Electronic states in large-gap organic insulators: a first-principles study

Sandro Scandolo
The Abdus Salam ICTP
Trieste
Italy

ABSTRACT

Thanks to their insulating electrical properties and chemical inertness, large-gap organic insulators are widely used in applications. Polyethylene, a 9-eV gap polymer with -CH$_2$- repeat unit, is the material of choice for high-voltage cables, and alkane thin films are very promising as coating materials for microelectronic devices. In spite of their relevance, our knowledge of the microscopic processes involved in the transport and injection of carriers in these systems is still vague.

In this talk I will present results of first-principles simulations which indicate that in polyethylene the hole mobility is band-like, while excess electrons prefer to localise between chains and form polarons through the creation of conformational defects.

Moreover, polyethylene surfaces possess an empty surface states below the conduction band minimum, which might have a role in the ageing process. I will also show some preliminary results on the behavior of the tunneling current in alkane-thiols thin films on Au(111), as a function of the film thickness and of the tail group, which highlight the sensitivity of charge injection to the presence of surface dipole layers.