In the present study we have measured the dielectric dispersion for different kinds of aqueous DNA solutions, among them 2.4 kbp plasmid DNA and 47 kbp Lambda DNA. The optical absorbance ratio  $A_{260}/A_{280}=1.84$  indicated a good purity of the samples from proteins. Complex permittivity measurements were carried out by means of a computer controlled vector network analyzer over the wide frequency range from 70 kHz to 110 GHz. We used an open-ended 1.19 mm diameter precision 50 Ohm semirigid coaxial line immersed in the sample, and the input reflection coefficient was measured at the tip of the coaxial probe. We were able to reduce the sample volume down to 10  $\mu\text{l}$ . All measurements were performed at temperature of 25 °C. Results of well defined DNA prepared by molecular biology methods are compared to samples of eukaryotic DNA.

## 9: Dielectric Characterisation of Polymer Structures with an Inclusion of a Metal Center

V.T. Avanesyan and E.G. Vodkailo

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Poster M: Mon 18:00, Chem

Since recently, new methods are intensively developed for obtaining polymers in which highly dispersed metal particles are formed directly in the monomer structure [1]. This kind of materials includes high molecular systems synthesized by electrochemical oxidation polymerization of transition metal complexes with Schiff bases, in particular, poly-[CumSalpn-1,3] [2], which possess such properties as electro- and photoactivity. One of the informative methods determining the relationship between the molecular structure of a polymer and its macroscopic properties is the dielectric spectroscopy. The dielectric losses taking place in high-molecular compounds may have different character depending on the size and eigen frequency of oscillatory motion of kinetic fragments of macrochains [3]. In this work, we present the results of studying the polarization characteristics of thin-film metal-dielectric structures on the basis of a copper Cu(II) complex formed on a conducting substrate outside electrolytic medium. Using a E7-20 broadband imittance measurer, frequency dependences of the capacitance  $C$  and the dielectric loss tangent ( $\delta$ ) were measured in the ranges of frequencies  $f = 102\text{--}106$  Hz and temperatures  $T = 293\text{--}340$  K. The results of dielectric measurements in the frequency and temperature ranges indicate the development of active relaxation processes in thin-film poly-[CumSalpn-1,3] structures. The obtained

dispersion regularities are satisfactorily approximated by the Cole-Cole relationship and reflect the Debye nature of relaxation, caused by inhomogeneity and reorganization of the structure of the metal-polymer under study. The frequency dependence of the electric conductivity  $\sigma$  of the thin-film poly-[Cu(mSalpn-1,3)] under study can be described by relationship  $\sigma \sim f^s$ , where the exponent of the reduced function for the results of measurements under normal conditions was within  $s = 0.58\text{--}0.63$ . The experimental temperature dependence of conductivity  $\sigma$  consist of two regions, which correspond to certain values of the activation energy. In the frequency interval studied, these energies fall within 0.12–0.24 and 0.84–0.98 eV for the low- and high-temperature regions, respectively. An analysis of the obtained experimental data showed that the conductivity of the samples exhibits features that are characteristic of the hopping mechanism of charge transfer, which is accompanied by the exchange of carriers related to the presence of metal centers distributed in the polymer structure. Acknowledgements: This work was supported by Ministry of Education and Science of the Russian Federation under Grant 6/12-GZF.

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## 10: Electrical Conduction and Dielectric Properties in Piezoelectric Fibre Composites

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Poster M: Mon 18:00, Chem

A series of 1-3 connectivity PZT fibres/epoxy resin composites with different volume fraction is studied by means of dielectric spectroscopy in the wide frequency range 0.1 Hz-100 kHz and temperature varying from the ambient to 210 °C. The conduction phenomenon is analyzed using the "universal power law" and its scaling is studied by the Jonscher's universal power law. At low frequencies ac conductivity tends to be constant, while in the high frequency region verifies the exponential law of conductivity. In the intermediate frequencies, the examined systems exhibit strong dispersion with frequency and the produced fitting curves deviate from the experimental data by not being able to describe the recorded relaxation and pointing out that in the vicinity of the relaxation peaks the power law is not applicable. Finally, dipolar relaxation

mechanisms and interfacial or Maxwell-Wagner-Sillars relaxation were revealed in the frequency range and temperature interval of the measurements.

## **11: Dielectrophoretic response of DNA determined by impedance measurements**

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Poster M: Mon 18:00, Chem

Using microelectrodes for dielectric spectroscopy allows the investigation of small sample volumes down to a few microlitres. We have combined this with the dielectrophoretic attraction and concentration of DNA in aqueous solutions near the electrodes. Monitoring impedance changes allows to study the dielectrophoretic response of macromolecules and nanoparticles without labeling or optical access. Above that the local enrichment of molecules close to the electrodes by dielectrophoresis helps to increase sensitivity of impedance based biosensors. Experimental results on various DNA samples are presented.

## **12: Giant permittivity and low dielectric loss in new three phases: BaTiO<sub>3</sub>-carbon nanotube / polyvinylidene fluoride composite**

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Poster M: Mon 18:00, Chem

A three-phase composite with multi-walled carbon nanotubes (MWNTs) and barium titanate BaTiO<sub>3</sub> particles embedded into polyvinylidene fluoride (PVDF) was prepared by using a simple blending and hot molding technique. The dielectric measurement results show that the effective dielectric constant of the composite is slightly dependence on the frequency below 0.1 MHz but increases rapidly with the MWNTs concentration when the concentration is very close to the percolation threshold. It is thus possible to reach a high dielectric constant equal to 7000. These films may lead to a large energy capacity storage.

### **13: Studies of dielectric relaxation of nanocomposites materials of natural rubber reinforced by natural nanofibres**

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Poster M: Mon 18:00, Chem

Cellulose whiskers and Microfibrillated cellulose (MFC) was extracted from the rachis of date palm tree and characterized. The cellulosic nanoparticle was used as reinforcing phase to prepare nanocomposite films using latex of natural rubber as matrix. These films were obtained by the casting/evaporation method. The properties of the ensuing nanocomposite films were investigated using differential scanning calorimetry, and dynamic dielectric analysis by means of broadband dielectric spectroscopy. The dielectric properties of the composites showed a strong dependence on nanofiller content, testing frequency and temperature. The presence of nanocellulosic fibres in the composite gives rise to other relaxation associated to MWS interfacial polarization. The MWS relaxation arises from the trapping of electric charges at the interfaces between the nanofibres and the matrix. The reinforcing effect was shown to be higher for nanocomposites with MFC compared to whiskers.

### **14: Modified Polymer Dynamics in PDMS Nanocomposites: Dielectric and Thermal Studies**

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Poster M: Mon 18:00, Chem

Molecular dynamics, phase transitions and interfacial relaxation phenomena in various poly(dimethylsiloxane) (PDMS) nanocomposites were studied using the following experimental techniques: Differential Scanning Calorimetry (DSC), Thermally Stimulated Depolarization Currents (TSDC) and Dielectric Relaxation Spectroscopy (DRS) in the temperature range -170 to 40 °C. Samples consisted of linear PDMS chemically sorbed mainly onto the surfaces and pores of: fumed silicas (A380 /13-32nm / 342 m<sup>2</sup>/g and OX50 / 4-5 nm / 58 m<sup>2</sup>/g) and mesoporous silica gel (Si60, 0.3-0.5 nm, 384 m<sup>2</sup>/g) [1]. The inorganic phase was also modified by the addition of small zirconia nanoparticles (ZrO<sub>2</sub>, 3-8 nm) [1]. Polymer/filler content varied between 100/0 (wt%) to 40/60 (wt%). The strong polymer-filler interactions were found

to affect significantly the mobility of PDMS, suppressing crystallization and changing the development of glass transition. Dielectric measurements (TSDC, DRS) showed four contributions to the segmental dynamics associated with the glass transition arising, in the order of decreasing mobility, from the confined polymer chains in the pores of silica gel ( $\alpha_p$  relaxation), from the bulk (unaffected) polymer fraction ( $\alpha$ ), from polymer chains restricted between condensed PDMS crystals ( $\alpha_c$ )[2] and from the polymer in an interfacial layer with strongly reduced mobility due to interactions on the nanoparticle surface ( $\alpha'$ )[2].

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## 15: Phase transitions and dynamics in semifluorinated side-chain poly(methacrylate) random copolymers studied by dielectric spectroscopy and other techniques

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Poster M: Mon 18:00, Chem

Semifluorinated side chain polymers show a specific microphase separation between polymer backbone and semifluorinated side chains, forming an ordered layered structure. In the present work the phase transitions and dynamics in poly(methyl methacrylate)/semifluorinated side-chain methacrylate (PMMA/PsfMA) random copolymers are studied. Random copolymers with different molar amounts of PsfMA ranging from 11 to 68% and PMMA homopolymer were prepared. Phase transitions in copolymers were studied by temperature dependent small angle X-ray diffraction (T-SAXS), differential scanning calorimetry (DSC) and dielectric relaxation spectroscopy (DRS) techniques. DRS technique in a broad frequency and temperature range was used for the study of molecular dynamics. A highly ordered structure with stable side chain packing was observed for the copolymers with molar content of PsfMA, higher than 30%. Copolymer with 11mol% PsfMA is characterized by a single glass transition, while for the copolymers with higher PsfMA molar contents (31-68%) except from glass transition temperature, melting and isotropization temperatures were recorded. Alpha relaxation related to the glass transition and beta relaxation

of PMMA, were recorded in all copolymers. In addition, copolymers exhibit a relaxation not observed in PMMA which is assigned to local motions of semifluorinated side chains. When microphase separation occurs an additional relaxation emerges.

## 16: Study of the dynamic heterogeneity in poly(ethylene-ran-vinyl acetate) co-polymer using nano-Dielectric Spectroscopy (nDS)

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Poster M: Mon 18:00, Chem

Dielectric relaxation is a useful technique for studying the dynamic behaviour of polymers[1]. In particular, characterization of the relaxation processes at nanoscale is of great interest as it will give a deeper insight into the complex mechanisms involved in the processes. One of the most useful approaches typically used for studying the dielectric relaxation of polymer is broadband dielectric spectroscopy (BDS)[2]. This technique is well established and allows measuring the dielectric relaxation process of polymers over a wide range of frequency and temperature. However, BDS measurements have limitations in the analysis of dynamically heterogeneous samples in the sense that this analysis is model dependent[2]. To overcome this constrain we have studied the dynamic heterogeneity in random co-polymers using a recently developed experimental approach (nDS) that allows measuring dielectric relaxation process of thin polymer films with nanoscale spatial resolution by means of electrostatic force microscopy (EFM)[3-5]. This experimental method enables dielectric contrast mapping of the polymer together with its topography and mechanical phase. Regions of the sample at which relaxation dynamics are studied were determined from dielectric contrast imaging. In this work we study the dynamic heterogeneity in thin films of ethylene-vinyl acetate (EVA) random copolymer. We measured the dielectric spectra in vinyl acetate rich amorphous regions and ethylene dominated semi-crystalline regions separately, and compared then with the one obtained from standard BDS measurements.

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## 17: Cole-Cole spectra broadening as the signature of dipole-matrix interaction in aqueous solutions

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Poster M: Mon 18:00, Chem

Whenever the water molecules interact with either dipolar or charged systems, a bulk water dielectric relaxation peak broadening takes place. If a solute has the dipole nature, the new clusters (compared with the bulk) are created due to the dipole-dipole interactions. It leads to the "red shift" of the dielectric loss maximum frequency. In the case of ionic solutions another cluster structure developed due to dipole-charge interactions and the "blue shift" is observed. In the general case when a solute molecule has both charged and dipole groups, the dielectric loss maximum demonstrate "red" or "blue" shifts depending on the entity concentration. In both cases the water and solute interactions can be considered as dipole-matrix interaction in which water is the dipole subsystem. The 3D trajectories phenomenological approach [1] was applied to the results of isothermal dielectric measurements of non-ionic (D-glucose and D-fructose) and ionic (NaCl and KCl) aqueous solutions [2,3]. In case of hydrocarbons the, number of hydrated water molecules is decreased with the concentration of sugars, in ionic solutions, this number is reached some limited value. The similar approach was applied to the aqueous solution of ATP and AMP. The dynamic/structural behavior indicates the solute concentration regions where dipole-dipole or dipole-charge interactions are dominated.

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## 18: Dielectric characterization of gold nanoparticles / antiferroelectric liquid crystal composites

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Poster M: Mon 18:00, Chem

By its very nature, nanotechnology is of immense academic and industrial interest as it involves the creation and exploitation of materials with structural features in between those of atoms and bulk materials, with at least one dimension limited to between 1 and 100 nm. Most importantly, the properties of materials with nanometric dimensions are, in most instances, significantly different from those of atoms or bulk materials. An important subset of nano-structured materials is represented by the so-called nano-composites which consist of nano-particles dispersed in a continuous three-dimensional matrix. In this context the nano-composites obtained by dispersing metallic nano-particles in liquid crystal materials are of particular interest. Liquid crystals by their very nature are suitable candidates for matrix-guided synthesis and self-assembly of nanoscale materials [1]. Since liquid crystals are anisotropic materials they provide an excellent support for self assembling of nano-particles into larger ordered superstructures. Moreover, as the liquid crystals responds to small external forces (electric, magnetic, mechanical stress), dispersed nano-particles can be forced to follow the molecular order of the hosting medium effectively controlling the order of the superstructure. Interesting results has been obtained by dispersing ferroelectric nano-particles [2] in nematic liquid crystals (NLCs). Low concentration of such nano-particles increase the orientational order of the hosting NLCs, the nematic-isotropic transition temperature and decrease the Frederiks transition threshold voltage. We present our recent investigations on the electric properties of W-129, an orthoconic smectic liquid crystal mixture, and on the same liquid crystal mixture doped with gold nanoparticles. W-129 presents both ferroelectric and antiferroelectric smectic C phases and an high spontaneous polarization ( $> 300 \text{ nC/cm}^2$  at room temperature) in virtue of its tilted chiral structure. The gold nanoparticles are functionalised with a polymer which presents both hydrophilic and hydrophobic properties in dependence of temperature. In the present study, dielectric relaxation of W-129 and W-129 doped with gold nanoparticles has been studied in a planar aligned cell as a function of the frequency of an applied electric field and as a function of temperature through Dielectric Spectroscopy technique. For this purpose the Havriliak-Negami function [3] has been used to determine the distribution parameters, the dielectric strengths and the relaxation frequencies as a function of temperature. In addition to that, we present a first attempt to study the morphological and ferroelectric properties of a thin layer

of W-129 and W-129 doped with gold nanoparticles deposited on ITO using Atomic Force Microscopy techniques. The differences found in the dielectric spectra are evidence of the influence of gold nanoparticles. They represent an interesting result from the theoretical and experimental point of view. These results are relevant for fundamental nano-science because they show how nano-sized particles can be coupled with the orientational order of macroscopic systems. Of course potential applications are envisioned in the field of soft nanotechnology and optical materials.

