TURKISH CHEMICAL SOCIETY

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IUPAC

International Union of Pure and Applied Chemistry

Bridging Continents & Bridging Molecules

MACRO 2016

World Polymer Congress Istanbul 17-21 July

46th IUPAC WORLD POLYMER CONGRESS

July 17-21, 2016 / Istanbul / Turkey

Halic Congress Center

BOOK OF ABSTRACTS

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Scientific Sessions

1 - Recent Developments in Polymer Synthesis

a) Controlled/Living Polymerization
Co-organizer: Prof. Masami Kamigaito
Coordinator: Prof. Remzi Becer

b) Complex Macromolecular Structures
Co-organizer: Prof. Filip Du Prez
Coordinator: Assoc. Prof. Amitav Sanyal

c) Light-induced Reactions in Polymer Science
Co-organizer: Prof. Xavier Allonas
Coordinator: Assoc. Prof. Binnur Aydogan Temel

d- Condensation Polymerization and Thermoset
Co-organizer: Prof. Tsutomu Yokozawa
Coordinator: Assoc. Prof. Baris Kiskan

2 - Polymer Characterization by New and Combined Techniques
Co-organizer: Prof. Michael Hess
Coordinator: Prof. Levent Demirel

3 - Macromolecules & Nanotechnology
Co-organizer: Prof. Gyula Julius Vancso
Coordinator: Assoc. Prof. Tamer Uyar

4 - Macromolecules in Biotechnology & Medicine
Co-organizer: Prof. Martina Stenzel
Coordinator: Asst. Prof. Muhammet Kahveci

5 - Energy, Optics, & Optoelectronics
Co-organizer: Prof. Levent Toppare
Coordinator: Assoc. Prof. Ali Çırpan

6 - Polymer and Polymer-Based Membranes
Co-organizer: Prof. S. Birgul Tantekin-Ersolmaz
Coordinator: Assoc. Prof. Tuba Erdogan Bedri

7 - Smart and Functional Polymers
Co-organizer: Prof. Richard Hoogenboom
Coordinator: Prof. Faruk Yilmaz

8 - Renewable Resources and Biopolymers
Co-organizer: Prof. Henri Cramail
Coordinator: Assoc. Prof. Huseyin Esen

9 - Polymer Engineering, Processing, and Characterization
Co-organizer: Prof. Mukerrem Cakmak
Coordinator: Assoc. Prof. Ali Durmus

10 - Polymer Physics
Co-organizers: Prof. Dimitris Vlassopoulos and Kurt Kremer
Coordinator: Asst. Prof. Deniz Ceylan Tuncaboylu

11 - Polymer Education
Co-organizers: Prof. Christopher Ober and Patrick Theato
Coordinator: Assoc. Prof. Mustafa Sözbilir

12 - Industrial Polymers
Co-organizer: Dr. Johan-FGA Jansen (DSM)
Coordinator: Asst. Prof. Huseyin Esen

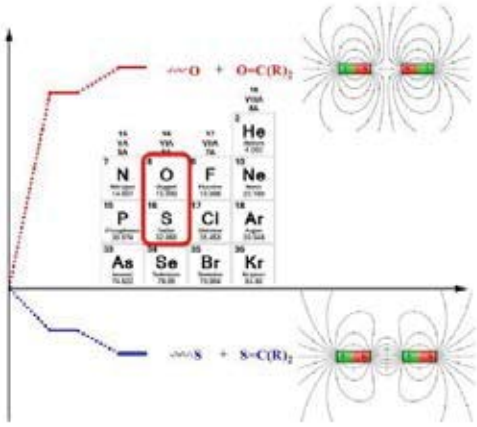
13 - Porous Polymer and Gels
Co-organizer: Prof. Michael S. Silverstein
Coordinator: Prof. Ali Tuncel

14 - Modeling and Simulation of Polymers
Co-organizer: Prof. Stefano Valdo Meille
Coordinator: Assoc. Prof. Nurcan Tuzun

based on thiruam disulfides.

