高分子物理学セミナー2013

日時：2013 年 5 月 14 日（火）　15:00 – 17:00

場所：化学研究所 5 階会議室 (N-531C)

主催：京都大学化学研究所 化学関連分野の深化・連携を基軸とする先端・学際研究拠点

共催：日本レオロジー学会関西レオロジー研究会

講師：Professor Dimitris Vlassopoulos

IESL-FORTH and Department of Materials Science and Technology, University of Crete, Heraklion, Crete, Greece

演題：Entanglement dynamics in ring polymers: Recent progress and open challenges

講師：Professor Ralph Colby

Department of Materials Science and Engineering and Chemical Engineering, Pennsylvania State University, University Park, PA, USA)

演題：Ionomer Design, Synthesis and Characterization for Ion-Conducting Energy Materials

高分子物理学分野で世界の研究を主導している Vlassopoulos 教授、Colby 教授が、日本レオロジー学会 40 周年記念にあわせて来日されます。この機会に、上記の最先端の研究成果についてセミナーを開催致します。奮ってご参加下さい。

連絡先：分子レオロジー研究領域　渡辺宏 (内 3135)

Entanglement dynamics in ring polymers: Recent progress and open challenges

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Rings represent a unique class of architecturally complex polymers. Their detailed structure and dynamics have been the subject of debates for three decades. Yes understanding their response is one of the remaining grand challenges in polymer physics and molecular rheology, with implications in biological functions and microprocessing. In this presentation we briefuly review the field with emphasis on the rheology of entangled rings. We discuss the main issues and earlier controversies and then present recent progress and the current state-of-the-art from the standpoint of experiments, modeling and simulations. Particular emphasis is given in the interaction of linear (unlinked) chains and rings (linked chains), which is believed to be of central importance, while we also address the problem of concatenation. Finally, we outline the key open issues in the field.

This work is part of a huge international effort involving the groups of Jülich (A. Bras, A. Wischnewski, W. Pyckhout-Hintzen, J. Allgaeir, D. Richter), Athens/KAUST (G. Sakellariou, N. Hadjichristidis), Pohang (Y. C. Yeong, T. Chang), North Carolina (M. Rubinstein) and Crete (R. Pasquino, D. Vlassopoulos). It is supported in part by the EU (Dynacop) and GGSRT (Aristeia).

Ionomer Design, Synthesis and Characterization for Ion-Conducting Energy Materials

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For ionic actuators and battery separators, it is vital to utilize single-ion conductors that avoid the detrimental polarization of other ions; the commonly studied dual-ion conductors simply will not be used in the next generation of materials for these applications. *Ab initio* quantum chemistry calculations at 0 K in vacuum characterize ion interactions and ion solvation by various functional groups, allowing identification of constituents with weak interactions to be incorporated in ionomers for facile ion transport. Simple ideas for estimating the ion interactions and solvation at practical temperatures and dielectric constants are presented that indicate the rank ordering observed at 0 K in vacuum should be preserved. Hence, such *ab initio* calculations are useful for screening the plethora of combinations of polymer-ion, counterion and polar functional groups, to decide which are worthy of synthesis for new ionomers. Single-ion conducting ionomers are synthesized based on these calculations, with low glass transition temperatures (facile dynamics) to prepare ion-conducting membranes for ionic actuators and battery separators. Characterization by X-ray scattering, dielectric spectroscopy, NMR and linear viscoelasticity collectively develop a coherent picture of ionic aggregation and both counterion and polymer dynamics. Examples are shown of how *ab initio* calculations can be used to understand experimental observations of dielectric constant, glass transition temperature and conductivity of polymerized ionic liquids with counterions being either lithium, sodium, fluoride, hydroxide (for batteries) or bulky ionic liquids (for ionic actuators).