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## 19: Impedance Spectroscopy as a Tool for Monitoring the Drying Behavior of Bulk Heterojunction Solutions for Polymeric Photovoltaic Devices

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Poster M: Mon 18:00, Chem

The drying behavior of bulk heterojunction [BHJ] solutions for polymeric photovoltaic devices is studied via impedance spectroscopy. Solutions of poly(3-hexylthiophene) [P3HT] and phenyl-C61-butyric acid methyl ester [PCBM] in chlorobenzene were prepared. Small amounts of octanedithiol (ODT) or chloronaphthalene (CN) were added to alter the resultant BHJ film morphology and drying time. The solutions were blade-coated onto interdigitated electrodes, and the impedance was monitored during solvent evaporation. As P3HT and PCBM solidify into a film, the alternating electric field causes an interfacial charge layer to develop on any formed precipitates, which is observed in the measured impedance. Impedance spectroscopy is able to accurately measure the drying time, as well as the onset of precipitate formation, and therefore holds the potential for on-line monitoring and process optimization during commercial manufacturing of large-scale printable solar cells.

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## 20: Dielectric Properties of Biocompatible and Biodegradable Polycaprolone and Polylactide and Their Nanocomposites in the Millimeter Wave Band

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Poster M: Mon 18:00, Chem

Polycaprolone (PCL) and polylactide (PLA) are widely used in biomedicine for coating wounds and in prosthetics, including tooth implantation [1,2]. The main advantage of these materials is their biological compatibility and slow biodegradation, releasing water and carbon dioxide; this makes these polymers an ideal ecologically pure packing material. There are literature data on the dielectric properties of PCL and PLA at frequencies from  $10^{-1}$  to  $10^6$  Hz, as well as data for PLA in the frequency interval 0.5 – 10 GHz. However, there are no data on the dielectric properties of PCL and PLA in the millimeter (MM) wave band. These data are important, in particular, in view of the growing application of MM waves in medicine. We measured the dielectric properties of crosslinked poly-caprolone (cPCL) and PLA, as well as of their composites with carbon nanotubes, in the range of frequencies from 85 to 100 GHz and in the temperature interval from 20°C to 90°C.

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## 21: Some considerations on Local Dielectric Spectroscopy

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Poster M: Mon 18:00, Chem

In the last years, a new AFM based dielectric spectroscopy approach was developed for measuring the dielectric response at the nanoscale, nano Dielectric Spectroscopy (nDS). In spite of the effort done so far, some experimental aspects of this technique remain unknown. In this work we address the study of two important aspects of the nDS, namely: the experimental frequency range and the dielectric signal intensity. Currently, the frequency range of this technique goes from 1Hz to 30kHz, approximately. We study the possibility of extending this range on both sides: on the one hand by increasing the measurement time and thereby reaching lower frequencies; and on the other hand by using frequencies above the limit imposed by the resonance frequency of the cantilever. In addition, intensity of the dielectric signal was studied by analyzing the amplitude of oscillation of the cantilever with different scan heights and distances to the lower electrode. All the proposed experimental methods are based on the detection of both, the topography and the electric force or force gradient between the tip and the sample surface. Thus, by means of a standard AFM setup, we are able to measure the electrical phase and amplitude over more than five decades in frequency as well as the dielectric contrast image at a given frequency and temperature.

## 22: Dynamics in sII structured clathrate hydrates

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Poster M: Mon 18:00, Chem

Clathrate hydrates are crystals consisting of water molecules forming cage like structures and guest molecules incorporated therein. Here we focus on cubic structure sII clathrate hydrates, where only the larger of the two cage species is filled with guest molecules. The host molecules, H<sub>2</sub>O, as well as the currently studied ring-type guest molecules exhibit permanent electrical dipole moments. Hence, dielectric spectroscopy is a powerful tool to investigate both host and guest dynamics in clathrate hydrates.

The water molecules constituting the hydrate lattice show reorientation rates that are similar to those of ice Ih [1]. A slight speed up of dynamics is observed [2] due to point defects created on the lattice through guest-host interactions. Even more interesting is to study the motion of guest molecules positioned inside the clathrate cages. Here we investigate and compare the ring molecules cyclopentane, tetrahydrofuran [3], dioxolane, tetrahydropyran and dioxane. Through a change of molecular diameter and electrical dipole moment the guest-host interaction can be modified and the effects on guest and host dynamics can be observed [4,5]. Below 40 K the reorientation of the guest dipoles slows down such that a dielectric freezing process can be detected. We compare these results with deuterium NMR measurements. Together with spin-lattice relaxation, spin-spin relaxation, and stimulated-echo experiments we are able to track guest dynamics over more than 10 decades in time.

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## **23: Water and protein dynamics in hydrated elastin over wide ranges of composition**

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Poster M: Mon 18:00, Chem

In this work we present a study of water and protein dynamics in case of hydrated elastin, over wide ranges of composition, from swollen compressed pellets 50 wt% in water, to practically dry protein pellets. The dielectric techniques employed are Broadband Dielectric Spectroscopy (DRS) and Thermally Stimulated Depolarization Currents (TSDC). In addition, Differential Scanning Calorimetry (DSC) and Water Equilibrium Sorption-Desorption Isotherms (ESI) techniques are performed. By ESI measurements a maximum value for water uptake of  $h=0.31$  (grams of water per grams of dry elastin, corresponding to 24 wt%) is found. DSC measurements show no crystallization effects of water for water compositions up to 24 wt%. On the contrary, crystallization and melting of water occurs in case of swollen samples. The glass transition of the system, is studied only by DSC. The glass transition temperature ( $T_g$ ) of the dry Elastin is located at 464 K in agreement with literature data [1] and a reduction of the  $T_g$  with increasing water composition is observed. DRS and TSDC

studies focus on water dynamics in the system, and follow three dielectric relaxations. The two faster relaxations at low temperatures correspond to the motion of small protein polar groups of the protein surface, triggered by hydration water, and/or hydration water molecules themselves [2,3,4]. The origin of the slower relaxation at higher temperatures [3] is not clear. The dielectric loss data are analyzed by model functions.

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## 24: Dielectric properties and hydration of DNA complexes with biologically active compounds

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Poster M: Mon 18:00, Chem

Hydration is one of the most important factors that affect ligand binding to DNA. Since interaction of DNA and ligand takes place in water environment the investigation of changes in hydration shell of nucleic acid can give information about mechanisms of the complex formation and the role water plays in its stabilization. We carried out such investigation using dielectric method that bases on the direct measurement of the difference of attenuation and phase shift coefficients between water and aqueous solutions of compounds under investigation. The study was done using an original high-sensitivity EHF differential dielectrometer at 39.5 GHz. We studied hydration of 4 biologically active substances (proflavine (PF), ethidium bromide (EB), propidium iodide (PI), chlorophyllin (CHLN)) and their complexes with DNA. The changes of dielectric parameters under the process of complex formation were registered. We found that hydration changes accompany complex formation for all ligands except EB. The difference in the number of bound water molecules between the complex and its components ( $N_w$ ) calculated taking into account the ratio of DNA-phosphate and drug concentrations was different for each ligand. The values found for  $N_w$  per one nucleotide were the following: PF, +3; PI, +2; CHLN, -6. For EB binding to DNA a value of  $N_w +0.5$  was found, indicating that interaction of EB with DNA induces only a slight hydration increase. The possible causes of the effects observed are discussed.

## 25: Effect of slight crosslinking on the dielectric and mechanical relaxation behavior of poly (2-ethoxyethyl methacrylate) chains

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Poster M: Mon 18:00, Chem

The thermal, dielectric and mechanical characterization of poly 2-ethoxyethyl methacrylate without (PEOEMA) and with (CEOEMA) crosslinking agent are reported. The relaxation spectra exhibit in the glassy state two relaxations called in increasing order of temperature  $\gamma$  and  $\beta$  processes followed by a prominent glass-rubber transition or  $\alpha$  relaxation. By decreasing the chains mobility by slightly crosslinking the polymer chains (using 1% (mol) of 2-ethoxyethyl dimethacrylate as crosslinking agent), the  $\beta$  relaxation disappears and the peak maximum of the glass-rubber relaxation is shifted from 10K to higher temperatures. The dielectric spectra, at high temperatures and low frequencies is dominated by electrode-polymer interfacial processes. The activation energy of the  $\gamma$  relaxation for the crosslinked and uncrosslinked polymers is ca. 30 kJ mol<sup>-1</sup>, about 10 kJ mol<sup>-1</sup> below than that of the  $\beta$ -relaxation. The X-rays pattern of the crosslinked polymer presents two peaks at  $q = 5.6 \text{ nm}^{-1}$  and  $12.76 \text{ nm}^{-1}$  resembling the X-ray patterns of poly(n-alkyl methacrylate)s. The peaks in poly(n-alkyl methacrylate)s were attributed to the formation of nanodomains integrated by side chains flanked by the backbone. However, whereas this heterogeneity produces an  $\alpha_{PE}$  peak in poly(n-alkyl methacrylate)s with  $n \geq 2$ , this microheterogeneity gives rise to a Maxwell-Wagner-Sillars (MWS) relaxation in the crosslinked polymer located at lower frequencies than the glass rubber relaxation.

## 26: Dynamics and cold crystallization of poly(pentamethylene terephthalate) as revealed by dielectric spectroscopy

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Poster M: Mon 18:00, Chem

The structure-dynamics relationship in poly(pentamethylene terephthalate)(PPT) has



been investigated by means of X-ray scattering and dielectric loss spectroscopy experiments. The  $\beta$  relaxation qualitatively follows the same trend of other polyesters based on terephthalic acid, like poly(trimethylene terephthalate) and poly(buthylene terephthalate), being a bimodal process. This is somehow expected, due to the local character of the  $\beta$  relaxation. We propose that the high frequency secondary relaxation  $\beta_1$  is associated to the most flexible part of the repeat unit, whereas the low frequency mode  $\beta_2$  has been assigned to the carbon-oxygen link of the ester groups. Regarding the  $\alpha$  process, as temperature goes up a lower frequency process appears ( $\alpha'$ ) that increases at expenses of  $\alpha$ .  $\Delta\epsilon_\alpha$  tends to zero and the lower frequency process becomes the characteristic  $\alpha$  relaxation of the crystallized material. Moreover, the evolution of the  $\beta$  and  $\alpha$  relaxations during isothermal crystallization has been studied in a single dielectric experiment, by opportunely varying the temperature. The  $\beta$  relaxation provides information on the crystalline structural development while the  $\alpha$  relaxation allows us to obtain a deeper knowledge about the evolution of the amorphous phase dynamics.

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## 27: Changes in the dielectric properties of medaka fish embryos during development studied by electrorotation

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Poster M: Mon 18:00, Chem

Medaka, *Oryzias latipes*, a small fish native of Southeast Asia has become a favorite model organism in developmental biology. This study explores the applicability of electrorotation (ROT) to analyze the dielectric properties of medaka embryos. Depending on the external conductivity, the ROT spectra of embryos at stages 10 and 20 (according to Iwamatsu nomenclature [1]) exhibited 2 or 3 anti- and co-field peaks, caused by the multilayered structure of fish eggs. A double or triple Lorentzian function matched very well the ROT spectra, thus yielding accurate values for the characteristic frequencies ( $f_{c1,2,3}$ ) and magnitudes of ROT peaks. The LF anti-field ROT peak centered at  $f_{c1}=5$  kHz resulted from the charging of the yolk membrane. The intermediate ( $f_{c2}$ ) and HF co-field peaks ( $f_{c3}$ ) were due to the polarizations of the chorion and yolk core, respectively. The chorion peak appeared only at the lowest conductivity ( $\sim 1$  mS/m). As the embryo progressed from stage 10 to stage

20, the major co-field peak ( $f_{c3}$ , yolk core) shifted to higher frequency from  $\sim 45$  to  $\sim 65$  MHz, and its magnitude decreased by  $\sim 30\%$ . At the same time, the yolk membrane ( $f_{c1}$ ) remained nearly unchanged. Upon development to stages 32–35, the amplitude of the yolk core peak further decreased, the chorion peak increased, and the anti-field peak shifted even below 1 kHz. Our data show that ROT technique is a useful non-invasive tool for studying the dielectric properties of live embryos during development.

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## 28: Preparation of Plastic Electrodes Based on Conductive Hybrid Polymers

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Poster M: Mon 18:00, Chem

Conductive polymers have both advantages of polymers (light weight, flexibility, low cost, and processability) and metal (high electrical conductivity). Polyaniline is a conducting polymer characterized with higher thermal stability and lower monomer cost compared to the other CP with tunable properties and easy synthesis. And hence has a numerous applications in various fields especially in supercapacitors and solar cells. But it is difficult to be processed due to infusibility, insolubility in the most common organic solvents. Also, it has bad mechanical properties due to both of intra- and inter-chain rigidity. So, a number of attempts were made to improve its solubility and flexibility by formation of composites. Dielectric relaxation spectroscopy provides vital information about the molecular dynamic, so enable us a detailed study of the conductivity and conductivity mechanisms. In this work we prepared some polyaniline and its composites with different polymers including; polystyrene, sulfonated polystyrene and polymethyl methacrylate, with different ratios and preparation methods including; copolymerization, in situ polymerization, and melt blending. the prepared samples were characterized using different techniques including; UV-Visible, FTIR, XRD, SEM, TGA and DSC. Also, some preliminary dielectric and electrical measurements were considered.

