XPS and NEXAFS Investigations of Organic Molecular Self-Assembly on Epitaxial Graphene

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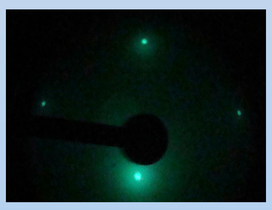
Motivations

Graphene is a promising candidate for next generation technology because of its novel electronic structures and properties. Epitaxial graphene grown on transition metal surface is a promising electronic material because of abundance, low cost and possible patterning using traditional lithography, which has many potential applications such as transparent electrode in organic electronic devices. Pentacene (Pn) and terephthalic acid (TPA), the much studied functional organic molecules, were selected to probe the molecular adsorption and interactions with graphene/Ni(111) surface investigated by NEXAFS and XPS. The orientation of molecules at the interface in organic devices plays key role on the electronic properties.

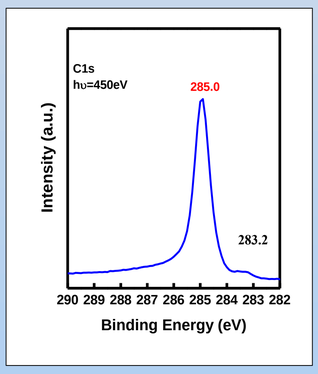
Experiment

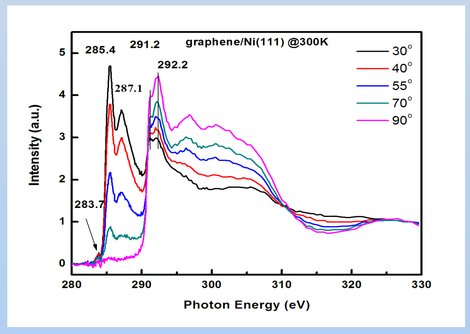
BESSY II , HE-SGM beamline. Partial electron yields (PEY) mode for NEXAFS with home-made MCP detector. SRXPS with VG Scienta R3000 analyzer.
Preparation of Graphene/Ni(111): ~850K, ethylene, 1.0x10^{-6} mbar, 10min
Molecules deposition: home-built K-Cell evaporator, OMBE.

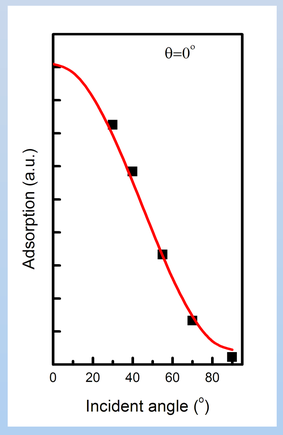
Confirmations of Graphene/Ni(111)



Graphene/Ni(111), E_p=120eV



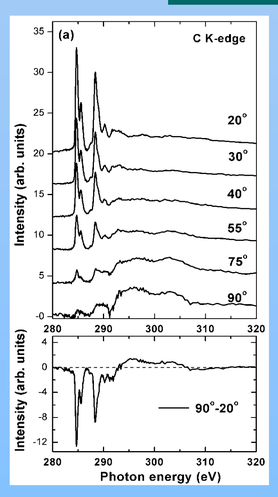


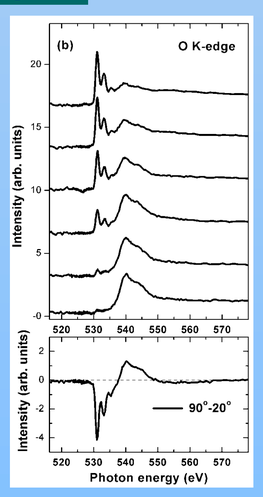


LEED, XPS and NEXAFS characterizations of single layer of graphene prepared by C_2H_4 cracking on Ni(111) surface. The state at 283.7eV may result from defect states. Dipole dependence of NEXAFS shows a highly parallel graphene layer on Ni(111) . The state at 287.1eV denotes strong hybridization between graphene with Ni(111).

TPA on graphene/Ni(111)

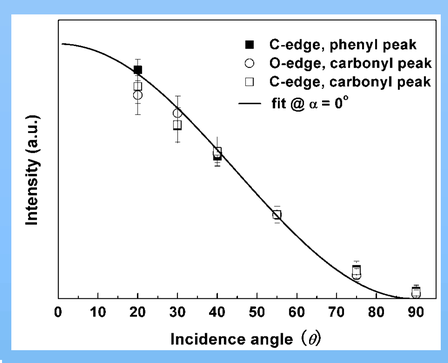
Monolayer

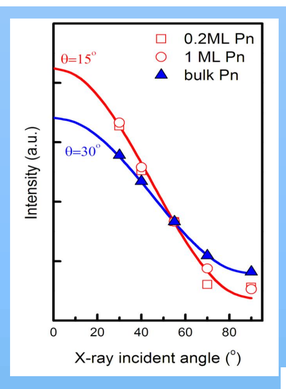




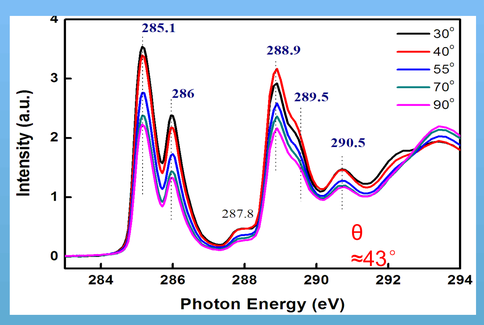
$$I = C \cdot \left(P \cdot \left(\cos^2 \alpha\right) \cdot \left[1 - 1.5 \cdot \left(\sin^2 \theta\right)\right] + 0.5 \cdot \left(\sin^2 \theta\right)\right)$$

