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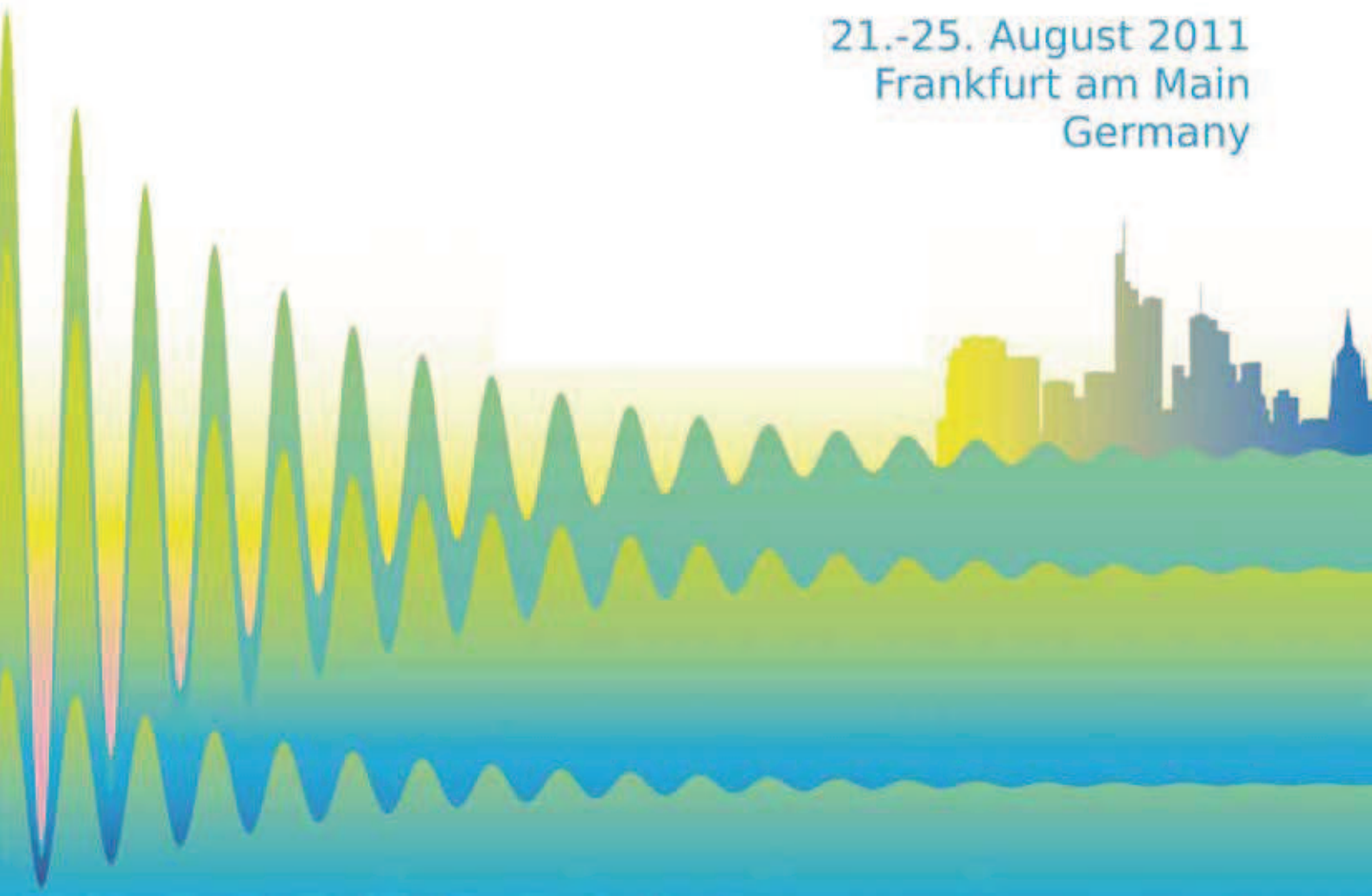