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## 29: Dielectric Relaxation of Water in Natural Layer Aluminosilicates

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The aluminosilicate minerals are an excellent group of natural adsorbents of different liquids and gasses. The water-clay interaction is of primary importance because of the intensive use in fields of pharmaceuticals, ecology, hydrogeology, agricultural chemistry, etc.. Thus, obtaining an accurate knowledge on main features of water adsorption in clays is an actual goal of the research. Two types of natural layered aluminosilicates-montmorillonite with the exchangeable K(I), Co(II), Ni(II), and Cu(II) cations and kaolinite with the exchangeable Na(I), Mg(II), and Cu(II) cations - were examined by means of Dielectric spectroscopy over wide temperature (-115°C to +300°C) and frequency (1Hz-1MHz) ranges. In all the samples studied the complex non-Debye dielectric behavior were observed. Obtained dielectric spectra can be described in terms of four distributed relaxation processes separated by different frequency and temperature ranges. The low temperature relaxation process was observed only in montmorillonites being subdivided into two processes each related to its specific hydration center. The cooperative behavior of water at the interface was observed in the intermediate temperature region together with a proton percolation process. The study demonstrates a deep understanding on water dynamics in the vicinity of different hydration centers of natural clay minerals.

## 30: Doping of ionic liquids into poly(vinylidene fluoride): How does it influence dielectric properties?

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Poster M: Mon 18:00, Chem

A small amount of ionic liquids doped in poly(vinylidene fluoride) (PVDF) induces ferroelectric properties in films without the need of stretching [1]. In this work, PVDF is

doped with different content of 1-ethyl-3-methylimidazolium nitrate ([EMIM][NO<sub>3</sub>]) which varies from 0.01 to 10 wt.%. It is found that nearly pure  $\beta$ -phase films are spin-coated from solutions containing [EMIM][NO<sub>3</sub>] of above 1 wt.%. Films with [EMIM][NO<sub>3</sub>] contents below 1 wt.% show both  $\alpha$  and  $\beta$  phases as evidenced by infrared (IR) spectroscopy and by scanning electron microscopy (SEM). Comparing with pure PVDF, the doped PVDF samples show a significant charge-carrier polarization. The corresponding loss-peak shifts to lower frequencies with increasing content of [EMIM][NO<sub>3</sub>]. It may arise from charge accumulation on the electrodes and on boundaries between crystalline and amorphous regions. The  $\alpha$  relaxation, associated with the glass transition in the dielectric spectra, tends to disappear for samples doped by more than 1 wt.% [EMIM][NO<sub>3</sub>]. The reason is still not understood. Dynamic mechanical analysis (DMA) and differential scanning calorimetry (DSC) measurements are now undertaken in order to clarify this unexpected behavior.

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### 31: Unusual dynamics of hydrogen-bonded heteroditopic molecules

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Poster M: Mon 18:00, Chem

The dielectric relaxation and rheological properties of self-complementary heteroditopic molecules have been investigated. Decoupling of dielectric structural relaxation from viscosity has been found in the vicinity of glass transition and the temperature dependence of viscosity appears to be stronger than that of dielectric structural relaxation. This unusual dynamic decoupling phenomenon is ascribed to the formation of hydrogen bonding.

### 32: Dielectric Study of Miscible Polymer Blend Thin Films

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Poster M: Mon 18:00, Chem

Molecular dynamics of Polystyrene (PS), Poly(vinyl methyl ether)(PVME) and their blend (PS/PVME) confined in thin film geometry have been studied by mean of

broadband dielectric spectroscopy (BDS). No thickness dependence of PS segmental dynamics was observed down to 14 nm. For pure PVME, three relaxation processes (Alpha, Beta and Gamma) were observed. The Arrhenius plots of the Beta and Gamma processes have activation energy of 38.3 kJ/mol and 20.5 kJ/mol, respectively. The relaxation rate of the Alpha process is well described by the Vogel-Fulcher-Tamman (VFT) equation. Thin films of PS/PVME polymer blend in the weight ratio of 25/75 have been investigated for different thicknesses. The broadening of the Alpha relaxation peak for the polymer blend was observed, the intensity of which increases with the temperatures. The glassy dynamics of the polymer blend thin films are independent of the layer thickness under study.

### 33: Dielectric phenomena vs. structural organization of the electroactive hybrid polymers containing ionic liquids

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The development, investigation and implementation of electrolyte systems of different nature, notably organic liquid electrolytes, ionic liquids, polymer electrolytes and inorganic solid electrolytes, are of interest. In brief the electrolyte systems can be conditionally divided as follows: - polymer + organic liquid (polymer gel); - polymer + ionic liquid; - polymer + inorganic solid electrolyte + ionic liquids; - polymer electrolyte + ionic liquid; - polymer electrolyte + ionic liquid + liquid organic electrolyte; - ionic liquids + liquid organic electrolyte; - polymer electrolyte + inorganic solid electrolyte. The blends consisting of two and more electrolytes are used and studied for obtaining EaPM with combined merits of selected electrolytes. The present work shows (by WAXS, FTIR, TOM and POM studies) that the doping of the hybrid organic-inorganic polymer systems (HOIS) based on urethane oligomers (UO) and metal silicate (MS) by the molecules of ionic liquids (IL) based on morpholine leads

to destruction of the mineral phase with the simultaneous formation of new crystalline structures due to MS/IL reactions. Contrariwise, synthesis of EaPM based on UO and IL results in amorphous grain-oriented structural organization and formation of the ion conducting cluster with the DC conductivity level  $\sigma_{DC} \sim 10^{-3}$ - $10^{-4}$  S/cm, AC conductivity level  $\sigma_{AC} \sim 10^{-2}$ - $10^{-3}$  S/cm and permittivity  $\epsilon \sim 10^5$ - $10^6$  (by the results of BDS, Im and cyclic VA spectroscopy).

## 34: Nonlinear dielectric response at the excess wing of glass-forming liquids

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 Poster M: Mon 18:00, Chem

We present dielectric relaxation spectra of two structural glass formers, measured with high excitation fields. They show nonlinear contributions at the high frequency flank of their  $\alpha$ -relaxation-peaks that vanish in the excess wing region. In earlier works [1,2], nonlinear dielectric spectroscopy was performed on glass forming glycerol and propylene carbonate (PC). A strong increase of the dielectric loss was found at the high-frequency flank of the  $\alpha$  peak while  $\Delta\epsilon$  was nearly zero at low frequencies. These results were fully consistent with a model assuming dynamical heterogeneities with closely correlated dielectric and thermal relaxation times. In the present work, we provide data on the high-field behavior of glycerol and PC in a frequency and temperature range extending well into the region of the excess wing. There, even at excitation fields as high as 671 kV/cm no field dependence of the dielectric loss exists. Possible implications for the microscopic origin of the excess wing and  $\beta$ -relaxation are discussed.

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### 35: Spin transition investigation in [Fe (H-trz) 2 (trz)] (BF<sub>4</sub>) complex using Broadband Dielectric Spectroscopy and Thermally Stimulated Polarization Currents

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Poster M: Mon 18:00, Chem

The high spin (HS)-low spin (LS) transition in spin crossover (SCO) complexes of iron (II) ions can be triggered by various external stimuli such as temperature, light, pressure or magnetic field [1]. The spin state change is accompanied by change of the dielectric properties as permittivity providing scope for applications as sensors or molecular memories [2,3]. Charge transport measurements (dc and ac conductivities) and spin state dependence of the conductivity were carried out on powder and thin film samples of [Fe(H-trz)2(trz)](BF<sub>4</sub>) complex using thermally stimulated polarization currents and broadband dielectric spectroscopy. A large thermal hysteresis (25 K) of the dc conductivity of the SCO powder is observed and assigned to the spin transition. These results are in good agreement with magnetic susceptibility measurements and optical reflectivity [4]. The conductivity is founded to be higher in the (LS) state than in the (HS) state. The frequency dependence of the ac conductivity exhibits a power law behavior while the loss electrical modulus M'' dispersion reveals two dielectric relaxations in the frequency range between 10<sup>-2</sup> and 10<sup>6</sup> Hz. The presence of these two relaxations in the entire investigated temperature range shows that residual HS or LS domains exist in the SCO powder. In thin film (100 nm thickness), TSCP data corresponds to the conduction through small aggregates of 2-3 nanoparticles and a thermal hysteresis of the dc conductivity is also detected.

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### 36: Segmental dynamics in silica nano-particles SBR rubber compounds by using broadband dielectric spectroscopy

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For silica nano-particles SBR rubber compounds, five different relaxation processes are observed by broadband dielectric spectroscopy (BDS). The dominant mechanisms at high temperatures or low frequencies are the segmental (or alpha) relaxation process and the interfacial MWS polarization process. Moreover, three additional relaxation processes, related to the presence of silica particles, are observed in the low temperature range. The main purpose of this work is to investigate the effect of the silica nano-particles on the dynamics of SBR rubber networks through the study of the alpha relaxation using BDS. For the silica filled SBR, the MWS polarization overlaps with the alpha relaxation making difficult the corresponding analysis. By drying the samples the MWS process shifts to lower frequencies and the alpha relaxation process can be studied for heterogeneous systems where the MWS process is close to the segmental relaxation. Besides the MWS polarization process, the dielectric relaxations associated with the presence of the silica nano-particles, are also affected by the drying process. We will also show in this work how the water content affects the dielectric properties of the silica filled rubber compounds.

### 37: Electrode Polarization effects in broadband dielectric spectroscopy

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Poster M: Mon 18:00, Chem

Electrode polarization (EP) leading to blocking electrodes (BEs) is a frequently encountered phenomenon when investigating ion conducting materials with dielectric



spectroscopy [1,2,3]. Due to the ions that accumulate at the electrodes, where they form a space-charge region, the dielectric constant rises to giant values and the conductivity drops drastically towards low frequencies. If EP cannot be avoided experimentally it has to be modeled mathematically to separate its contributions from the bulk properties of the sample. This is commonly done by describing the BEs using a simple equivalent circuit or a constant-phase-element [4,5]. However, in our experience both approaches have certain drawbacks when analyzing broadband dielectric spectra, where contributions from EP are observed over several frequency decades. Instead we propose the use of a parallel RC-circuit-element with a distribution of characteristic times, which accounts for the often fairly broadened spectral features arising from EP. Excellent fits of the frequency spectra of a variety of different samples such as salt solutions, ionic liquids and melts, biological materials and electronic semiconductors could be achieved [6]. Moreover the data reveals the presence of a second dispersion region due to EP at very low frequencies which seems to be a common phenomenon in ionic conductors and could be an indicator for an additional very slow charge-transport process in the space-charge region.

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### 38: A simple and economic way to measure low-temperature quasi-isothermal dielectric spectra

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Poster M: Mon 18:00, Chem

In dielectric spectroscopy measuring the temperature dependence of the dielectric response of the materials is of great importance. For the investigation of the most of the materials very low temperatures need to be reached. In addition measurements

under isothermal conditions are highly recommended. Although this task is easily executable with dedicated cryosystems, purchasing these state-of-the-art cooling systems is difficult for groups on a lower budget. Moreover, using such cryosystems for parallel pilot measurements is rather prodigal on resources even for well-funded laboratories. Here we present an easy and economic way to carry out dielectric spectroscopic measurements from low temperatures on under quasi-isothermal conditions. The basis of the technique is Newton's law of heating; a sample holder with reduced heat transfer to the environment heats up at such a low rate which allows measurements to be made from e.g. 170 K to room temperature in the 30 mHz-10 MHz range with an initial temperature error of  $\sim\pm 0.5$  K (decreases towards higher temperatures). We discuss the limitations and errors of our method and present some typical example dielectric measurements on materials of very different kinds: low-molecular-weight glass-forming liquid/water mixtures, carbohydrate aqueous solutions, polymeric materials, ionic liquids. The evaluation of the obtained spectra is compared to those measured with dedicated cooling devices.

### **39: Role of H-bonding on the Structure and the Dynamics of Concentrated Polymeric Solutions**

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Poster M: Mon 18:00, Chem

Water plays a fundamental role in biological processes. The deep understanding of such processes requires clarifying the structure and dynamics of water in a biological environment and how it interacts with the surrounding medium. Aqueous polymer solutions can be considered as suitable simple model systems to approach these questions since polymers are much less complex than biological systems. In recent works we have investigated the component dynamics in concentrated aqueous solutions of polymeric macromolecules (poly(vinyl methyl ether) (PVME), poly(dimethyl amino ethyl methacrylate) (PDMAEMA) and polyamide (PA)) [1]. We have found a similar peculiar phenomenology of the dynamics, including extreme stretching and deviations from Gaussian behavior that can be attributed to the existence of diverse environments in the samples. In the case of the polymer we also find that the formation of H-bonds with water plays a crucial role. An important arising question is whether the underlying structural heterogeneities, invoked to explain the results, are a consequence of the H-bond formation. We performed dielectric spectroscopy experiments on dry PDMAEMA and concentrated solutions of PDMAEMA with tetrahydrofuran

(THF), which do not form H-bonds. The percentage in weight was  $w_{\text{THF}} = 30\%$ . Dry polymer data reveal two different dynamics, at low and high temperature respectively. The high-T one has been analyzed by using an HN function and shows a VFT dependence on temperature suggesting an alpha-like relaxation nature, while it has been used a CC function to describe the low-T relaxation and it has been found to have an Arrhenius temperature dependence (beta-relaxation). Adding THF, it's not possible to observe the high temperature relaxation, while the low-T region is characterized by the presence of two components having an Arrhenius temperature dependence. It is possible to associate the fast one to the beta relaxation of the polymer, while the slow one is related to the presence of the solvent and shows an energy activation, 0.47 meV, similar to that of hydration water. No VFT-Arrhenius crossover has been found in both relaxations.

