First-principles calculations – Bonding of benzene on indium oxide

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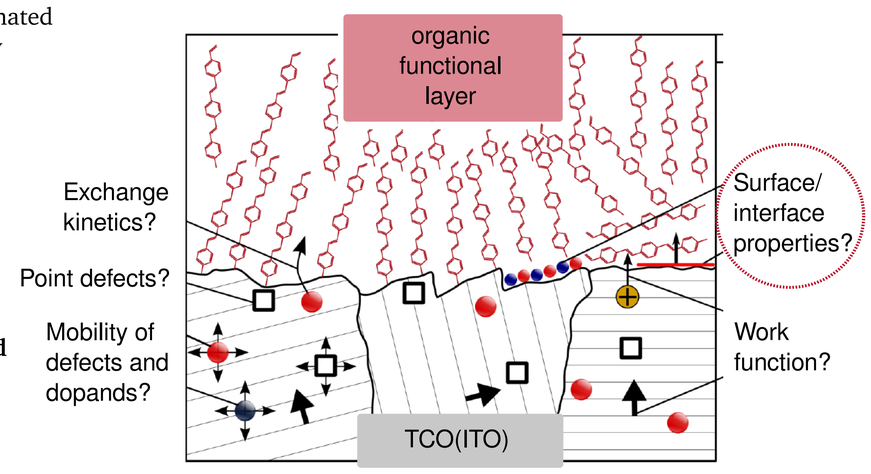
Project C2

Motivation

Properties of TCO/organic interface

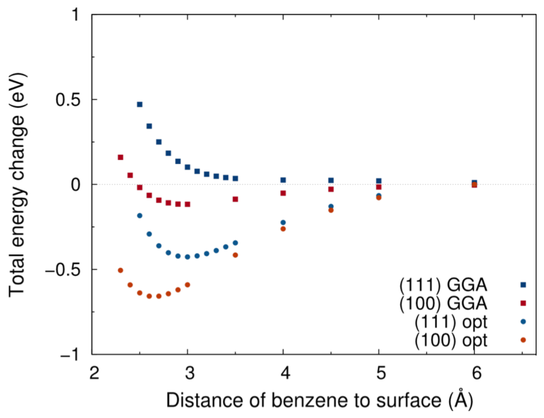
A few years ago the flat panel display market was dominated by Liquid Crystal Displays (LCDs). Recently, new display technology based on the organic light emitting diode (OLED) has emerged. Mobile displays based on OLEDs are already realized.
Despite recent technological advances in display fabrication 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?
- Energetics of adsorption and/or absorption process?
- Nature of chemical bonds between TCO and organic molecules?

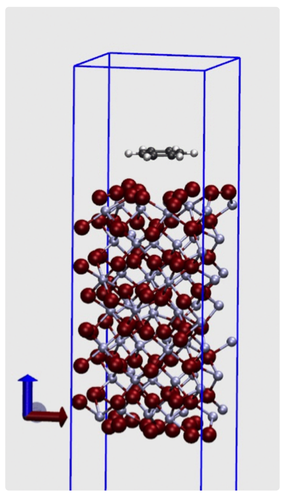


Method

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



Slab geometry for surfaces

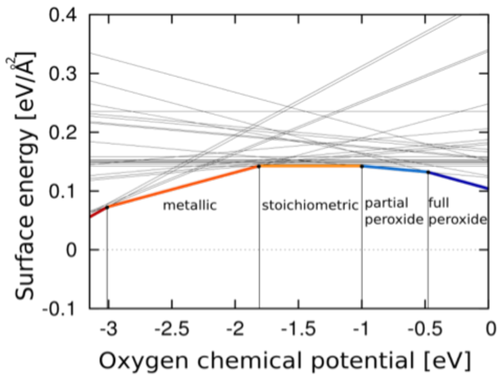


Nudged-elastic band (NEB) calculations for reaction barriers

Results

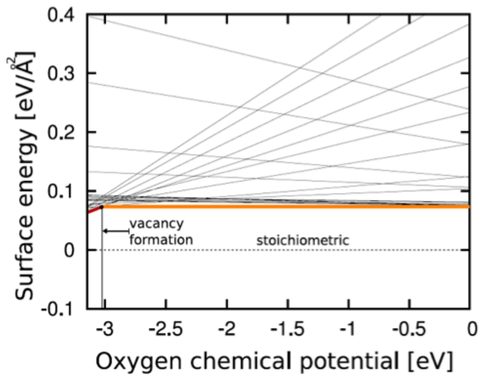
In_2O_3 surfaces: thermodynamic stability

