restricted Hartree Fock closed- shell wave function. The minimizations were terminated at r. m. s. gradient of less than 0.01 KJ-mol^{-1} Å^{-1}. The optimized geometry of the structure displays significant change in the orientation of thiophene rings thereby resulting participation of such rings in the C-H…O and C-H… π interactions. The Semi-empirical Quantum Chemical C alculations were also performed on the analogous structure that has the substitution of two thiophene rings at position 2 to pentadiene moiety and these results will be compared with the present one and their detailed analysis will be presented later.

Keywords: bis-chalcones, hydrogen bond interactions and MOPAC 2009

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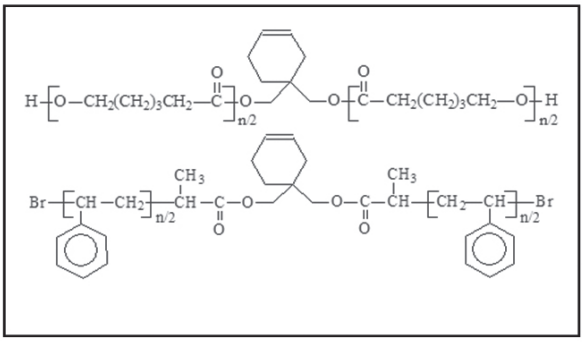
Characterization of some di-block copolymers and investigation of their temperature-dependent structural behaviors

Ilghar Orujalipoor,[a] Caner Tükel,[b] Ömer Çelik,[c] Semra İde,[d] Nasrettin Genli,[e] Mustafa Değirmenci,[f] *[a]Hacettepe Univ., Dept. of Nanotechnology and Nanomedicine, Ankara (Turkey). [b]Hacettepe Univ., Dept. of Nanotechnology and Nanomedicine, Ankara (Turkey). [c]Dicle Univ., Dept. of Physics, Diyarbakir (Turkey). [d]Hacettepe Univ. Dept. of Physics Engineering, Ankara (Turkey). [e]Harran Univ., Dept. of Chemistry, Şanlıurfa(Turkey). [f]Harran Univ., Dept. of Chemistry, Şanlıurfa (Turkey).* E-mail: ilghar.orujalipoor@gmail.com

The synthesis and characterization of novel polymeric materials is crucially important for new scientific researches and technological applications. The present research is focused on Cyclohexene Mid-Chain polymers containing polystyrene (PS) and [Poly(ε- Caprolactone)] (PCL) functional groups. These polymers, because of their easily crystallization feature, can make some blends with other polymers, that have a wide technological utilization field [1]. The usage of an apolar aliphatic polyester [Poly(ε- Caprolactone)] and polystyrene which has a low melting point can cause radical polymerization controlling with light and cationic polymerization. Thus, molecular weight of the polymer and end-groups of the polymer chains can be also controlled. So, the physical properties of the polymers can be changed by adding different functional end groups (such as PS and PCL) to the Cyclohexene Mid-Chain.

In the present work, X-Ray diffraction (XRD) and X-Ray scattering methods (SAXS and WAXS) have been used to characterize these type polymeric structures (Figure 1.) in solid and solution forms. On the other hand, because of their big importance in living radical polymerization, thermo response behaviors of the novel synthesized polymers (in solution form) have been also examined.



[1] G.C. Eastmond *Adv. Poly. Sci.* **2000**, *149.*

Keywords: SAXS, WAXS, copolymer

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A SAXS Study of an enzyme-reponsive self-assembling polymer/ peptide conjugate

Ian W Hamley, Valeria Castel*)*letto, *Department of Chemistry, University of Reading, Whiteknights, Reading RG6 6AD, (UK).* E-mail: I.W.Hamley@reading.ac.uk

Enzyme-responsive biopolymer systems are attracting considerable interest for applications in biocatalysis, drug delivery, tissue scaffolding and other applications. Recent work in our group led to the development of an enzyme-responsive nanocontainer delivery and release system [1].

The micelles are formed by PEG/peptide conjugates comprising a core of amyloid peptide βAβAKLVFF. This peptide has been the subject of recent investigation by our group, having interesting self-assembly properties [2] and the potential to develop amyloid inhibition systems with therapeutic applications [3]. In the PEG/peptide construct, the polymer-peptide linkage is selectively cleaved using the model enzyme α-chymotrypsin which cleaves between phenylalanine (F) residues. This produces products βAβAKLVF and F-PEG3000 (PEG with molar mass of 3 kDa). Remarkably, the product βAβAKLVF was found not to aggregate into amyloid fibrils, in contrast to the parent peptide βAβAKLVFF, pointing to the importance of aromatic interactions and the presence of two phenylalanine residues in driving self-assembly. The relase of unassociated non-amyloid peptide may be useful in applications.