Keywords: Self-healing polymers, radical thiol-ene reactions, quantum chemical calculations, G3(MP2)-RAD method

Reaction profile for the addition of thiyl radicals to thioketones and alkoxyl radicals to ketones



MSP-O-008 [Modeling and Simulation of Polymers]

Study on the physics of polymer crystallization based on the rod-coil multi-blocks chain model

Ping Tang, Faqiang Liu, Hongdong Zhang, Feng Qiu, Yuliang Yang

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Only considering the long-chain characteristics of polymers can we understand the physics behind polymer crystallization. We aims to construct the microscopic molecular theory to describe polymer crystallization based on the more accurate chain model, which can both consider the long-chain conformation entropy and the segment orientation. By developing the self-consistent field theory for multi-block rod-coil copolymers as a model system, we can investigate the effect of chain structure such as the comonomer composition, comonomer sequence (such as polyolefins) on the crystallization degree and crystal structures. We also expect to simulate the chain folding mechanism to compare with the phenomenological crystallization model. The developed work will be helpful to understand the physical mechanism and essence of polymer crystallization and to guide the design of crystal structures.

Keywords: polymer crystallization, rod-coil multiblocks chain model, self-consistent field theory, chain folding

MSP-O-007 [Modeling and Simulation of Polymers]

Determining and modelling polymer crystal structures: the perspective of a polymer crystallographer

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From its very beginnings, polymer crystallography has been extensively interrelated with molecular and crystal modelling. The relationship has never been unidirectional, as the two fields have substantially benefitted from the respective developments. Specifically, detailed molecular models have been and still are very often a prerequisite to solve polymer crystal structures. As the quality and the reliability of molecular models is increasing, so does their role in polymer crystallography. On the other hand experimental crystal structures, lattices and symmetries, not to speak of crystal morphologies and their evolutions represent essential testing grounds of modelling abilities. They can still hardly be predicted from molecular data, but rationalization of properties and of structural developments from known arrangements, is becoming on the other hand increasingly viable. Polymer crystal structures, as compared to low molecular mass structures, present often unique properties related to the unique features of polymer chains for which intramolecular properties tend to play a more significant role. Also the small size and the inherent anisotropy of crystals, the extensive role of disorder, the stability of mesophases, often dependent on molecular masses, the role of conformational chirality and of chain directionality in determining packing of chains, are very different than in low molar mass materials. In the present communication selected recent examples in the fields of conjugated polymers but also of more traditional polyolefins will be reported and discussed, especially with reference to the significance of so called "limited ordered" models and to the treatment of disorder in crystallographic and in modelling perspectives.

A. Buono, G. Raos, S. V. Meille et al.: Macromolecules, 43, 6772 (2010).
A. Buono, A. Famulari, S. V. Meille et al. Macromolecules, 44, 3681 (2011).
A. Famulari, S. V. Meille et al. J. Phys. Chem. B, 116, 14504 (2012)

Keywords: crystal structures, modelling, simulation

MSP-O-009 [Modeling and Simulation of Polymers]

Crystallization of Double Crystalline Binary Polymer Blends

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Polymer blends are known to be one of the exciting materials to prepare nanoscale devices via self-assembly. The thermodynamic and mechanical properties largely depend on their mutual miscibility. Miscible blends usually give a single glass transition temperature, whereas immiscible blends produce two distinct glass transition temperatures. Since the components in the blend are chemically dissimilar they phase separate via macrophase separation. We report dynamic Monte Carlo simulation results on the crystallization of A/B binary polymer blends with varying composition, wherein both the components are crystallizable. We model A-polymer as high melting component and hence its crystallization precedes the crystallization of B-polymer upon cooling from a homogeneous melt. The morphological development is controlled by the interplay between crystallization driving force (attractive) and de-mixing energy (repulsive) between the components. With increasing the composition of B-polymer, macrophase separation, crystallization and lamellar thickness follow a non-monotonic trend. This non-monotonic trend is attributed to the composition-heterogeneity in the blend. When one component is relatively less compared to the other, its mobility is reduced affecting transition temperature during crystallization. As a result, transition happens at a relatively lower temperature (viz., enhanced thermal driving force). Isothermal crystallization reveals that the crystallization behavior and crystal morphology strongly depends on the mode of cooling. Two-step, compared to on-step isothermal crystallization provides better crystalline structures.

Keywords: Binary blend, Crystallization, Monte Carlo Simulation