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## 40: From bulk to attograms of matters: applications of Broadband Dielectric Spectroscopy in polymer nanoscience

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Poster M: Mon 18:00, Chem

Investigations on attograms of material (1 attogram= $10^{-18}$  grams) open the door for fundamental questions in soft-matter physics, such as for instance "What is the minimum amount of matter necessary to "define" the material properties?" and-in the same time-offer new routes to be explored for enhancing the performance of macromolecular materials. The present contribution aims to demonstrate the strength of Broadband Dielectric Spectroscopy in measuring extremely small amounts of material. It will be shown that dielectric measurements on attograms of matter are possible by using a novel experimental concept which employs nano-containers as measurement cells.

## 41: The Scaling Laws of Electrode Polarization

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Poster M: Mon 18:00, Chem

A quantitative description is suggested for electrode polarization, an ubiquitous phenomenon which takes place at the interface between metallic and ionic conductors and results in an increase by many orders of magnitude in the net dielectric response of the sample cell. Based on the fact that, due to coulombic interactions, the mobility of charge carriers is drastically reduced at the metal/ionic conductor interface, the approach quantitatively reproduces the observed scaling laws and enables one to determine-by means of a novel formula-the DC conductivity of the material under study.

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## 42: The Dynamic Properties of Water Confined in Chrysotile Asbestos

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Poster M: Mon 18:00, Chem

Water is one of the most interesting objects due to many special peculiarities and abnormal properties and some of them are not well understood up-to-now. The crystalline forms of water have been studied for a long time and many efforts are concentrated on study of glassy structure of water. Water forms a non-crystalline structure under certain conditions for example water confined in ultra small pores. This glassy state should be characterized by specific peculiarities at low temperature. In this contribution the dynamic properties of water confined in chrysotile asbestos fibers have been studied by dielectric spectroscopy. The fibers possess sets of macroscopically long, parallel channels with a characteristic diameter of about 5 nm. The complex dielectric permittivity has been measured using a Novocontrol BDS80 at frequencies  $10^{-1}$ - $10^7$  Hz and in the temperature range from 150 to 300 K. Multiple relaxation processes in asbestos with low and high concentrations of water were observed and

analyzed. Neutron and X-rays studies have shown that there is no peaks corresponding to an ice structure in these samples with small water concentration. Moreover the data of quasielastic neutron scattering have clearly shown an abrupt increase in the elastic scattering due to the freezing of water in the asbestos nanochannels at 237 K [1]. From analysis of dielectric response the relaxation process demonstrating the anomaly in the temperature dependence of characteristic relaxation time in vicinity of 240 K was found. This contribution is supported by RFBR grants 10-02-00576, 11-03-00747 and 12-02-00230.

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### **43: Dielectric Properties of Hybrid Unsaturated Polyester-based Composite Reinforced with Alfa and Wool Fibres**

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Poster M: Mon 18:00, Chem

Alfa fibres were hybridised with wool fibres in order to better cohesion between non-woven natural fibres. The reinforcing effect of these fibres in unsaturated polyester resin was characterized by dielectric measurements in the frequency range 0.1 Hz- 1 MHz and temperature interval from ambient to 150°C. This study revealed the presence of two dielectric relaxations in the matrix. These relaxations were attributed to the  $\alpha$  mode relaxation and the conductivity effect occurred for high temperature above glass transition temperature and low frequencies. The incorporation of the fibres in the matrix showed the presence of two additional relaxations associated with the interfacial polarization and the orientation polarization imputed to the presence of polar water molecules in fibres. Furthermore, the influence of natural fibres on the thermal and dielectric properties of this composite was demonstrated by means of several characterization techniques such as Fourier Transform Infrared Spectroscopy (FTIR), Differential Scanning Calorimetry (DSC) and Scanning Electron Microscopy (SEM).

## 44: Self-assembly and Dynamics of Discotic Liquid Crystals of Nanographenes

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Poster M: Mon 18:00, Chem

Discotic liquid crystals (DLC), consisting of rigid disk-shaped aromatic cores and disordered alkyl substituents tend to organize into columnar supramolecular structures with applications as molecular wires. Their self-assembly is driven by noncovalent intermolecular interactions favoring the  $\pi$ -stacking of aromatic cores and the unfavorable interactions between the cores and the alkyl chains leading to nanophase separation [1]. The role of aliphatic chains is also important as they provide with the required solubility and further impart a rich thermotropic behavior and fast molecular dynamics[1]. X-ray scattering revealed two main columnar structures in HBCs: a liquid crystalline phase (Col<sub>h</sub>) at higher temperatures composed of columns that are further organized in a hexagonal lattice and a crystalline phase (C<sub>r</sub>) at lower temperatures composed of columns of tilted disks (i.e. "herringbone") in a monoclinic unit cell. The kinetics of phase transformation was investigated by Infrared Spectroscopy and Related Techniques [2] over an extraordinary broad time-window (1-105 s). Identical kinetics were found suggesting that both the core and the alkyl chains simultaneously drive the system from the under cooled Col<sub>h</sub> to C<sub>r</sub> phase. Non-linear phenomena on the phase transformation were also studied. Applications of DLC as nanoscale conductive devices (i.e. molecular wires) rely on the optimal stacking of the aromatic cores that allow for charge carrier mobility along the columnar axis. Herein we report on the effect of molecular structure on the thermodynamics[4,5,8], self-assembly [6,7], the hierarchy of dynamics[3,4], the kinetics of structure formation [6,7] and the viscoelastic properties of a class of DLC, the hexa-peri-hexabenzocorenes.

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## 45: Molecular order and dynamics of Tris (2-ethylhexyl) phosphate confined in uni-directional nanopores

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Poster M: Mon 18:00, Chem

Infrared Transition Moment Orientational Analysis (IR-TMOA) and Broadband Dielectric Spectroscopy (BDS) are combined to study molecular order and dynamics of the glass forming liquid Tris(2-ethylhexyl)phosphate (TEHP) confined in unidirectional nanopores with diameters of 4, 8, and 10.4 nm. The former method enables one to determine the molecular order parameter of specific IR transition moments. It is observed that the central P=O moiety has a weak orientational effect (order parameter) due the nanoporous confinement, in contrast to the terminal C-H groups. BDS traces the dynamic glass transition of the guest molecules in a broad spectral range and at widely varying temperature. An enhancement of the mobility takes place when approaching the glass transition temperatures and becomes more pronounced with decreasing pore diameter. This is attributed to a slight reduction of the density of the confined liquid caused by the 2-dimensional geometrical constraint.

## 46: Dielectric and Viscoelastic Behavior of Polymerized Ionic Liquids with Various Counterions

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Poster M: Mon 18:00, Chem

The macro and micro dynamics of poly(1-butyl-3-vinylimidazolium)-based polymerized ionic liquids with various counterions X-(PC4VIX) were investigated using rheological and dielectric relaxation techniques to extract the role of counterions in the bulk polyelectrolyte system. All PC4VIX species showed two dielectric relaxation modes, the faster mode and the slower mode. The fast mode could be attributed to the rotational motion of the polymer side chain and the slow mode to the lifetime of the

ion-pairs. The time-temperature superposition principle was found to be valid for all the PC4VIX species, and the segmental dynamics of polymer chains in bulk PC4VIX depends only on the glass transition temperature  $T_g$ . The relaxation time of the dielectric slow mode is shorter than the rheological relaxation time of the Kuhn monomer for all the PC4VIX species at a given temperature. This finding strongly suggests that the slow dielectric relaxation mode is due to the ion-pair motion. The temperature dependence of the slower relaxation time agrees well with that of the direct current conductivity, which is described by the Arrhenius type temperature dependence below  $T_g$ . This indicates that the ion transport mechanism is due to the repetitive ion-pair formation and dissociation processes below  $T_g$ . Above  $T_g$ , this value deviates from the Arrhenius line, which implies the presence of the VFT-component. Hence, around  $T_g$  there are two contributions.

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## 47: Investigation of Dielectric and Mechanical Properties of Polypropylene/Montmorillonite Nanocomposites

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Poster M: Mon 18:00, Chem

Polypropylene/organomodified montmorillonite (PP/OMMT) nanocomposites were investigated by broadband dielectric spectroscopy in order to analyze the filler effect on the molecular mobility of the polymer chains. The frequency and temperature dependences of the imaginary part of the relative permittivity  $\epsilon''$  of the composites on the OMMT contents have shown the presence of two relaxation processes, whereas for pure PP the relaxation transitions are not revealed. The relaxation peak around 10 °C has been corresponded to the glass-rubber transition ( $\beta$ -relaxation) of the amorphous phase of the polymer. The second peak around (80-100) °C has been attributed to the molecular dynamics of the amorphous phase which confined between the crystalline lamella or on the lamella surface ( $\alpha$ -relaxation). The  $\beta$ -relaxation was better described by a VTF equation. The VFT parameters obtained for the  $\beta$ -relaxation have shown that presence of OMMT does not influence on glass transition of PP matrix. The calculated value of the  $T_g$  coincides with the value, obtained by the dynamic mechanical analysis method. The  $\alpha$ -relaxation was better described by the Arrhenius equation. From the obtained data it was concluded that OMMT has influence on the relaxation process in crystalline phase of PP matrix, videlicet the value of activation energy is growth with increasing of filler content. The results



obtained via dielectric spectroscopy method had a good correlation with the results obtained by the DMA method.

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## 48: Dielectric spectroscopy of medaka fish embryos using electroration

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Poster M: Mon 18:00, Chem

In the last years, *oryzias latipes* (medaka) has become a favorite vertebrate model organism for basic biological research and aquaculture. In the aquafarming, management of the development and viability fish embryos is important to control their hatchability. The detailed knowledge of the dielectric properties of fish eggs might be useful for monitoring the conditions of fish embryos. In the present study we explore the dielectric structure of early-stage medaka embryos by means of the single-cell electroration (ROT). The ROT spectra of live medaka embryos exhibited up to three well-resolved peaks in the kHz-MHz frequency range, resulting obviously from the multilayered structure of fish eggs. Using the approach developed by Jones [1], we elaborated a three-shell dielectric model (TSM) that describes very well the complex ROT response of medaka embryos over wide ranges of field frequency and external conductivity. The TSM also yielded accurate numerical values for the dielectric properties of the four major structural units of medaka embryos. In sharp contrast, dead/undeveloped eggs exhibited only one ROT peak, shifted markedly to lower frequencies. In conclusion, the ROT technique has proved a powerful non-invasive tool for studying the dielectric properties of live fish embryos, which may be useful for discrimination of their development stage, for analyzing changes in embryos' viability, as well as for toxicological and environmental studies.

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## **49: Dielectric investigation of charge accumulation and depletion at the interface between a ferroelectric polymer and an organic semiconductor**

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Poster M: Mon 18:00, Chem

Thin-film metal-insulator-semiconductor capacitor and field-effect transistor (FET) structures based on the ferroelectric polymer poly(vinylidene fluoride-trifluoroethylene) (P(VDF-TrFE)) as insulator and poly(3-hexylthiophene) (P3HT) as organic semiconductor were prepared and investigated by use of dielectric spectroscopy, capacitance-voltage (C-V) and nonlinear current-voltage (I-V) measurements. Essentially, the influence of the ferroelectric polarization on charge accumulation and depletion at the insulator-semiconductor interface is studied. From the dielectric spectrum, it can be deduced that the insulator-semiconductor interface does not remain in a stable depletion state, i.e., charge starts to accumulate already before the ferroelectric polarization switches. With C-V measurements as well as FET output and transfer characteristics, it is shown that this lack of stable depletion behavior is caused by a permanent trapping of negative charges at the insulator-semiconductor interface, not by a decay of the insulator's ferroelectric state. These charges partially neutralize the effect of the ferroelectric polarization that would otherwise maintain the interface in depletion until it becomes reversed by application of the respective coercive field [1], [2]. These findings lead to a deeper understanding of charge trapping and polarization phenomena in polymer-based ferroelectric FET structures that are promising candidates for all-organic non-volatile memory devices.

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## 50: Towards homogeneous dynamics in incompatible blends by selective transesterification

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Poster W: Wed 18:30, Chem

The evolution from two component dynamics towards homogeneous dynamics in originally incompatible blends of biodegradable aliphatic polyesters has been followed by dielectric spectroscopy. Transesterification reactions are the responsible for the compatibilization process. However, our results indicate that the segmental dynamics is strongly modified even before any transesterification process is detected by <sup>13</sup>C-NMR. This modification in the dynamics can be explained by incipient reactions at the interphase between the homopolymer rich regions, which further evolves to the interior of those phases by the formation of block copolymer of gradually decreasing block length. This process produces finally a random copolymer that forms a single phase with a single segmental relaxation.

## 51: Intra- and inter-molecular dynamics probing the molecular signature of the dynamic glass transition in polymers

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Poster W: Wed 18:30, Chem

The intra- and intermolecular interactions of glass forming polymeric model systems (polystyrene, PS; polyvinyl acetate, PVAc and polymethyl-metacrylate, PMMA) are studied by Fourier-Transform Infrared (FTIR) and Broadband Dielectric Spectroscopy (BDS). By analysing the temperature dependencies of the spectral position and the oscillator strength of specific IR absorption bands, it is demonstrated that each

molecular moiety in the polymer has its own characteristics in the course of the dynamic glass transition. Particularly, for PS and PVAc discontinuities in the temperature dependencies are observed well below the calorimetric glass transition temperature  $T_g$  for vibrations of the aromatic rings and the carbonyl group, respectively; whereas for the main-chain vibrations a pronounced kink is found only at  $T_g$ . In contrast, the carbonyl and C-O stretching bands of PMMA exhibit distinct changes at  $T_g$ , with no additional features for lower temperatures. These findings enable one to unravel the detailed molecular interactions in the evolution of the liquid to glass transition beyond coarse-grained models.

