Surface states of organic crystals

Jaroslav Tóbkí, Andrea Dal Corso, Sandro Scandolo, Erio Tossati

1 SISSA, via Beirut 4, 34014 Trieste, Italy
2 INFM/F1 Postdoctoral Fellowship
3 INFM Democritos, via Beirut 2-4, 34014 Trieste, Italy
4 ICTP, strada Costiera 11, 34100 Trieste, Italy

Abstract:

Organics molecular crystals attract the attention of the physics community and of electronic industry as promising materials. So far their main problem - difficulty of doping, and small carrier mobility - has limited the interest of these materials, but there is significant research activity aimed at finding technological and physical conditions where those materials can operate with results comparable to conventional semiconductors. Because many of these materials have very small or negative electron affinities, the states of electrons near surfaces need to be particularly clarified. Moreover, in view of existing attempts at field doping, this is of particular interest in order to understand the electronic structure of their surfaces in an external electric field.

In this study we present ab-initio electronic structure calculations as well as model calculations for benzene and anthracene surfaces, first without and then with an electric field, ranging from weak to strong. The ab-initio calculations are conducted on thin slabs within density functional and with ultra-soft pseudopotential techniques. They show that at zero field the surface differs very little from the bulk, while for strong field they clarify the involvement of the surface in the screening process. Above a critical field partial electron transfer takes place from the negative to the positive face, mimicking electron and hole field-induced surface doping. The precise nature of the surface field doping level is then pursued for weaker, more realistic field strengths by means of model calculations in the semi-empirical effective mass approximation.