Ss624

Molecular Dynamics of F8BT Polymer Film: Correlation with Opto-Electronic Properties

Gregório C. Faria[1,2], Roberto M. Faria[1], Heinz von Seggern[2] and Eduardo R. deAzevêdo[1]

[1]*Instituto de Física de São Carlos, Universidade de São Paulo, SP, Brazil;* [2]*Technischen Universität Darmstadt, Darmstadt, Germany.*

Poly(9,9 '-dioctylfluorene-*co*-benzothiadiazole) (F8BT) is currently one of the most promising material for use as active layers in polymeric electronic devices, such as polymer light-emitting diodes (PLEDs) and polymer field effect transistor (P-FET). It is well known that both polymer structure and dynamics affects either the luminescence or transport properties in thin films, making worthwhile to investigate them. Dynamical aspects of F8BT were first investigated by Dynamical Mechanical Thermal Analysis (DMTA), Differential Scanning Calorimetry (DSC) and ^{1}H Nuclear Magnetic Resonance (NMR). The results revealed the presence of two main relaxation process, which occurs at about 225 K (β-relaxation) and 370 K (α -relaxation). The molecular processes responsible by such relaxations were investigated by specific NMR experiments, such as Dipolar Chemical Shift correlation (DIPSHIT) and Centerband Only Detection of Exchange (CODEX). The results showed that, in the temperature range of 220 to 373 K, the lateral chain execute molecular rotations with average correlation times ranging from 10^{-4} – 10^{-7} seconds. On the other hand, from 300 to 350K the backbone carbons execute slow libration motions with reorientation angles that increase as a function of temperature. Those results could be correlated with the Current-Voltage characteristics of thick ITO/F8BT/Al devices carried out a several temperature (70 until 490 K).The drift charge mobility in the device was studied as a function o temperature by Time of Flight techniques (TOF), showing relatively abrupt change on the activation energy near both relaxations (β and α). Based on these results, a model that explains the behavior of the charge transport as a function of temperature based on the occurrence of the molecular relaxation was proposed.

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Amplifying the effects of molecular motion in DIPSHIFT-like experiments

Márcio F. Cobo[1]; Eduardo R. deAzevedo[1]; Anja Achilles[2]; Detlef Reichert[2]; Kay Saalwachter[2]

[1] *Instituto de Física de São Carlos, Universidade de São Paulo, Brazil;* [2]*Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany).* marciofcobo@gmail.com

Dipolar Chemical Shift Correlation (DIPSHIFT)[1] is frequently used to study molecular motions by probing the reorientations through the modulation introduced in the dipolar CH coupling and T_2.[2] In systems where the coupling is weak or the reorientation angle is small, a variant of the DIPSHIFT experiment, where the effective dipolar coupling is amplified by a REDOR π - pulses train, is applied. However, the previously described experiment is not sensitive to the T_2 modulation introduced by the motion,[3] which avoid the observation of motions with rates ranging from hundreds of Hz to few kHz. We present a DIPSHIFT implementation which amplifies the dipolar couplings and is sensitive to T_2 effects. Spin dynamics simulations, analytical calculations and experiments demonstrate the sensitivity of the technique to molecular motions and the best experimental conditions to avoid imperfections. Furthermore, an in-depth analysis of the DIPSHIFT experiments was done, which allowed explaining the physical origin of many artifacts found in the literature data. We also show that in DIPSHIFT-like experiments, simple Lee-Goldburg homonuclear decoupling may perform as good as, or even better than, its more intricate variants, such as Frequency Switched and Phase Modulated Lee-Goldburg. To demonstrate the use of the technique, we show recent applications to membrane lipids

REFERENCES
1. Munowitz M., Griffin R. et al, *Journal of the American Chemical Society*, 103, 2529-2533 (**1981**)
2. deAzevedo E.R.; Saalwächter K. et al, *Journal of Chemical Physics.,*128, 104505 (**2008**)
3. Hong M.; Gross J. D. et al, *J.Mag. Res.,*129, 85-92 (**1997**)