## **52: Interface dielectric response in silica filled rubber compounds using standard- and nano-dielectric spectroscopy**

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Poster W: Wed 18:30, Chem

For nano-particles filled polymers an additional dielectric process is usually observed in the loss dielectric spectra at frequencies lower than the segmental relaxation. This process has generated some controversy in the literature due to the different (sometimes contradictory) interpretations given to explain its physical origin. Some authors understand this process as a second segmental relaxation due to the reduced mobility of the polymer close to the filler surface. However, other authors argue that the segmental dynamics of the polymer matrix is not affected by the presence of nano-particles. We present in this work a systematic study by means of two different dielectric spectroscopy techniques. On the one hand, we use standard broadband dielectric spectroscopy in combination with thermal analysis, to understand the physical origin of the low frequency process. By using this approach we will demonstrate that this process is compatible with a MWS polarization process, enhanced by the presence of water molecules at the silica surface. On the other hand, we use an AFM based approach to locally measure the dielectric behaviour of the interacting polymer layer,

i.e. the thin layer of polymer around the filler particles. This approach enables us to study the relaxation dynamics of interacting polymer layer with a spatial resolution better than 20 nm. The measurements were performed in bulk-like rubber (matrix) and over the filler particles, probing bulk dynamics of reinforced rubber and local dynamics of interacting rubber layer, respectively. In addition, we compared the relaxation spectra obtained at these points with previously measured spectra for unfilled rubber, obtained using the same approach. Dielectric relaxation spectra obtained for the interacting rubber for different temperatures overlap with those obtained for the matrix (bulk behaviour), which indicates that the segmental mobility of these layers is not restricted compared to their bulk counterparts.

### 53: Biophysical properties of starch blended with poly vinyl alcohol for drug delivery purposes

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Poster W: Wed 18:30, Chem

Starch (St) was blended with polyvinyl alcohol (PVA) with various compositions and the permittivity  $\epsilon'$  and the dielectric loss  $\epsilon''$  were measured in the frequency range 0.1 Hz up to 5 MHz and at temperatures ranging from 30 °C up to 90 °C. The effect of the temperature on the dielectric behavior of the investigated systems is also studied. The data for the loss electric modulus  $M''$  were calculated and the analyses revealed three relaxation processes which are related to the rotation of the main chain and its related motions. The possibility of using St/PVA blend systems as coating agents for oral colonic delivery of protein drugs was studied. The mechanical properties of the polymeric film coatings with different blend ratios were studied to estimate the risk of the accidental crack formation which will be developed during storage, and especially when exposed to aqueous media. The utility of using St/PVA coatings for oral colonic delivery of protein drugs was studied by conducting the drug release studies in the physiological fluids of the gastrointestinal tract (GIT). The investigation of the effect of various formulations (e.g., polymer blend ratio and coating level) on drug release is also included. It is taken in to consideration the effect of adding enzymes of the GIT fluids to check the possible enzymes influence on the release profiles.

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## **54: Low-cost planar interferometric microchannels for dielectric measurements in the GHz range**

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Poster W: Wed 18:30, Chem

High-sensitivity dielectric measurements have many applications for sensing, diagnostics, and industrial process monitoring. While broadband measurements have definite advantages over single frequency measurements, especially in a research setting, a less costly single frequency interrogation method can be sufficient to monitor a process or chemical change. We report the design and fabrication of a microstrip waveguide-based interferometer centered at 10 GHz using traditional printed circuit board manufacturing techniques. The interferometer consists of a splitter, two identical transmission lines, one for reference transmission and a second for introduction of test materials, a phase shifter, combiner, and microwave connectors. Microchannels are milled into the multilayer printed circuit board substrate through which fluids and gases can be pumped [1]. The microchannel board and waveguide board are bonded in an oven using standard pre-impregnated composite binding material. The device transmission coefficient is measured using a network analyzer and compared with numerical computations predicting the broadband impedance characteristics of the design. Performance of the device for measurement of common gases and liquids passing through the interferometer are reported.

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## 55: Effect of Imidazolium Ionic Liquid Type on the Properties of Nitrile Rubber Composites

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Poster W: Wed 18:30, Chem

The purpose of this work was to investigate the impact of hydrophobic and hydrophilic imidazolium ionic liquids characterized by high ionic conductivity on morphological, thermal, mechanical and ionic conductivity properties of nitrile rubber composites. Room temperature ionic liquids RTILs: EMIM TFSI and EMIM SCN were used. Magnesium-aluminium layered double hydroxide MgAl-LDH was added in XNBR whereas fumed silica Aerosil 380 was used for NBR as reinforcing fillers. NBR rubber compounds were vulcanized using a conventional sulfur based crosslinking system whereas XNBR compounds were cured with layered double hydroxide MgAl-LDH. The nitrile rubber composites contained various loadings of EMIM TFSI and EMIM SCN and were characterized by differential scanning calorimetry DSC, dynamic mechanical analysis DMA, AC measurements and scanning electron microscopy SEM. Thermal analysis showed that EMIM TFSI and EMIM SCN effected on increase in conductivity of nitrile rubber composites from  $10^{-11}$  S/cm to  $10^{-8}$  S/cm and  $10^{-9}$  S/cm respectively. The presence of ILs in the NBR compounds slightly affected the  $T_g$  whereas the presence of EMIM TFSI in XNBR contributed to shifting  $T_g$  toward lower temperatures from  $-23$  °C to  $-31$  °C at 15 phr loading, what can be attributed to a plasticizing behaviour of EMIM TFSI in XNBR system. A slight improvement in tensile strength from 18 MPa to 23 MPa was observed for NBR composites containing 5 phr EMIM TFSI.

## 56: Microwave dielectric spectra and concentration transition in acetonitrile-water mixtures

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Poster W: Wed 18:30, Chem

Complicated spectra of AN-water mixtures are determined by the solvation and the

initial compound association. There may be follow types of relaxation processes: 1) the molecular motions are averaged in the framework of the one Debye relaxation function; 2) the elementary interactions are reflected in the own individual relaxation parts of Debye's type; 3) there are a cooperative molecular motion in bulk water and solvation shell (or in different solvation shells) for different subsystems with separate Debye processes. Last case was considered for mol. fraction AN  $0 < X < 1$ . The variants are considered using standard and new fitting procedure for different subdivisions of microwave spectra (using own and literature experimental data). If  $X(\text{AN}) > 0.8$  the one main relaxation is observed. It describes the cooperative motion of AN molecules in the initial and hydrated states. At the  $X = 0.5-0.3$  only hydrated AN molecules are present. There are the hydration specification for polyfunctional molecule of AN. The second Debye relaxation in the area  $x = 0.5-0.6$  is determined by the hydrophilic and hydrophobic hydration in the complicated hydration shells. The two types of hydration water there are at  $x < 0.4$ , but this range is more complicated. The separate Debye relaxation is determined by hydrophobic hydration of nonpolar group. It is difficult, but possible, to divide the hydrated AN and Debye relaxation of water with weak AN-H<sub>2</sub>O bonds in distorted water structure.

## **57: Kinetics of Thermo-Stimulated Volume Phase Transition in Hydrogels Based on Poly(2-(2-MethoxyEthoxy)Ethyl Methacrylate) Obtained via ATRP or FRP**

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Poster W: Wed 18:30, Chem

The biggest disadvantage of stimuli-responsive hydrogels is their insufficiently quick response to an applied stimulus. One of the solution of this issue is the introducing hydrophilic dangling chains into a polymer network. Their role is to prevent to some extent aggregation of hydrophobic chains and maintain channels for water diffusion. In this work the gels containing dangling chains poly(MEO2MA) were compared with the analogous not containing any dangling chains. There were compared also the



materials with the same contents, obtained via atom transfer radical polymerisation (ATRP) or free radical polymerisation (FRP) methods. Relaxations of polymer chains during volume phase transition were analyzed with use of BDS and DMA. The water-molecular interactions during VPT were studied by Raman Spectroscopy. Investigations show at least three phase of VPT with different kinetics. First phase is very quick and is shorter for the sample without any side chains. For sample with dangling chains this stage is slower the most probably because of more complicated structure. Second phase reversely is quicker for the samples with the side chains. Then there is one more stage, very slow, but it is very difficult to estimate exact end time of this phase because of hazard of water evaporation during long measurements. Similar tendency was seen in all used techniques. This project was supported by Polish Ministry of Science and Higher Education (grant no. NN209200738).

## 58: Dielectric Spectroscopy of Swellable and Non-Swellable Clays at Low Moisture Levels

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Poster W: Wed 18:30, Chem

Clays are widely used in industrial and environmental applications, such as construction of geotechnical barriers of hazardous waste disposal sites. Swellable clay minerals are characterized by high specific surface area and high water uptake capacity. Water binding mechanisms of swellable clay minerals such as smectites are complex, since they adsorb water on the silicate surface and within the interlayer. Many applications where clays are present require a water content monitoring that is fast, destruction free and applicable in-situ and over wide area coverage, which can be achieved by dielectric spectroscopy. Former dielectric studies were mostly conducted on clays at high moisture levels or suspensions. Still, the majority of the applications for clays require water content determinations at low moisture levels. A study was performed to assess the dielectric properties of swellable and non-swellable clays at low moisture levels at two frequency ranges ( $2 \cdot 10^8$ - $1.1 \cdot 10^9$  Hz,  $1 \cdot 10^{-4}$ - $1 \cdot 10^6$  Hz). Several material-intrinsic properties were identified that hinder the parameterization of water content from real permittivity. In the low frequency range, processes in addition to bound water relaxation, e.g. electrode polarization and conductivity contribution, impeded deriving the water content from real permittivity. The suitability of different

mixing equations was compared for low moisture level clays and a new equation was developed considering clay specific properties.

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## **59: Comparative dielectric studies of Ag nanoparticles in matrix of polymers and monomers**

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Poster W: Wed 18:30, Chem

In this work the results of BDS study ( $10^{-3}$ - $10^5$  Hz, 140-180°C) of Ag nanoparticles (NPs) synthesized in different matrix (polymers and monomers) are presented. The frequency dependence of specific AC conductivity and complex electric modulus was used to estimate the temperature-frequency intervals of charge transfer by long and short distances, respectively. With increasing the concentration of Ag NPs, specific AC conductivity increases. In low frequency region, the AC conductivity dependence transformed into plateau, that corresponded to DC conductivity. The temperature dependence of specific DC conductivity show considerable deviation from Arrhenius dependence, that points to the significant contribution of cooperative effects in the charge carriers transport mechanism. In the sols and films of Ag NPs the considerable increase of Vogel temperature and glass-transition temperature,  $T_g$ , in sols in comparison with pure solvent was found. Although the dielectric characteristics of sols generally controlled by the conductivity relaxation, the dielectric response was observed in the high-frequency range ( $1\text{-}10^3$  Hz) at low temperature (-50 - +10°C). This response was resulting from the presence of NPs in the solution. It was supposed that the relaxation was caused by motion of ion impurities on the Ag NPs surface within the carboxylate ligands shell. In contrast to the sols and films of Ag NPs in the epoxide and Ag NPs nanocomposites the  $T_g$  was varied from 90 to 96°C.

## 60: Study of electrical and dielectric properties of nanopowders of hydroxyapatite with added piezoelectric material

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Poster W: Wed 18:30, Chem

Bones piezoelectric properties play an important role on their growth and regeneration. Besides their strength natural hydroxyapatite (HAp), an apatite ceramic, and collagen and movement of ions in fluids gives this piezoelectric characteristic to bone. In many biomedical applications related to bone and dental replacement is used a synthetic hydroxyapatite whose piezoelectric properties can be enhanced by adding a piezoelectric material, usually barium titanate ( $\text{Ba TiO}_3$ ) [1]. In this work a study of a nanopowders of HAp produced via sol-gel were mixed with tetragonal micro-powders of barium titanate. Different compositions were used: 5, 10, 15 and 20% w/w of barium titanate. The aggregation and distribution of two different size powders was studied by SEM in order to understand the influence of powder distribution on the properties of the composite. Main interested was on electrical and dielectric properties, which were investigated by dielectric spectroscopy and isothermal and thermally stimulated currents measurements. After, selected samples were polarized and stability of polarization was studied so to select the more stable for bioactivity tests.

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## 61: Very low frequency dielectric relaxation and DC conductivity in dielectric materials

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Poster W: Wed 18:30, Chem

Symmetric bipolar triangular-voltage signals of very low slope (very low frequency) and different amplitudes can be used to measure the resistive component and the

capacitive component of the current. We have measured the current for polar (Nylon 11) and nonpolar polymers (Kapton) for a large range of temperatures (isothermal and non-isothermal measurements) and applied fields. Thermally stimulated discharge current was used to check if there is trapped charge in the material and to measure the amount of the charge trapped in the material for different experimental conditions. The experimental results show that when an electric field is applied on the dielectric material besides the polarization charge, electric charge is injected/extracted into/from the material. This charge is partially transported and partially trapped into the material, depending on the material properties and on the experimental conditions. As a consequence, the structure is decorated with space charge. The space charge will influence the behavior of the material. Even for a very long time periods, at low and moderate applied fields DC conductivity can not be observed. The results can not be explained in terms of ohmic conduction and a new conduction mechanism is proposed. The contribution of the electrode effects and bulk effects is analyzed, especially by combining short-circuit and open-circuit isothermal and non-isothermal measurements.

## 62: Glassy dynamics of isolated polymer coils

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Poster W: Wed 18:30, Chem

For the first time, the glassy dynamics of randomly distributed, isolated poly(2-vinylpyridine) (P2VP) polymer coils is studied by means of Broadband Dielectric Spectroscopy (BDS). This is achieved by recently developed nano-structured electrode arrangements where isolated polymer coils are deposited onto ultra-flat, highly conductive silicon electrodes. Atomic Force Microscopy scans of the identical sample before and after the BDS measurement prove that the volume of the coils matches, within a factor of 10 (reflecting the broad molecular weight distribution), with the expected volume of a single chain (considering bulk density and the respective molecular weight). The observed dynamics resembles that of the bulk but the mean relaxation time is slowed down by about one decade. This is attributed to attractive interactions of the P2VP segments with the supporting silica surface.

