up to 25 cm2/Vs at 150 K), whereas in TCNQ and F4-TCNQ FET the mobility is 0.1-0.2 cm2/Vs at room temperature and decreases upon cooling. Moreover, we performed a comparative analysis of the crystal and electronic structures for the three materials and found several aspects distinguishing F2-TCNQ: the primitive unit cell of F2-TCNQ crystals contains a single molecule so that all the molecules in crystal are oriented parallel to each other; the electronic structure of F2-TCNQ crystals is clearly three-dimensional and shows a very large band width. These properties are conducive to a more pronounced electron delocalization, which could account for the remarkable behavior of F2-TCNQ single-crystals FETs.

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14:45 **Non-contact, Non-destructive Probing of Charge Carrier Transport in Conductive Molecular Materials**

Authors : Shu Seki, Tsuneaki Sakurai, Akinori Saeki, and Daisuke Sakamaki
Affiliations : Department of Applied Chemistry, Osaka University Department of Molecular Engineering, Kyoto University

Resume : Understanding charge carrier transport processes at interfaces is one of the most important subjects in organic electronics. Charge carriers are injected or extracted through metal/semiconductor interfaces in most electronic devices, while carrier transport occurs at insulator/semiconductor interfaces rather than in the bulk in the major organic electronic devices.1,2 However, analytical techniques for evaluating such interfacial carrier transport phenomena are still limited, and this remains a challenging issue. We have recently reported a technique, referred to as time-resolved microwave conductivity (TRMC)3, and the system has been extended into field-induced TRMC that combines charge carrier injection via gate bias applied into working devices and microwave-based non-contact probing of intrinsic and local charge carrier motion. Using this technique, it was determined that a Au/pentacene/PMMA/SiO2/Au MIS device had hole and electron mobilities of 6.3 and 0.3 cm2V?1s?1, respectively.4,5 Non-contact, fully experimental evaluation of intra-domain carrier mobility at interfaces is quite unprecedented and is a characteristic feature of this system. In this paper, we further report that the FI-TRMC technique can distinguish between mobile charge carriers at the interface and immobile charges trapped at defects, thus enabling quantification of both the charge carrier mobility and the density of trap sites at insulator-semiconductor interfaces. References: 1) G. Horowitz an

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15:00 **Unraveling Charge Transport Over Multiple Length Scales in Supramolecular Fiber Transistors**

Authors : Emanuele Orgiu1, Jeffrey M. Mativetsky1, Ingo Lieberwirth2, Wojciech Pisula2, Paolo Samori1
Affiliations : 1Institut de Science et d'Ingénierie Supramoléculaires (I.S.I.S.), 8 allée Gaspard Monge, 67083, Strasbourg, France 2Max Planck Institute for Polymer Research, Ackermannweg 10, 55124 Mainz, Germany

Resume : Band-like transport of delocalized charge carriers over a few molecules has been previously observed in high quality vapor-grown crystals1. However, description of band-like transport in a solution-processed n-type semiconductor has been elusive1. The present work2 focuses on a N,N'-1H,1H-perfluorobutyl dicyanoperylenecarboxydiimide (PDIF-CN2) molecule and shows that crystalline order, attainable through solution-based self-assembly, and specific molecular orientation, resulting in reduced dipolar disorder, leads to transport via delocalized carriers, and enhanced mobility. These findings have been obtained by comparing the electrical performance of conventional spincoated organic transistors with transistors consisting of either single or multiple supramolecular fibers, while carefully considering the dependence of electrical transport on structure at multiple length scales. Despite an earlier report on apparent band-like behavior for a solution processed p-type semiconductor, we provide here the first example of measurable band-like transport from an air stable solution processed n-type semiconductor. Further, we observe that the activation energy Ea is strongly related to crystalline order, with spin-coated and fiber-based devices exhibiting two distinct transport mechanisms. References 1. N. A. Minder, S. Ono, Z. Chen, A. Facchetti, A. F. Morpurgo, Adv. Mater. 2009,19,1–9. 2. J. M. Mativetsky, E. Orgiu, I. Lieberwirth, W. Pisula, P. Samori Adv. Mater. 2014, 26, 430–435

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15:15 **Simulation of Charge Carrier Mobility in Organic Crystals**

Authors : Nenad Vukmirović
Affiliations : Scientific Computing Laboratory, Institute of Physics Belgrade, University

of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Resume : Despite a large interest in understanding the electrical transport properties of small molecule based organic crystals, there is still a lack of consensus about the proper framework for the calculation of charge carrier mobility in these materials. Band transport theory may be applicable only in the limit of small electron-phonon coupling, while Marcus theory is applicable in the limit of large electron-phonon coupling and large temperature. In this work, we present a theoretical framework and a computational scheme for the calculation of charge carrier mobility in small molecule based organic crystals. The first step of the approach is the calculation of band structure, phonon modes and electron-phonon coupling constants using density functional theory and density functional perturbation theory [1]. Next, these results are used to construct a tight-binding Hamiltonian with electron-phonon interaction in the basis of single molecule orbitals. Charge carrier spectral functions, lifetimes and mobility at different temperatures are then calculated from such a Hamiltonian. Application of the approach to the calculation of temperature dependence of charge carrier mobility in naphthalene crystal will be presented. [1] N. Vukmirović, C. Bruder, V. M. Stojanović, Phys. Rev. Lett. 109, 126407 (2012).

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15:30 **Coffee Break**

16:00 **PLENARY SESSION**

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