In2O3 surfaces: thermodynamic stability

Properties of TCO/organic interface

A few years ago the flat panel display market was dominated by Liquid Crystal Displays (LCDs). Recently, new display technology based on the organic light emitting diode (OLED) has emerged. Mobile displays based on OLEDs are already realized. Despite recent technological advances in display fabrication little is known about the TCO/organic interface and its role in the degradation processes of OLEDs.

Using first-principles calculations we addressed the following questions concerning TCO surfaces and TCO/organic interfaces:
- Structures and stabilities of the TCO surfaces?
- Influence of Sn-doping on surface stabilities?
- Structures and stabilities of the TCO surfaces?
- Nature of chemical bonds between TCO and organic molecules?

Results

In2O3 surfaces: thermodynamic stability

Benzenesorption on In2O3 surfaces: reaction paths

Chemical bonds: differential charge density

Method

Exchange correlation functional: Combination of GGA and van der Waals functional (opt) necessary to capture interaction of benzenewith surface

Mudged-elastic band (NEB) calculations for reaction barriers

In the first-principles calculations – bonding of benzene on indium oxide,

Arno Fey¹, Paul Erhart², Karsten Albe¹

¹Technische Universität Darmstadt, Fachgebiet Materialmodellierung, Darmstadt, Germany
²Chalmers University, Department of Applied Physics, Gothenburg, Sweden

Publications last funding period


5 key publications (2003-2014)