## 63: Molecular dynamics of cis-1,4-polyisoprene in 1-D and 2-D confinement

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Poster W: Wed 18:30, Chem

Broadband Dielectric Spectroscopy (BDS)-in combination with a nanostructured electrode arrangement [1] is used to study thin layers of cis-1,4-polyisoprene (PI). Being a Type A polymer [2], cis-polyisoprene enables the investigation of two distinct relaxation modes taking place at two different length scales: the segmental motion which involves structures of about one nanometer in size, and the normal mode which represents the dynamics of the whole macromolecule. Down to 7 nm, for three molecular weights (44.5, 53 and 75 kg/mol), it is observed that:(i) the segmental mode as a local relaxation process is unaffected by the 1-D confinement; and (ii) the normal mode becomes faster with decreasing layer thickness, in dependence on molecular weight. The former result underscores a thickness- and molecular weight-independent (dynamic) glass transition (at least in the range studied here) [3,4], while the latter is a clear indication of an alteration of chain conformation. Furthermore, results of the measurement of the molecular dynamics of PI under the 2-D confining geometry of unidirectional Anodic Aluminium Oxide (AAO) nanopores are also presented.

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## 64: Kirkwood Spheres for Transient Dipolar Entities - Correlation in Weakly Ergodic Systems

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Poster W: Wed 18:30, Chem

Accounting for dipole correlations in systems that exhibit weak ergodicity breaking is no straight forward matter. For example, the original Kirkwood-Frohlich theory, is insufficient, in that it does not allow for systems with non-rigid dipolar entities.

The new method presented here provides a bridge extending Frohlich's insights to include these weakly non-ergodic, fluctuating virtual dipoles. The analysis provides a testable parameter derived primarily from the static dielectric parameters and is based upon evaluating the dielectric strength of any type of transport or hopping process. A number of distinct examples are presented, including Porous Silicon, Porous Glass, and Ferroelectric Crystals, demonstrating the model's versatility and wide range applicability.

## 65: Terahertz time-domain spectroscopy on proteins and polypeptides

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Poster W: Wed 18:30, Chem

When protein expresses the function, a large structural change often occurs. This change is induced by the collective motions of many atoms in protein, corresponding to the low-frequency motion below a few tens of wavenumbers. Therefore, the low-frequency spectra of protein contain information on the motions relevant to the function of protein. Native myoglobin (Mb) is called holo-Mb and Mb without the heme which is active center of Mb is called apo-Mb. When Mb expresses the function, its conformation changes locally by desorption of oxygen, suggesting that the heme is important for the conformational change. In this work we studied effects of hydration and temperature on the low-frequency spectra of holo-Mb and apo-Mb. Furthermore, we studied influence of the heme on the low-frequency dynamics of protein, by measuring the low-frequency spectrum of holo-Mb and apo-Mb by terahertz time-domain spectroscopy (THz-TDS). We have also studied microscopic environment around a tetraalkylammonium cation, a hydrophobic probe, in aqueous solutions by THz-TDS. For recent years, we have applied THz-TDS to investigate low-frequency spectra of solute molecules in solution in the THz frequency region [1-5]. The solute contributions to the observed spectra are obtained by subtracting the solvent contribution from the solution spectra. In this work we apply this technique to the aqueous solutions to investigate THz response in the hydrophobic hydration.

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## 66: Impact of finite size effects and interfacial interactions on the cold crystallization of poly(ethylene terephthalate) between two attractive interfaces

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Poster W: Wed 18:30, Chem

We investigated the impact of nanometric confinement on the cold crystallization of ultrathin films of poly (ethylene terephthalate), PET. Upon reduction of the thickness, in agreement with previous investigations of other polymers [1,2], we observed an increase of the cold crystallization temperature during heating scans, and of the characteristic crystallization time during isothermal experiments. We propose a model of the time evolution of the dielectric strength during isothermal experiments, taking into account both crystallization and adsorption, which permitted us to discriminate between interfacial and size effects. While for thicker films we could explain the reduction in crystallization rate by mere nucleation effects, around 100 nm we determined the onset of interfacial interactions, and below 20 nm we observed total inhibition of the crystallization. Remarkably, the last threshold corresponds to the thickness of the polymer layer irreversibly adsorbed [3] onto the attractive aluminum electrodes, at the timescale of the experiment. Contrary to the general idea on the impact of interfaces on the dynamics of confined systems, we verified that the interfacial energy is not a reliable parameter to predict the deviations from bulk behavior.

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## 67: Study of HEA-HEMA hydrogels by dielectric spectroscopy and thermoanalytic methods

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Poster W: Wed 18:30, Chem

Hydrogels prepared by copolymerisation of 2-hydroxyethylacrylate (HEMA) and 2-hydroxyethylmethacrylate (HEA) have shown potential for various biomedical applications due to an easy control over their physicochemical properties by changing the

monomer ratio in the reaction mixture. In this work, eleven samples with different HEA/HEMA compositions with 10 mol% step were synthesized by three-dimensional free-radical copolymerisation [1]. The hydrogel samples were incubated in aqueous solutions with salt, glycerol, or model drugs. Broadband Dielectric Spectroscopy (BDS) and other techniques (TGA, DSC, SEM and drug release assay) were engaged to study the effect of HEA-HEMA composition on the water-polymer molecular dynamics and properties of water in the hydrogels. BDS (Novocontrol Alpha system) spectra were recorded in frequency range from 0.1Hz to 1MHz and temperature range from -140 °C to 80 °C and revealed different behavior in HEMA-rich and HEA-rich samples. One relaxation process with the activation energy  $\sim 20$  kJ/mol was registered for samples with HEA content greater than 50 mol%, whereas for HEMA-rich samples two relaxation processes can clearly be distinguished. TGA measurements performed in temperature range 25-200 °C have shown that water is evaporated from hydrogels in two steps related to free water and bound water. DSC measurements were aimed to analyse the freezing and melting processes in temperature range: 25 °C- > -40 °C- > 25 °C.

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## **68: Structure, dielectric and magnetic properties of ferriiferous two-phases and porous alkali borosilicate glasses**

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Poster W: Wed 18:30, Chem

The structure and properties of the two-phase borosilicate glasses (BSG), doped by different amount of hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) (Fe25-25% of iron oxide, Fe20-20%, Fe15-15%) and microporous (Fe20-MIP) and macroporous (Fe20-MAP) glasses on base of Fe<sub>2</sub>O have been studied. These materials demonstrate magnetic properties and could be considered as a very perspective media for production so-called "artificial" multiferroics. At preparation of two-phases ferriiferous glasses the transition of initial  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> into the magnetite (Fe<sub>3</sub>O<sub>4</sub>) takes place. Fe<sub>2</sub>O glass demonstrates



the largest value of dielectric permittivity and conductivity and this type of magnetic glasses have been chosen as a base for porous magnetic matrices. Temperature dependencies of porous magnetic glasses DC-conductivity were obtained from hodographs of impedance. These dependencies demonstrate thermal activation behavior. From magnetic-force microscopy measurements and magnetometry data we have estimated the coercive field for magnetic nanoclusters ( $\sim 90$  mT). At the temperature 120 K we can see some peculiarities on the curves corresponding to the Verwey transition in the bulk magnetite. The lattice parameters, particle sizes of magnetite ( $\text{Fe}_3\text{O}_4$ ) and occupations of iron octahedral ( $\text{Fe}^{2+}$ ) and tetrahedral positions ( $\text{Fe}^{2+}/\text{Fe}^{3+}$ ) for two-phase Fe<sub>20</sub> (150(5) Å), Fe<sub>20</sub>-MIP (168(7)Å) and Fe<sub>20</sub>-MAP (180(5)Å) were determined.

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## 69: The role of molecular mobility in governing physical stability of glass-forming liquids

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Poster W: Wed 18:30, Chem

Despite years of studies glassy formation is still incomprehensible in many aspects. Understanding what drives supercooled liquids and glasses towards crystallization is fundamental not only in the context of unsolved problems of condensed matter physics, but also many practical applications. Herein, the role of molecular mobility in governing the physical stability of glass-forming materials will be discussed in the context of pharmaceutically important substances. Based on dielectric data it was concluded that molecular mobility is certainly an important parameter that controls crystallization abilities of glass-formers, however, there must be other factors of much greater authority. As will be presented in the context of glucose and its acetyl derivatives by changing the character of intermolecular interactions from hydrogen bonding to typical van der Waals, the resistance against crystallization can be drastically changed. This points out that the character of molecular interactions and molecular architecture, might have the crucial importance on the physical stability of glass-forming liquids. Finally, results from crystallization kinetics experiments under elevated pressure will be presented for pharmaceutical, ibuprofen, showing that that pressure slows down its crystallization progress, possibly even inhibit it.

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## 70: Quantifying the dielectrophoretic response of DNA by impedance measurements

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Poster W: Wed 18:30, Chem

Biological macromolecules like proteins and DNA can be concentrated and immobilised in strongly inhomogeneous electrical AC fields by dielectrophoresis. For a systematic optimisation of experimental parameters proper knowledge about the underlying phenomena is advisable. Typically, molecular dielectrophoresis is monitored by fluorescence microscopy, which, however, is problematic to be applied to quantitative studies due to photobleaching. Here we present a purely electrical method to monitor the dielectrophoretic response of DNA in solution by measuring impedance changes between the collecting electrodes. Dielectrophoretic spectra were determined between 1 kHz and 3 MHz for DNA which varied in size from 100 bp to 48 kbp. The capacitive part of the corresponding impedance changes was acquired at 1 kHz with an automatic capacitance bridge. Interdigitated microelectrodes of 1.4  $\mu\text{m}$  width and 1.1  $\mu\text{m}$  gaps were used. Maximum response was found around 3 kHz and 3 MHz and for both very long DNA and quite short 100 bp fragments. This combination of dielectrophoresis with impedance measurements allows quantitative dielectrophoretic studies on macromolecules without the need for any optical access or labeling. Since it is purely electrical, laborious image analysis can be avoided and automation is rather simple.

## 71: Relating conductivity to morphology in Poly(ethylene oxide)/Lithium Triflate polymer electrolytes) Blends

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Poster W: Wed 18:30, Chem

Polymer electrolytes form the basis of solid-state lithium batteries and their structural

and electrical properties have been extensively investigated. However, even in the archetypal polymer electrolyte, poly(ethylene oxide)/lithium triflate, little is known how the local and global organization affects the ionic conductivity. Herein we explored the thermodynamic states (DSC), the structure (with X-rays, POM and IR), the viscoelastic properties (with Rheology) and the electrical conductivity (with BDS) in a series of PEO/LiTf electrolytes. We found a composition different than the stoichiometric giving rise to the local organization responsible for the high ion mobility.

## 72: Dielectric relaxation study of butanenitrile with 1,2-dichloroethane through time domain spectroscopy

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Poster W: Wed 18:30, Chem

The dielectric relaxation study of 1,2-dichloroethane has been carried out with butanenitrile in the frequency range of 10 MHz to 20 GHz using time domain spectroscopy (TDS) in the temperature range 15°C to 45°C for 11 different concentrations of the system. The relaxation in these systems can be described by a single relaxation time using the Debye model. The dielectric parameters viz. static dielectric constant ( $\epsilon$ ) and relaxation time ( $\tau$ ) have been obtained by the least squares fit method. Excess properties and Kirkwood correlation factor of the mixture have been determined. The static dielectric constants for the mixtures have been fitted with the modified Bruggeman model.

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## 73: Equations of state in the thermodynamic scaling regime-theoretical, experimental and simulation studies

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 Poster W: Wed 18:30, Chem

Recently, we have suggested [1,2] two equations of state (EOS) to study glass formers in the thermodynamic scaling regime, in which dynamic quantities such as structural relaxation time and viscosity can be scaled vs the scaling quantity ( $\text{density}^{\gamma_{\text{gamma}}}$ )/temperature, where the exponent gamma is a material constant. In the proposed talk, our latest successful tests [3] of these EOS by using molecular dynamics (MD) simulations of the Kob-Andersen Lennard-Jones binary liquid (KABLJ) are to be discussed. These EOS lead in case of the KABLJ model to a perfect scaling of volumetric (PVT) data with the same value of the scaling exponent gamma as that found for structural relaxation times. This meaningful result will be compared with that earlier found for experimental dielectric and PVT data of real glass formers. Further, these findings will be used to formulate an EOS for the activation volume, which is an important parameter commonly used to characterize how pressure changes affect molecular dynamics of glass former. The EOS for the activation volume also predicts a scaling behavior of the activation volume, which is successfully tested [4] by using MD simulation data for the KABLJ liquid and experimental dielectric and PVT data for real glass formers. Finally, unexpected pressure dependences of the isothermal bulk modulus for the activation volume calculated from structural dielectric relaxation times of real glass formers and the KABLJ liquid will be demonstrated.

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## 74: Molecular dynamics study of amorphous anti-inflammatory drug celecoxib stabilized by octaacetylmaltose

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Poster W: Wed 18:30, Chem

Many crystalline drugs, including celecoxib (CEL, a non-steroidal anti-inflammatory agent), are poorly water soluble, and therefore they are characterized by low bioavailability. It has been shown that the aqueous solubility of amorphous CEL is significantly higher than that of its crystalline counterpart [1]. However, we found that amorphous CEL is physically unstable and easily crystallizes above the glass transition temperature  $T_g$  as well as during storage in normal conditions at  $T=20\text{ }^{\circ}\text{C}$  (more than  $30\text{ }^{\circ}\text{C}$  below its  $T_g$ ). A key question that arises in the case of such materials is "how does their molecular mobility influence their stability?". Performing broadband dielectric measurements of CEL, we are able to determine time scales of molecular motions in the glassy and liquid states to find some correlations of the molecular mobility with the tendency of the material to crystallization [2]. Moreover, we present a novel way of stabilization of amorphous CEL against recrystallization by preparing binary amorphous celecoxib-octaacetylmaltose (CEL-acMAL) systems by quench-cooling of the molten phase. We found that such a system is characterized by a much better solubility and stability than pure CEL. By dielectric measurements we found that the molecular mobility of the mixture of CEL with 10wt% acMAL in the glassy state is much more limited than that in the case of pure CEL, which correlates with the better stability of the amorphous binary system [3,4].

