14:00 **Electronic properties of grain boundaries in polycrystalline naphthalene**

Authors : Marko Mladenovic, Nenad Vukmirovic, Igor Stankovic
Affiliations : Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Serbia

Resume : Thin films of small molecule based organic semiconductors have a polycrystalline form, which is composed of many different crystalline grains. It is currently well understood that grain boundaries are the most limiting intrinsic factor for efficient charge transport in these materials. However, there is still a lack of understanding of the specific mechanism by which grain boundaries affect the charge transport. In this work, we investigated the influence of grain boundaries on electronic properties of polycrystalline organic semiconductor naphthalene. Atomic structure of grain boundaries was found using a Monte Carlo method, while electronic structure calculations were performed using the density functional theory based charge patching method [1]. We found that grain boundaries introduce trap states within the band gap of the material. Our results show that spatial positions and energies of trap states can be predicted solely from geometrical arrangement of molecules near the boundary. Wave functions of these states are localized on closely spaced pairs of molecules from opposite sides of the boundary. The energies of trap states are strongly correlated with the distances between the molecules in the pair. These findings were used to calculate the electronic density of trap states, which was found to exhibit a qualitatively different behavior for grain boundaries perpendicular to the a and b direction. [1] N. Vukmirovic and L.-W. Wang, J. Chem. Phys. 128, 121102 (2008).

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14:00 **Semi-transparent electrodes for solid-state hybrid solar cells**

Authors : Konrad Wojciechowski, Henry J. Snaith
Affiliations : Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK; Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK

Resume : Solution processable transparent electrodes are required for flexible hybrid solar cells on metal foil, building-integrated semi-transparent photovoltaic windows on glass substrates or for top illumination in multi-junction architectures with a wide gap hybrid solar cell as a top cell. One of the most promising solutions is utilization of metal nanowires. Rough surface of the nanowire mesh and its susceptibility to detach from the substrate can be overcome by blending it with n-type or p-type materials, like metal oxide nanostructures or conducting polymers. Short-range charge transport in a semiconductor can be combined with long-range conductivity throughout the metal nanowire network resulting in efficient charge collection. Here we present an approach to nanowire based transparent electrodes, fabricated through a low-temperature process, employed in solid-state dye-sensitized and perovskite solar cells. We investigate the influence of the type of nanostructure material, its doping level and post-deposition treatment on conductivity of transparent electrodes and solar cell operation.

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14:00 **Component compositional dependence of methyl ammonium lead halide thin -film perovskite solar cells**

Authors : Mingzhen Liu, Michael Johnston and Henry J. Snaith
Affiliations : Clarendon Laboratory, University of Oxford

Resume : Perovskite solar cells have been achieved almost 11% efficiency by our group. We have showed that the perovskite, methylammonium lead iodide chloride (CH3NH3PbI2Cl), is a good absorber of light energy and also a good charge conductor by making the presence TiO2 redundant. The latest breakthrough in our group was making the perovskite solar cells from the use of mesoporous alumina as an inert scaffolds so that the electrons have to reside in and be transported through the perovskite for achieving the 11% efficiency cells. Because of the low-cost and intense absorptivity, we believe that perovskite solar cells have a very promising future. In order to investigate the optimal compositions of the materials, here we will present a study looking at the influence of the stoichiometry of MA to Pb to I and Cl in MAPbI3-xClx thin film perovskite solar cells. We focus on both the change in crystal structure, UV-vis absorption and solar cell operation. We observe a strong sensitivity on the precise composition and film thickness, but observe good solar cell operation with optimum conditions.

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