The release of the peptide from the PEGylated nanocontainer delivery system upon enzymatic cleavage was studied by mass spectrometry, circular dichroism, SAXS, TEM (including cryo-TEM) and FTIR spectroscopy. These materials are under further study as bio-responsive self-assembling systems, with potential applications in detection and delivery.

[1] V. Castelletto, J.M.E. McKendrick, I.W. Hamley, C. Cenker, U. Olsson, *Langmuir* **2010,** *26*, 11624. [2] V. Castelletto, I.W. Hamley, R.A. Hule, D.J. Pochan, *Angew. Chem., Int. Ed. Engl.* **2009,** *48*, 2317. [3] V. Castelletto, I.W. Hamley , T. Lim, M. de Tullio, E.M. Castano, *J. Pept. Sci.* **2010,** *16*, 443.

Keywords: peptide, enzyme, SAXS

MS04.P02

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Characterization by SAXS of lignin from modified straw and bagasse sugarcane

Priscila Maziero,[a] Mario de Oliveira Neto,[b] Aldo Felix Craievich,[c] Igor Polikarpov,[b] Adilson Roberto Gonçalves,[a] *[a]Engineering School of Lorena. [b]Institute of Physics of São Carlos. [c]Institute of Physics of São Paulo. University of São Paulo, Brazil.* E-mail: priscila.maziero@debiq.eel.usp.br

A biorefinery deals with process of converting biomass like bagasse and straw sugarcane into a variety of products [1]. Different useful products derived from sugarcane bagasse and straw can be obtained via separation process of hemicellulose, cellulose and lignin matrix [2]. Separation processes consists of a pretreatment that removes hemicellulose and the remaining product is submitted to a delignification procedure leading to a final product composed of pure lignin. Lignin can be modified for generation of a variety of novel and useful chemical agents and substances.

A standardized lignin for industrial applications is required to minimize the costs of reagents and processing power. In this work the effects of different pretreatment and delignification processes

on the structural features of lignin obtained from straw and bagasse sugarcane were studied using synchrotron small angle X-ray scattering (SAXS). Bagasse and straw were pretreated under three different types of pretretament -hidrothermal, diluted acid and steam explosion. The delignification was carried out by means of either soda pulping or soda/antraquinone processes. Our SAXS study was performed for aqueous solutions containing 5 mg/mL of lignin using the SAXS1 beamline of the Synchrotron Light Laboratory (LNLS), Campinas, Brazil. Data treatment was carried out by using Beaucage model for two structural levels [3].

SAXS results revealed that dilute solutions of both lignins, from bagasse and from straw, are composed of a mixture of colloidal nanoparticles and aggregates. It was observed that the aggregates in solutions of lignins from straw are in general larger than those of lignin from bagasse. The nature of the assymptotic behavior of SAXS curves at high angles allowed us to conclude that, under similar pretreatment and delignification processes, lignin aggregates from straw exhibits a fractal external surface while aggregates of lignin from bagasse shows a mass fractal structure. Our SAXS results also indicated that the diluted acid pretretament promotes a higher fragmentation of the aggregates of lignin from bagasse.

Lignins obtained from steam explosion pretreatment under different conditions of temperature do not exhibit significant changes in the fragmentation effect on aggregates and colloidal particles. The main difference regards the nature of the fractal structure, the aggregates corresponding to lignin pretreated under severe steam explosion exhibiting a fractal surface while those of lignin pretreated under softer conditions a mass fractal structure. SAXS results also indicated that delignification by means of the soda/antraquinone process promotes a lower fragmentation of the aggregates than the process of soda delignification.

Industrial applications as dispersing agent in textile segment or wastewater treatment require the use of highly fragmented lignin. Our SAXS results suggest that lignin produced by acid diluted pretreatment followed by soda pulping delignification would promote a higher yield in industrial processes.

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[1] *NREL Biomass Research*:http://www.nrel.gov/biomass/biorefinery.htm [2] D. Fengel, G. Wegener, *Wood Chemistry, Ultrastructure, reactions*,Walter de Gruyter, Berlin. **1989** [3] G. Beaucage, T.A. Ulibari, E.P. Black , D.W. Schaefer; *Hybrids Organic-Inorganic Composites* **1995,** *585,* 97-111.