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## 75: Boson Peak in Hydrogen-Bonding Liquids

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Poster W: Wed 18:30, Chem

Boson peak is commonly observed as dielectric dispersion in THz frequency range for hydrogen-bonding liquids, supercooled-liquids and glasses. Origin of the boson peak must be very important to understand nature of amorphous substances. However, we still have some difficulties to explain the boson peak. One of the reasons is considered to be that behavior of the boson peak doesn't depend on substances very much. It has been reported that density of -OH group and the hydrogen-bonding structure is reflected in behavior of the terahertz dielectric loss for many simple alcohols [1-4]. It has been also indicated that the terahertz dielectric loss for several different pentanol isomers strongly depends on their chemical structure [2]. We are going to discuss about relation between the terahertz dielectric dispersion and dynamics of local structure composed of several -OH groups. This approach is very helpful to understand the fact that the loss peak observed in simple alcohols is connected to the boson peak observed in polyhydric alcohols such as glycerol.

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## 76: Relaxation dynamics of protein solutions

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Poster W: Wed 18:30, Chem

We provide broadband dielectric spectra on aqueous lysozyme solutions of various concentrations and analyze the three dispersion regions commonly found in the physiological temperature range. The beta-dispersion, occurring in the frequency range around 10 MHz and the gamma-dispersion arising around 20 GHz can be attributed to the rotation of the polar protein molecules in the aqueous medium and the reorientational motion of the free water molecules, respectively. The nature of the third relaxation (delta-relaxation) around 100 MHz, which is often ascribed to the motion

of protein-bound water molecules, is not yet fully understood and the hydration-shell dynamics of biomolecules is an ongoing field of research [1-6]. Additional insight can be gained by analyzing the subzero temperature spectra, where the beta- and gamma-dispersions, which partly superimpose the delta-relaxation in the physiological temperature range, disappear due to the freezing of the bulk water. In contrast, the water molecules in the protein hydration shell are known to remain in the liquid state well below the freezing point. This allows to investigate the delta-relaxation in an extended temperature range and to shed new light on the hydration-shell dynamics of biomolecules.

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## 77: Broadband Dielectric Spectroscopy for checking bonded assemblies

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Bonded assemblies are currently used in satellites manufacturing to answer increasing requirements of structures lightening. For checking these assemblies, accelerated testing based on space industry knowledge [1] and standards have been performed. The purpose of this study is to estimate the influence of these ageing parameters. Differential scanning calorimetry and dynamic mechanical analysis are performed to follow and understand the effect of ageing on bulk adhesives. BDS is a convenient non-destructive technique to study adhesives in a representative configuration, i.e bonded assembly. Dielectric measurements were performed using a Novocontrol BDS 4000. The samples were round plate assemblies (200  $\mu\text{m}$  in thickness) using aluminum alloy substrates as electrodes. The isotherm network of polyepoxy adhesives has been fitted

by the Havriliak-Negami function. The temperature dependence of relaxation times has been described by activation parameters in the vitreous state; for the rubbery state, the Vogel-Tammann-Fulcher parameters have been considered. Their evolution with ageing conditions (humidity, temperature, thermal cycling or radiations) highlights ageing phenomena like chain scissions, crosslinking, plasticization, physical ageing. BDS gives us molecular interpretations of adhesive properties evolutions to predict service life of assemblies. Data collected help us to optimize accelerated ageing test and to formulate new adhesives for future applications.

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## **78: Probing the internal morphology of different poly (N-isopropylacrylamide) systems by dielectric spectroscopy**

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Poster W: Wed 18:30, Chem

Dielectric Relaxation Spectroscopy (DRS) is applied in a frequency range of  $10^{-1}$  to  $10^6$  Hz and temperature range of  $15^{\circ}\text{C}$  to  $50^{\circ}\text{C}$  to aqueous solutions of linear Poly(N-isopropylacrylamide) (pNIPAM) with different polymer concentrations and to aqueous dispersions of pNIPAM microgels with different crosslinking densities. In aqueous media pNIPAM shows a lower critical solution temperature (LCST) at about  $32^{\circ}\text{C}$  where a coil-to-globule transition in the case of linear pNIPAM and a volume phase transition (volume contraction) in the case of pNIPAM microgels can be observed. The structural change at the LCST can be monitored by both the temperature dependence of the DC conductivity and the frequency dependence of the conductivity spectra. The latter one is due to a Maxwell/Wagner/Sillars polarization and can be related to the formation of a "soft particle" at the LCST at which charge carriers are blocked. The frequency and temperature dependence of the conductivity was investigated in dependence on different parameters such as the polymer concentration, the heating/cooling rate and the crosslinking density. The dielectric measurements were accompanied by dynamic light scattering (DLS) and zeta potential measurements in order to relate the dielectric data with results obtained by well established methods.



## 79: Dynamic and structural characteristics of water in the hydrated amino acids and protein powders

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Poster W: Wed 18:30, Chem

The dielectric study of water in a variety of complex systems can clarify its structural and dynamic interaction with other molecular environment. If in aqueous solutions the starting point of water state considered as a bulk one, which interacts with the solute only partially, the state of water adsorbed in heterogeneous materials is determined by various hydration centers of inhomogeneous material (the matrix) and is significantly different from the bulk. In both cases, the dielectric spectrum of water is symmetrical and can be described by Col-Cole (CC) function. This universal feature allowed the application of a unified phenomenological consideration based on 3D trajectories in the phase space of CC parameters to completely different water contained systems [1]. Here we report the results of dynamic and structural study of the hydrated amino acids with variability of their polarity. We investigated powders with various humidity in the wide temperature (-120 – 50°C) and frequency (0.1 Hz – 1 MHz) ranges. The knowledge gained on water in the vicinity of amino acids was used for elucidation of water-protein interactions in powders.

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## 80: Dielectric properties of polyvinylidene fluoride (PVDF)/TiO<sub>2</sub> nanocomposites

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Poster W: Wed 18:30, Chem

Polymer nanocomposites based on polyvinylidene fluoride (PVDF) matrix filled with TiO<sub>2</sub> nanoparticles (1,2,3 and 5% by v/v%) were studied by broadband dielectric spectroscopy (BDS) in order to investigate the filler effect on the molecular mobility of the polymer chains. The formalism of electric modulus was used to analyze the dielectric response, thus three relaxation processes were observed. In fact, the first

one, which is around  $-40^{\circ}\text{C}$  at 10 Hz, is attributed to the glass transition at low temperature. As for the second phenomenon, around  $30^{\circ}\text{C}$  at 10 Hz, it is related to the dipolar relaxations in the crystalline phase. Regarding the third one, around  $100^{\circ}\text{C}$  at 10 Hz, it can be due to the interfacial polarization (IP). The crystallinity ratio decreases and the electric modulus of the interfacial polarization increases with the increase of the  $\text{TiO}_2$  content.

## 81: Highly conductive metallic nanowires-polymer composites for aeronautical applications

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Poster W: Wed 18:30, Chem

Conductive polymer nanocomposites have attracted much attention. Obtaining the lower percolation threshold with the lower volume fraction of conductive particle was the mainly objective of most part of studies during the past decades. Balberg have shown[1] the dependence of percolation threshold with the aspect ratio of conductive particles. On this way, nanomaterials such as CNTs[2] and nanowires[3] enable the formation of poorly filled conductive composites. A recent study[4] has shown a low percolation threshold ( $p_c$ ) of 2.2 vol% and an electrical conductivity of 100 S/m above  $p_c$  for composites of P(VDF-TrFE) filled with gold nanowires. The value of electrical conductivity obtained above the percolation threshold is unusual at this low content of conductive filler and is observed for the first time. The composite conductivity seems to be dependent of the intrinsic particle conductivity. The polymer layer between particles drives the electrical conduction mechanisms. The BDS was used to study the electrical conductivity of composites. This technic is well adapted to the understanding of charge transport in solids. Dc and ac conductivity are examined with varying parameters. The conductivity temperature and frequency dependence give identification on behavior laws (tunneling, hopping). These low filled composites are excellent candidates to formulate high conductive composites polymer for multifunctional applications as conductive composites for aeronautical structures.

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## 82: Complementary study by dielectric spectroscopy of a multilayer film exposed to UV radiations

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Poster W: Wed 18:30, Chem

Under the action of sunlight, polymer materials undergo many irreversible changes due to a series of oxidative reactions that lead to chemical degradation. These changes produce unwanted effects which are responsible for the damaging of the film integrity and the reduction in product lifetime [1]. In a lot of applications the film selected is a multilayer material. Their properties, like gas permeability or mechanical strength, are better than the monolayer film properties. The present study is devoted to multilayer films constituted of a PA6 film situated between two PET films bonded with an adhesive. The multilayer was exposed to ultraviolet radiations for seven days. The evolution of its properties was investigated by uniaxial tractions, UV-Visible and FTIR-ATR spectroscopies and DSC. Finally the molecular mobility evolution has been analyzed by BDS. The complexity of the multilayer thermograms recorded by DSC and BDS has required the study of each film constituting the multilayer in order to assess each one of their contribution. The results showed that the degradation is similar to PET film, typical to photooxydation, mainly localized at the exposed layer [2]. However, the BDS of the multilayer exposed to UV shows an evolution of the molecular mobility in the PA6. A temperature shift of the dielectric relaxation associated with the dielectric manifestation of its glass transition is observed. This phenomenon reveals the degradations also occur in this layer.

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## 83: Comparison of different models studying the molecular mobility evolution at the dynamic glass transition

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For many years the interest of scientific literature in the molecular mobility of glass forming liquids has been very important. More precisely, many studies concern the study of glass-former cooperative processes [1]. The theoretical models to estimate the length scales of these relaxations are multiple: Adam and Gibbs theory [2], Donth approach [3], Berthier model [4]. Comparisons of the results obtained using these different models are not easy due to different theoretical assumptions. The goal of this work is to compare the evolution of cooperative structural unit number  $N_{\alpha}$  calculated using a temperature fluctuation approach [5,6] and the number of dynamically correlated relaxation units  $N_{corr}$  calculated from a two-point dynamic correlation function,  $\chi^2_T(t)$  [6,7]. Comparison of the two models has been carried out discussing on the different hypotheses and assumptions included in the analysis and calculation protocols.

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## 84: Dielectric relaxation in bionanocomposites based on polyhydroxyalkanoates/organomodified montmorillonite

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Poster W: Wed 18:30, Chem

With growing environmental awareness, considerable researches and development interests are focused on the limitation of pollution by non-degradable petroleum plastics with long-lasting presence. The combination of biodegradable polymers with nanofillers seems to be a new way of processing for reducing the impact of packaging products. The elaboration of bionanocomposites combines different contributions:

the biodegradability exhibited by the polymer matrix and the favourable effect of the nanoclays on the mechanical, thermal and barrier properties of matrix. Polyhydroxyalkanoates (PHAs), a bio-polyester synthesized by various bacteria, has received considerable attention due to their good balance between gas barrier and mechanical properties [1]. The use of organomodified montmorillonite (OMMT), improves these properties [2]. The aim of this work was to study the amorphous phase mobility by dielectric spectroscopy to determine the impact of the incorporation of OMMT in semi crystalline PHA-matrix. This work is focused on two samples, a pure PHA and a PHA with 7.5wt% of OMMT. The obtained results in dielectric spectroscopy show a complex beta relaxation. After the data treatment, two contributions have been observed for both samples according to an Arrhenius law. A alpha relaxation is also observed and follows a Vogel-Tamman-Fulcher (VTF)-equation. The impact of incorporation of OMMT in PHA behaviour does not appear to affect alpha and beta relaxations of PHA. Acknowledgement: The authors acknowledge financial and equipment support from the "Région Haute-Normandie".

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## **85: Dielectric relaxation of carbon black-filled nitrile rubber composites and electric network structure**

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Poster W: Wed 18:30, Chem

Dielectric frequency spectra were recorded for carbon black filled nitrile-butadiene rubber (NBR) over a wide range of frequencies (0.1Hz–5MHz) and temperatures (20–100°C). The three layer condenser method introduced before by Goertiz, was used. This condenser is obtained by embedding the sample (partially conductive layer) between two insulating and loss free layers.  $\epsilon'' - f$  curves analyzed for unfilled sample revealed at 300C, two loss peaks at 10 and 106 Hz. Increasing temperature shifted these peaks to higher frequencies and a third peak appeared around 0.2 Hz at 80°C.  $\epsilon'' - f$  curves for CB-filled samples below percolation threshold revealed a 4th peak around 0.5 Hz at 30°C and shifted to 50 Hz at 90°C for the 20phr sample. While for 40phr CB, sudden increase in  $\epsilon''$  appeared at the percolation threshold. This sudden jump implies the formation of conductive network through the polymer matrix. For

50phr sample and at 90°C temperature more conductive paths are produced caused by the transport of electrons among CB particles connected with the tunnelling effect. The results are discussed.

## **86: Molecular Dynamics of a discotic liquid crystal**

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Poster W: Wed 18:30, Chem

The molecular dynamics of the discotic liquid crystal pyrene-1,3,6,8-tetracarboxylic tetra(2-ethylhexyl)ester is studied by dielectric relaxation and specific heat spectroscopy. Dielectric spectroscopy shows 3 processes, a  $\beta$ -relaxation at low temperatures, an  $\alpha$ -relaxation in the temperature range of the mesophases followed by conductivity. The  $\alpha$ -relaxation is assigned to glassy dynamics in the plastic crystal as well as in the liquid crystalline phase. Two Vogel-Fulcher-Tammann equations which differ in the both the Vogel temperature and the fragility can be used to describe the process. Dielectric and calorimetric data show a good agreement. Conductivity in the high temperatures exhibits different activation energies in the liquid crystal and the isotropic phase.  $\beta$ -relaxation at lower temperatures has a relatively low activation energy when compared to other liquid crystals which might be due to the short side chains and the location of a branch at the ester group of the molecule. Furthermore the material is studied when confined to nanoporous Alumina Oxide membranes with different pore sizes and the results are compared to those of the bulk material.