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



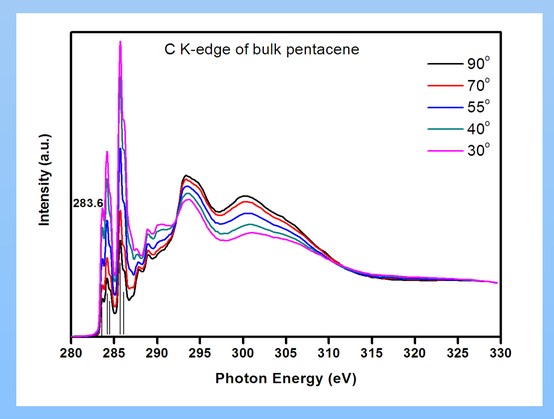


Multilayer

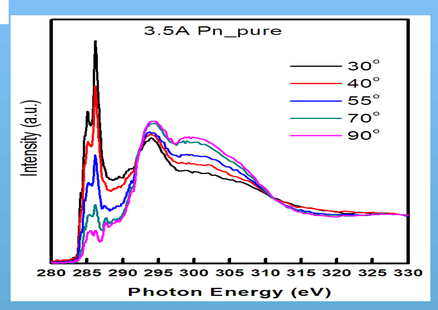


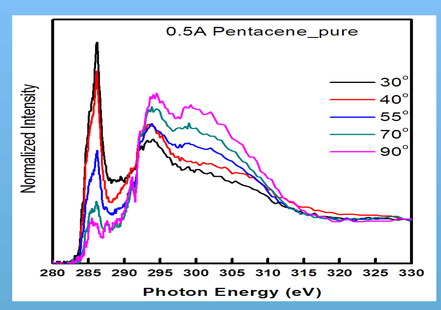
Pentacene on graphene/Ni(111)

Bulk

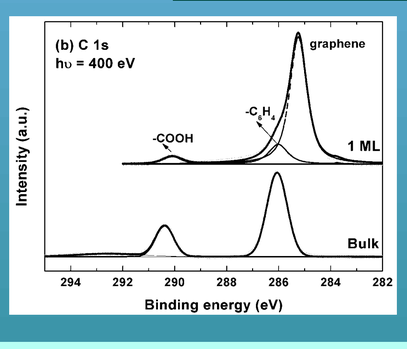


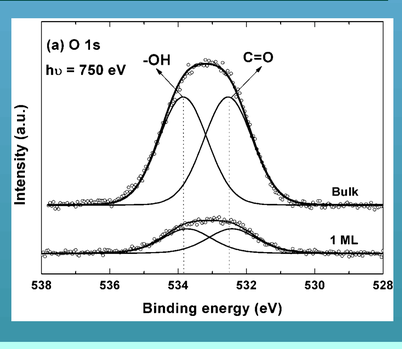
Sub- and monolayer





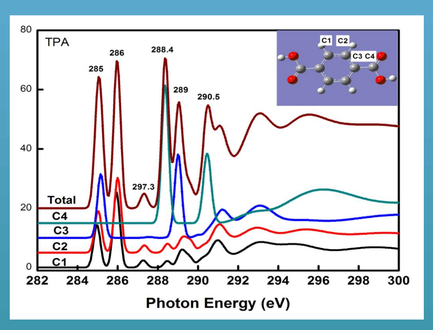
XPS of TPA on graphene/Ni(111):

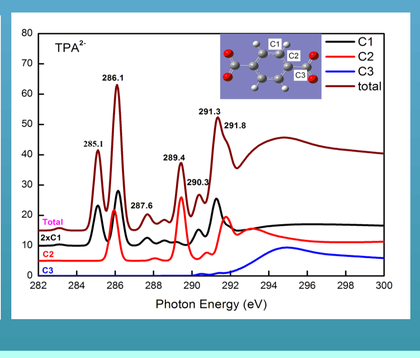


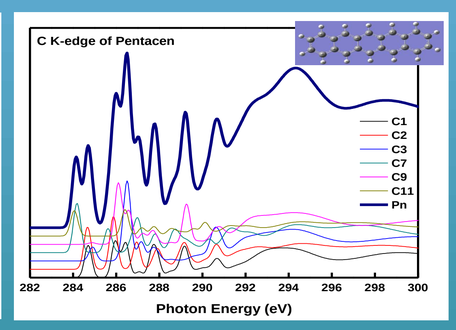


Interactions between TPA and graphene are very weak. TPA molecules are neutral and no deprotonation takes place.

Simulation of NEXAFS of TPA, deprotonated TPA and Pn molecule







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

Conclusions:

- Highly parallel single-layer of graphene was prepared by C_2H_4 cracking on Ni(111).
- Epitaxial graphene appears the similar properties to graphite for molecular deposition, but it can serve as a good support for the deposition of polycyclic aromatic hydrocarbons (PAHs) at lower coverages due to less interference of the signals from graphene support. Our experiments reveal that (sub-)monolayer pentacene molecules orientate orderly on graphene surface with a 15^o tilting angle.
- For 1 ML coverage TPA molecules aren't deprotonated and have a parallel orientation with respect to the graphene surface.

Acknowledgements:

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