(100) surfaces



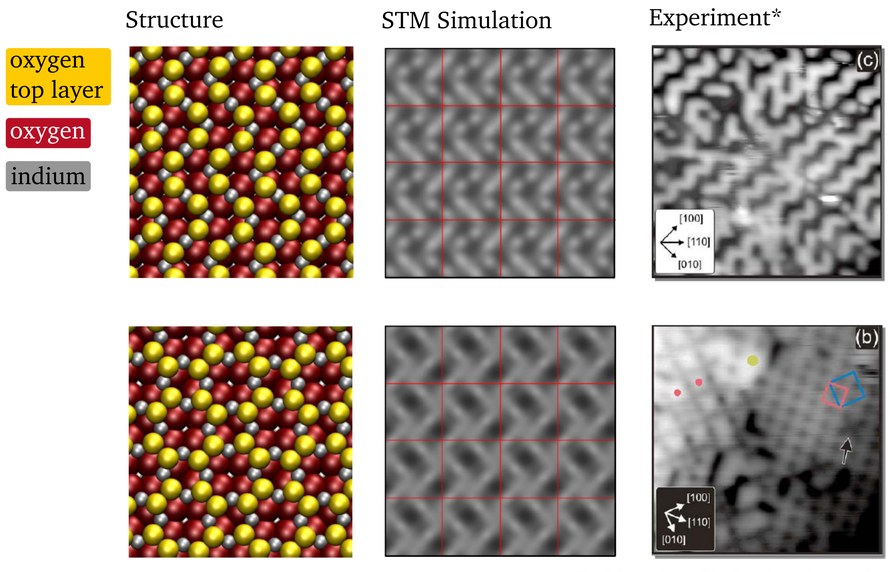
stoichiometry depends on oxygen chemical potential polar surfaces, **various surface phase transitions**

(111) surfaces



most stable surface, constant stoichiometry over large range of oxygen chemical potentials

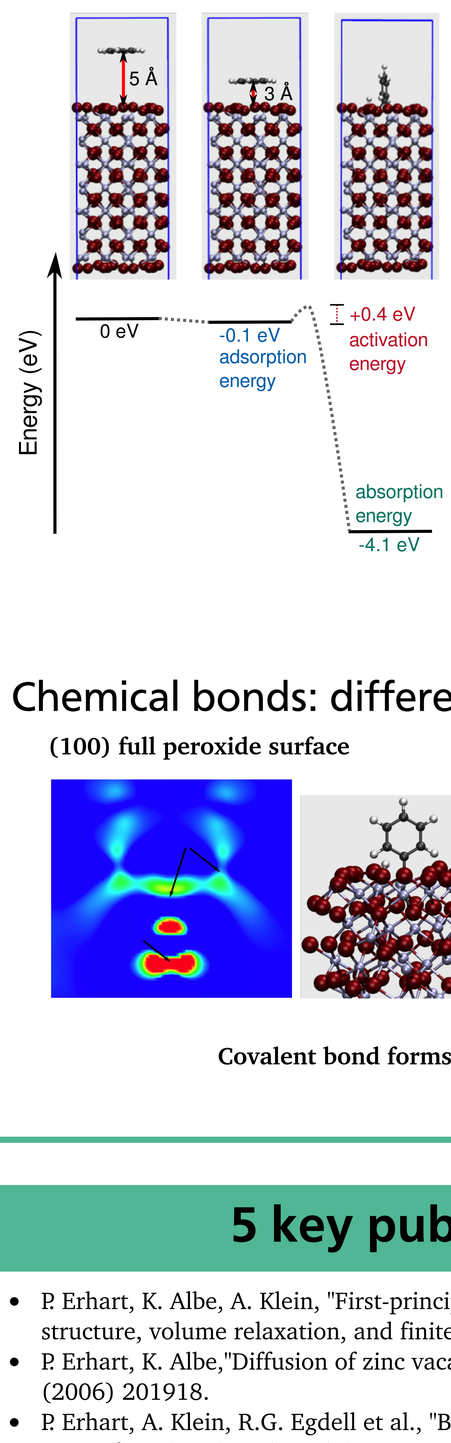
(100) surfaces of Sn-doped In_2O_3: simulation of STM images