## **87: Triphenylene-based discotic liquid crystals in the bulk and confined to alumina oxide membranes**

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Poster W: Wed 18:30, Chem

Discotic liquid crystals consist of a stiff aromatic core surrounded by flexible aliphatic side chains. As the disc-shaped molecules of the core self-organize into hexagonal columnar arrays, the alkyl chains fill the space between the columns yielding a nanophase

separated state. A series of triphenylene-based discotic liquid crystals (2,3,6,7,10,11-Hexakis[n-oxy]triphenylene (HATn,  $n=5,6,8,10,12$ ) is investigated by means of Dielectric Relaxation Spectroscopy, Differential Scanning, Specific Heat Spectroscopy, Neutron Scattering and X-Ray Scattering. Nanoporous alumina membranes with different pores sizes are filled with the triphenylene derivatives to study the influence of confinement on the dynamics in these discotic liquid crystals by means of Dielectric Relaxation Spectroscopy.

## 88: Piezo- and pyroelectric detection of space charges in human blood during coagulation

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Poster W: Wed 18:30, Chem

Coagulation, the process by which blood clots are formed, is of fundamental importance to all living things. For all mammals, it involves both a cellular (platelet) and a protein (coagulation factor) component. Exposure of blood to these proteins initiates changes to blood platelets and the plasma protein fibrinogen. Platelets form a plug at the site of initiation, while clotting factors form fibrin strands through a complex cascade, to strengthen the plug. Earlier work has shown that an electric potential can be measured if electrodes are placed in the blood during clotting[1]. Here, we attempt to measure the pyro- and piezoelectric activity of blood plasma after initiating the coagulation with a  $\text{CaCl}_2$  solution. In our experiment, a photo-thermal setup is used that shows strong similarities to a Scanning PyroElectric Microscope[2]: the output of a laser beam is modulated in time and produces a local thermal (diffusion) wave in the medium. This periodic change in temperature can lead to an alternating pyroelectric current, modulated at the same frequency. By scanning the laser over the surface of the sample, spatial information about the polarization or charge distribution[3] can be obtained from the pyroelectric current. Continuous scanning of the sample allows monitoring the kinetics of coagulation of human blood from the time-dependence in the polarization distribution. A high level of activity is expected at the phase front where an active charge separation is maintained.

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## 89: Single crystal dielectric spectroscopy on Metal Organic Framework MIL-68 in combination with pyroelectric microscopy

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Poster W: Wed 18:30, Chem

Using a highly sensitive dielectric analyzer, we attempt to obtain the dielectric spectrum of a single crystal of MIL-68 containing polar paranitroaniline (PNA) guest molecules. The large, hexagonal pores of the MIL-68 host structure allows multiple PNA molecules to align parallel to each other in the same pore[1]. Interactions both between the molecules in the same pore and between molecules in adjacent pores should introduce several relaxation processes. With the aid of a Scanning PyroElectric Microscope, the dielectric data obtained can then be compared to a pyroelectric current map of the same crystal, taken at several relevant temperature ranges. The local pyroelectric response can be related to the macroscopic polarization distribution present, and the mobility of the molecules in the pores[2].

[1] A.Fateeva, P.Horcadada, T.Devic, C.Serre, J.Marrot, J.M.Grenèche, M.Morcrette, J.M.Tarascon, G.Maurin, G.Férey, *Eur. J. Inorg. Chem.* 2010, 3789-3794.

[2] A. Quintel, J. Hulliger, and M. Wübbenhorst, *J. Phys. Chem. B*, 102, 4277-4283, 1998.

## 90: Novel Copolymers of Difluorine Ring-substituted 2-Phenyl-1,1- dicyanoethylenes with 4-Fluorostyrene: Synthesis, Structure and Dielectric Study

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Poster W: Wed 18:30, Chem

Copolymerization of difluorine ring-substituted 2-phenyl-1,1-dicyanoethenes,  $\text{RC}_6\text{H}_3\text{-CH}=\text{C}(\text{CN})_2$  with 4-fluorostyrene were prepared in the presence of a radical initiator



(ABCN) at 70°C. The composition of the copolymers was calculated from nitrogen analysis, and the copolymers were characterized by IR,  $^1\text{H}$  and  $^{13}\text{C}$ -NMR, GPC, DSC, and TGA. The monomer reactivity ratios for 4-fluorostyrene ( $\text{M1}$ ),  $r_1 = 0.6$  and 2-(2,4-difluorophenyl)-1,1-dicyanoethene ( $\text{M2}$ ),  $r_2 = 0$  were determined from Fineman-Ross plot. DSC curves showed that the copolymers were amorphous with high  $T_g$  in comparison with that poly(4-fluorostyrene) indicating a substantial decrease in chain mobility of the copolymer due to the high dipolar character of the trisubstituted ethylene monomer units. From the thermogravimetric analysis, the copolymers began to degrade in the range 214–260°C. Using dielectric spectroscopy, we have studied the dielectric properties of homo and copolymers of 4FST.  $\alpha$  relaxation processes occurred above the  $T_g$  in the copolymers was observed. In the copolymers, this strong primary relaxation was associated to the cooperative movements of the polar groups (CN) of the main chains. The values of dielectric relaxation increment were calculated and compared to the similar cyano copolymers. The  $\alpha$ -activation energies were also calculated. The relationship polarity-permittivity was discussed.

## 91: Dielectric phenomena vs. structural organization of the electroactive hybrid polymers containing ionic liquids

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Poster W: Wed 18:30, Chem

The blending of semi-crystalline polymer and elastomer is an attractive polymer blends to obtain high strength and elasticity material which called thermoplastic elastomer (TPE). Blends of poly(vinylidene fluoride) (PVDF) and epoxidized natural rubber (ENR) were prepared by internal mixer in melted state. The ENR with 50 mol% epoxide (i.e., ENR-50) was blended with PVDF according blend ratios of PVDF/ENR-50 = of 80/20 and 50/50 wt% to study relaxation behavior of the blends. Influence of blend ratio and phase structure of the blends was investigated by morphological, dynamical mechanical and dielectric properties to study relationship between phase structure and properties of the blends. Owing to the phase morphology is an important factor to determine properties of polymer blends. Phase morphology of the blends was studied by Scanning electron microscopy (SEM). Different structure were found according the composition of the PVDF/ENR-50 blends : 80/20 wt% of PVDF/ENR-50 presents ENR-50 which formed a dispersed phase in PVDF but 50/50

wt% of PVDF/ENR-50 was observed as a co-continuous phase structure. Dynamic mechanical studies showed storage modulus of the blends are intermediate between storage modulus of two component with storage modulus of 80/20 wt% is higher than 50/50 wt% of PVDF/ENR-50. The immiscible blends of PVDF/ENR-50 exhibited two relaxations on the loss factor versus temperature curves in dynamic mechanical and dielectric studies related to  $\alpha$ -relaxations of PVDF and ENR-50. These two  $\alpha$ -relaxations confirms phase separated of PVDF/ENR-50 blends. Differences observed in dielectric spectra of 80/20 and 50/50 wt% of PVDF/ENR50 blends were associated with different formation of the phase structure in the blends with affect the relaxation process in amorphous phase of PVDF, ENR-50 and crystalline phase of PVDF. Furthermore, the glass transition temperatures ( $T_g$ ) of PVDF and ENR-50 phases were shifted to higher and lower temperature, respectively which indicates the formation of partially compatible blends. The activation energy ( $E_a$ ) of the 2 blends relaxation was also calculated from frequency-temperature dependence of dynamic mechanical and dielectric properties.

## **92: Dielectric characteristics of new epoxy-phosphotungstic polymeric materials with ionic conductivity**

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Poster W: Wed 18:30, Chem

Epoxy composites are widely used for different applications in many technical areas due to their valuable properties, particularly as isolating adhesive materials with high mechanical properties. The original approach that allows receiving epoxy polymers with ionic conductivity is proposed in this work. The characteristics of epoxy composites depend on type of curing agents. Phosphotungstic heteropolyacid (PTA), which has a high catalytic activity and high proton conductivity, is a perspective hardener that in combination with epoxy resin creates epoxy-phosphotungstic polymer (EPTP) that can possess high ionic conductivity. Epoxy resins (ER) of different chemical nature (aromatic and aliphatic) have been used for synthesis of EPTP. EPTP polymers were synthesized due to cationic polymerization of the ER, which is caused by the catalytic effect of the PTA. This heteropolyacid was added to the reactive mixture as water solutions. The dielectric characteristics (permittivity, impedance, conductivity) in a wide range of frequencies ( $3 \times 10^{-1} - 1 \times 10^7$  Hz) and temperatures ( $-40 -$

$-200^{\circ}\text{C}$ ) have been studied. It is shown the influence of the structure on characteristics of the EPTP. The same content of the protons in every system (the protons source is 1% of the PTA in the reactive mixture) gives different level of conductivity depending on chemical nature of the ER and solvent (water) content in the reactive mixture. It is provided with the different activation energy of the protons moving within the epoxy matrix with different chain structure.

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## **BUFFET**

### SALADS

tender bitter lettuce with house topping  
tomatoes and Mozzarella with pesto  
salad with cucumber, tomato and pepper with cheese  
homemade salads of the season  
filled eggs with salmon caviar and cream

### SEVERAL COLD DISHES

chicken breast with exotic fruits  
variation of smoked fish with creamed horseradish  
seasonal potpourri prepared according to traditional recipes  
hot tartar with gherkins

### WARM DISHES

tomatoes soup with croutons and fresh herbs  
medallions of chicken  
with vegetable, mushrooms and potatoes potato pancake  
roasted fillet of fish with vegetables and rice  
gratin of tomato and spinach on noodle and backed with mozzarella

### SELECTION OF LOCAL CHEESE

with different kinds of bread and rolls, butter

### DESSERTS

cocktail of delicious fruits  
different varieties of homemade cakes  
red fruit jelly with vanilla cream  
white and dark chocolate mousse

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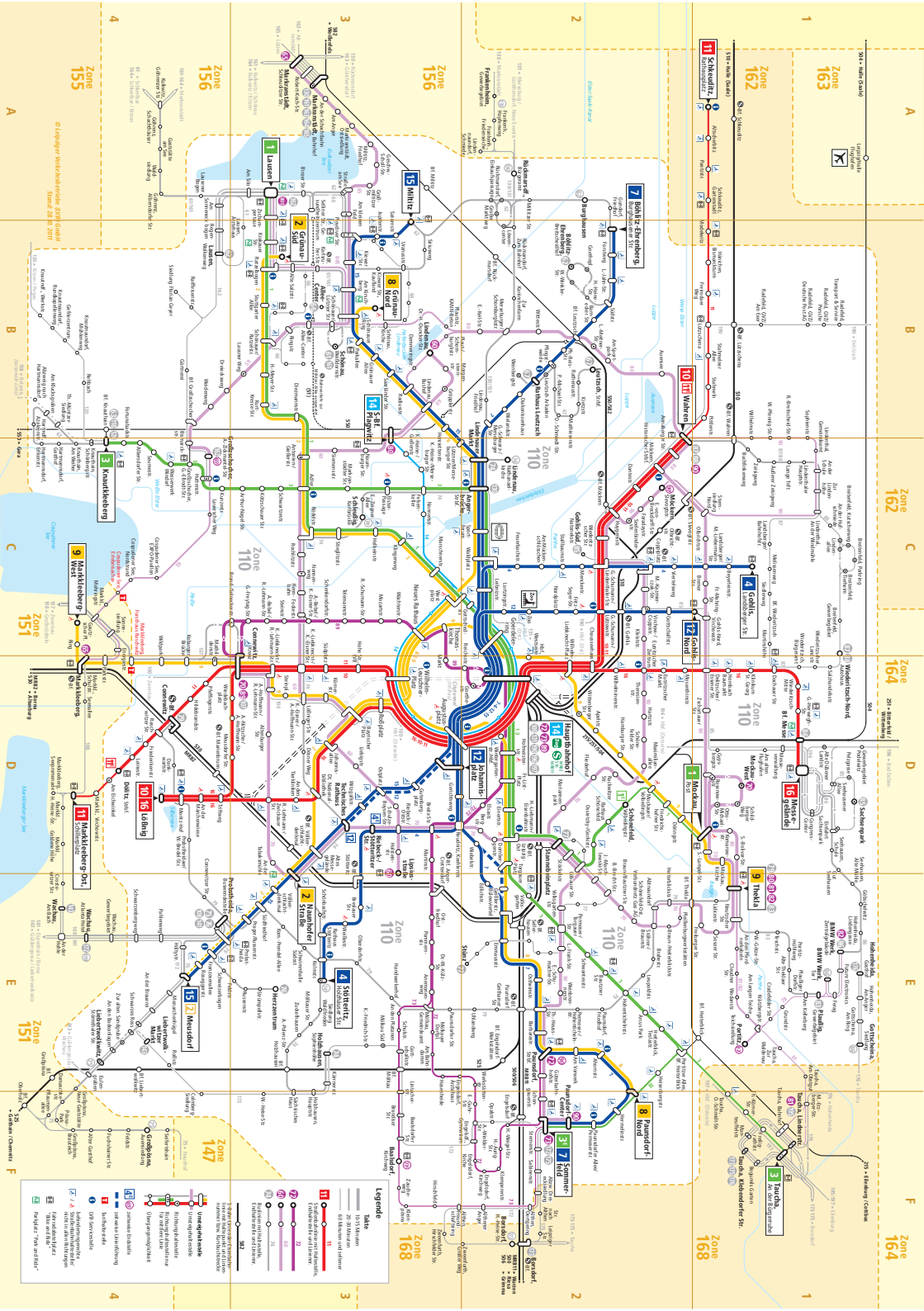
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**Legende**

**Linien**

- S-Bahn
- Tram
- Bus
- Bus Rapid Transit
- Seilbahn
- Fähre
- Fahrrad

**Stationen**

- S-Bahn-Station
- Tram-Station
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- Fähre-Station
- Fahrrad-Station

**Liniennummern**

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**Linienfarben**

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