Pentacene on Epitaxial Graphene: XPS and NEXAFS Investigations

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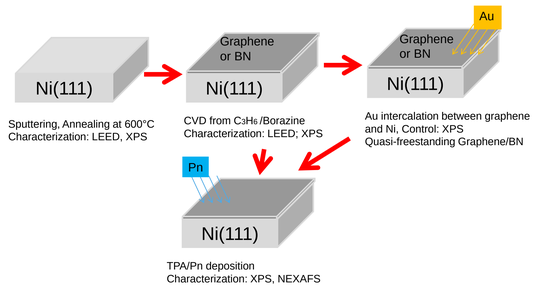
Motivation

Surface functionalization by self-assembly of organic ligands into 2d-networks is a method of growing interest for the development of functional, periodic nanometer-scale structures. Moreover, smooth interfaces are a prerequisite for future high-performance and low-cost organic electronic devices based on small conjugated molecules. Since all important charge transport processes are confined to the first several monolayers (ML), the quality of the first layer plays a key role on device performance. Pentacene ($C_{22}H_{14}$, Pn) stands out as a model molecule among organic semiconductors due to its ability to form well-ordered films showing a high field effect mobility. Moreover, the morphology of the first layer of a thin Pn film is known to be strongly influenced by the substrate termination, which further decisively affects the interfacial charge transport properties. Thus, information on the molecular orientation of pentacene in a case of (sub)monolayer coverages can provide a key information on improvement of device performance.

Sample preparation and layout of the experiment



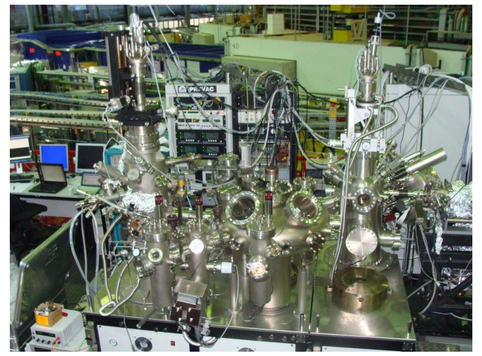
Sputtering, Annealing at 600°C
Characterization: LEED, XPS

CVD from C_3H_6 /Borazine
Characterization: LEED; XPS

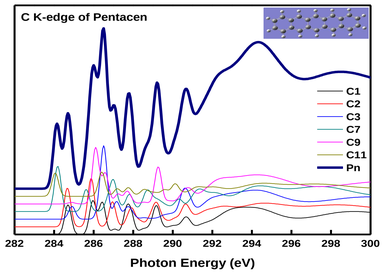
Au intercalation between graphene and Ni, Control: XPS
Quasi-freestanding Graphene/BN

TPA/Pn deposition
Characterization: XPS, NEXAFS

Experimental facility: HESGM @BESSY II

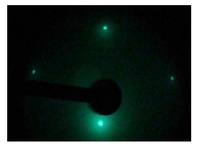


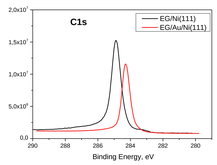
Simulation of NEXAFS of Pn molecule

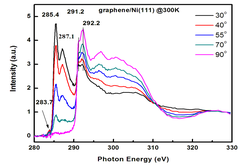


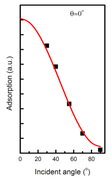
Atomic specific XAS calculations for carbon K-edge of free Pn molecule using StoBe package.

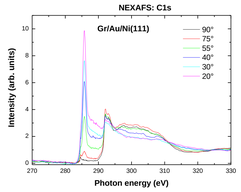
LEED, XPS and NEXAFS characterizations of graphene





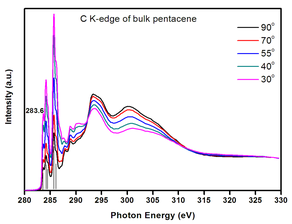


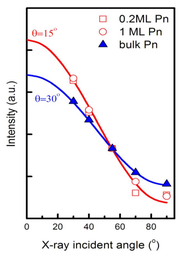




LEED, XPS and NEXAFS characterizations of single layer of graphene prepared by C_2H_4 cracking on Ni(111) surface without and with Au intercallation. Dipole dependence of NEXAFS shows a highly parallel graphene layer on Ni(111) . The binding energy of EG/Ni (~285 eV) and the state at 287.1eV in corresponding NEXAFS spectra denote strong hybridization between graphene with Ni(111).

Bulk



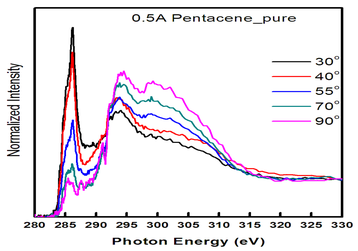


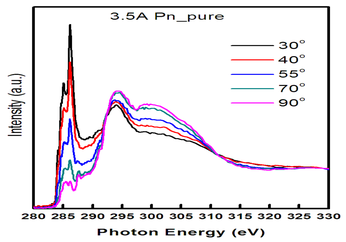
Dependence of π* resonance intensities on the X-ray incidence angle and the corresponding theoretical fittings with a polarization degree of P=0.91.

Pentacene on graphene/Ni(111)

Sub- and monolayer

EG/Ni(111)





EG/Au/Ni(111)