Keywords: characterization, lignin, SAXS

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GISAXS with nanoparticles on liquids and with multilayer films on a lab source

Joerg Wiesmann,[a] Bernd Hasse,[a] Carsten Michaelsen,[a] Peter Siffalovic,[b] Karol Vegso,[b] Eva Majkova,[b] Jozef Keckes,[c] Günther Maier,[d] *[a]Incoatec GmbH, Geesthacht (Germany). [b]Inst. of Physics, Slovak Academy of Science, Bratislava (Slovakia). [c]Erich Schmid Inst. of Materials Science, Leoben (Austria). [d]Materials Center, Leoben (Austria).* E-mail: wiesmann@incoatec.de

The method of small angle x-ray scattering enables the investigation of materials in the nanometer scale. It is used for mesoscopic structures like colloids, partially crystalline polymers and other soft-matter samples. For a long time SAXS was mainly developed and used at synchrotrons due to the lack of high brilliance lab-sources. With the introduction of microfocus X-ray sources with high flux densities and low divergence many of useful experiments are now also feasible in the lab-environment, even GISAXS (grazing-incidence SAXS).

In this contribution we show several SAXS measurements with our high brilliance microfocus source IμS for Cu radiation. The beam was collimated with a divergence of only 1mrad and a size of about 0.5mm. The IμS was compared with conventional sealed tubes by measuring standard samples like silver behenate. Multilayer structures of thin films, which were manufactured with different techniques like e-beam evaporation and magnetron sputtering, were investigated with GISAXS in the home-lab and for a comparison at a dedicated synchrotron beamline. Nanoparticles on a liquid sample were investigated with a special GISAXS setup with an IμS and a Pilatus pixel detector. Ordering phenomena could be observed in-situ during an increase of surface pressure. The particles were transformed from single islands to an almost vertically ordered structure of connecting particles.

Keywords: multilayer, SAXS, nanoparticles

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SAXS and SANS for the better understanding of polymer processing.

Yoshinobu Nozue,[a] Mitsuhiro Shibayama,[b] Edward B. Coughlin,[c] Julia A. Kornfield,[d] *[a]Petrochemicals Research Laboratory, Sumitomo Chemical Co., Ltd. [b]Institute of Solid State Physics, The Univ. of Tokyo. [c]Department of Polymer Science and Engineering, Univ. of Massachusetts. [d]Division of Chemistry and Chemical Engineering, Caltech.* E-mail: nozue@sc.sumitomo-chem.co.jp

The deeper understanding of the deformation and crystallization behavior of polymer under flow is needed for the better polymer design in industries and we have focused on the researches about polymer deformation. In this talk, we will mainly discuss 'shish-kebab', a highly oriented crystal structure having an excellent mechanical property. We have clarified the role of each molecular weight component of polymer on the formation of shish-kebab structure. Previously, it was believed that the shish is mainly formed by long chains, which is necessary for the effective shish-kebab formation. However, through SANS measurement, it was found that the long chains are not the main component of shish itself and the role of long chains is to recruit surrounding chains into shish [1]. Furthermore, we have found the novel methodology for the effective shish-kebab formation using not long chains but the interaction between inorganic particles. By synchrotron SAXS and WAXD, we observed the shish-kebab formation behavior of polymers copolymerized with inorganic particles during melt drawing and clarified that the shish-kebab formation can be accelerated by controlling the degree of interaction between particles.

[1] S. Kimata, S. Sakurai, Y. Nozue, T. Kasahara, N. Yamaguchi, T. Karino, M. Shibayama, J.A. Kornfield *Science* **2007**, *316,* 1014-1017.

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More possibilities of membrane permeation for antimicrobial peptides investigated with biophysical methods

Kuo-Long Lou,[a,b,e] Jia-Nan Jian,[a,f] Po-Tsang Huang,[b,f] San-Tai Shen,[a] Meng-Hsuan Hsieh,[a] U-Ser Jeng,[c] Huey W. Huang,[d] Ming-Tao Lee,[c] *[a]Graduate Institute of Oral Biology, National Taiwan University, Taipei, (Taiwan). [b]Institute of Biochemistry and Molecular Biology, National Taiwan University, Taipei, (Taiwan). [c]National Synchrotron Radiation Research Center, Hsinchu, (Taiwan).*