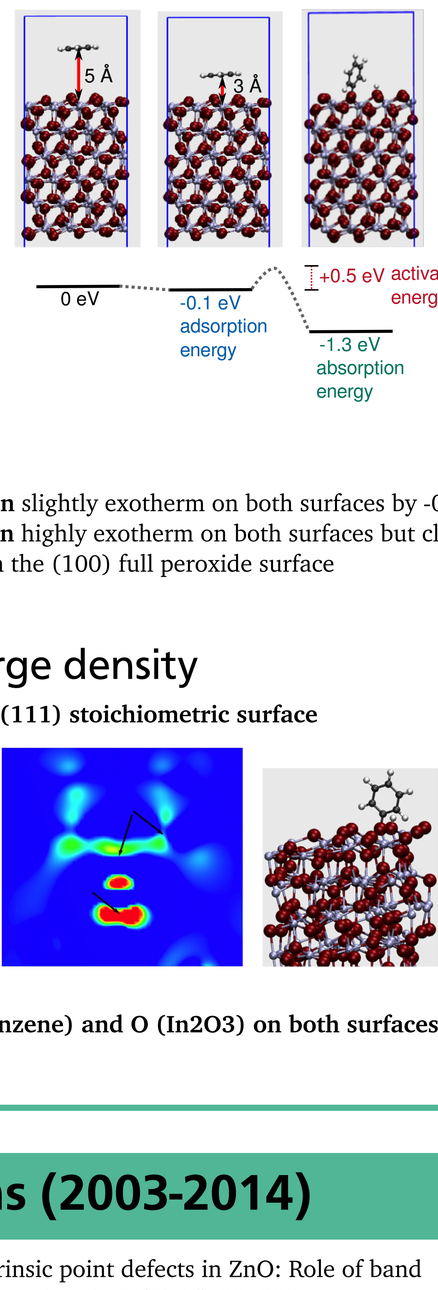
*E. Morales, U. Diebold, *Appl. Phys. Lett.* 139 (2009) 665-672.

Benzene absorption on In_2O_3 surfaces: reaction paths

(100) full peroxide surface



(111) stoichiometric surface



Adsorption slightly exotherm on both surfaces by -0.1 meV
Absorption highly exotherm on both surfaces but clearly favored on the (100) full peroxide surface

Chemical bonds: differential charge density

(100) full peroxide surface

(111) stoichiometric surface

Covalent bond forms between C (benzene) and O (In_2O_3) on both surfaces.

Publications last funding period

- P. Ágoston, K. Albe, "Thermodynamic stability, stoichiometry, and electronic structure of bcc-In_2O_3 surfaces", *Phys. Rev. B* 84 (2011) 045311.
- P. Ágoston, K. Albe, "Disordered reconstructions of the reduced SnO_2-(110) surface", *Surf. Sci.* 605 (2011) 714-722.
- P. Ágoston, K. Albe, R.M. Nieminen, M.J. Puska, "Reply: Comment on "Intrinsic n-type Behavior in Transparent Conducting Oxides: A Comparative Hybrid-Functional Study of In_2O_3, SnO_2 and ZnO", *Phys. Rev. Lett.* 106 (2011) 069602.
- C. Körber, A. Wachau, P. Ágoston et al., "Self-limited oxygen exchange kinetics at SnO2 surfaces", *Phys. Chem. Chem. Phys.* 13 (2011) 3223-3226.
- M.V. Hohmann, P. Ágoston, A. Wachau *et al.*,"Orientation dependent ionization potential of In2O3: a natural source for inhomogeneous barrier formation at electrode interfaces in organic electronics", *J. Phys.: Cond. Matter* 23 (2011) 334203.

5 key publications (2003-2014)

- P. Erhart, K. Albe, A. Klein, "First-principles study of intrinsic point defects in ZnO: Role of band structure, volume relaxation, and finite-size effects", *Phys. Rev. B* 73 (2006) 205203.
- P. Erhart, K. Albe,"Diffusion of zinc vacancies and interstitials in zinc oxide", *Appl. Phys. Lett.* 88 (2006) 201918.
- P. Erhart, A. Klein, R.G. Egdell et al., "Band structure of indium oxide: Indirect versus direct band gap", *Phys. Rev. B* 75 (2007) 153205.
- P. Ágoston, K. Albe, R.M. Nieminen, M. Risto et al. "Intrinsic n-Type Behavior in Transparent Conducting Oxides: A Comparative Hybrid-Functional Study of In_2O_3, SnO_2, and ZnO", *Phys. Rev. Lett.* 103 (2009) 245501.
- P. Ágoston, K. Albe, "Ab initio modeling of diffusion in indium oxide", *Phys. Rev. B* 81 (2010) 195205.