

## O 70: Invited talk (Nobuo Ueno)

Time: Thursday 15:00–15:45

Location: HE 101

## Invited Talk

O 70.1 Thu 15:00 HE 101

**First-principles experiment on electrical conductivity of organic devices with UPS: Charge delocalization, vibration coupling and band-gap states** — •NOBUO UENO — Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan

We will discuss following two topics, which are related to quantum mechanical/chemical studies of electrical conductivity in organic devices, by using UV photoelectron spectroscopy (UPS):

- (i) Energy band dispersion, electron-phonon coupling and polaron.
- (ii) Direct detection of very low density of electronic states in organic HOMO-LUMO gap.

As the electrical conductivity ( $\sigma$ ) is given by  $\sigma = ne\mu$ , where  $n$  is

the carrier concentration and  $e$  the charge and  $\mu$  the charge mobility, the topic (i) is a direct experimental study of  $\mu$  in molecular aggregates and in a molecule based on energy and momentum conservation rules, and the topic (ii) is related to study  $n$ , since  $n$  is related to the energy level alignment/the Fermi level position that must be controlled by unknown and undetectable electronic states in organic HOMO-LUMO gaps. The topic (ii) is thus related to elucidation of a well-known mystery; why do the transport types appear depending on molecules without impurity doping? In other words why does the Fermi level move in HOMO-LUMO gap? The mystery might be originated from a primary difference between organic semiconductors and their inorganic counter parts.