Adsorption of Pentacene (Sub)monolayer on Epitaxial Graphene and BN: Spectroscopy Studies

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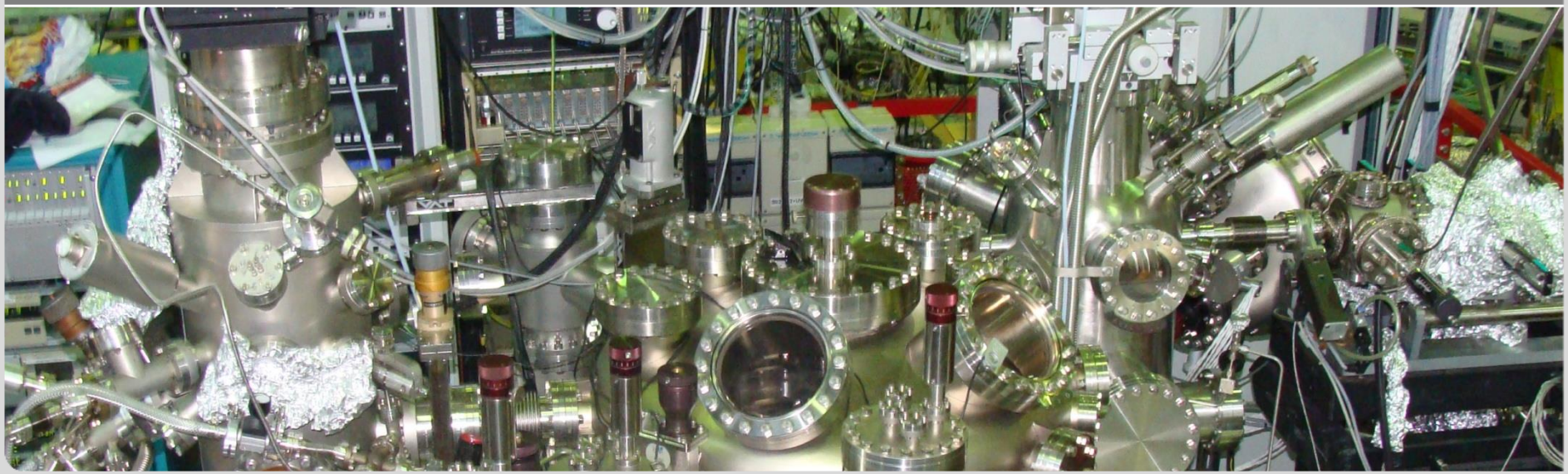


Motivation

- Pentacene and graphene are promice candidates for organic electronics:
  - behaviour on the interface between them is very important
  - flat orientation of the first pentacene layer is necessary

- Fundamental understanding of the interaction on graphene/metal interface:
  - „weak“ or „strong“

  Pentacene as a probe molecule

  Comparison of EG/Ni(111) *vs.* EG/Au/Ni(111) and h-BN/Au/Ni(111)

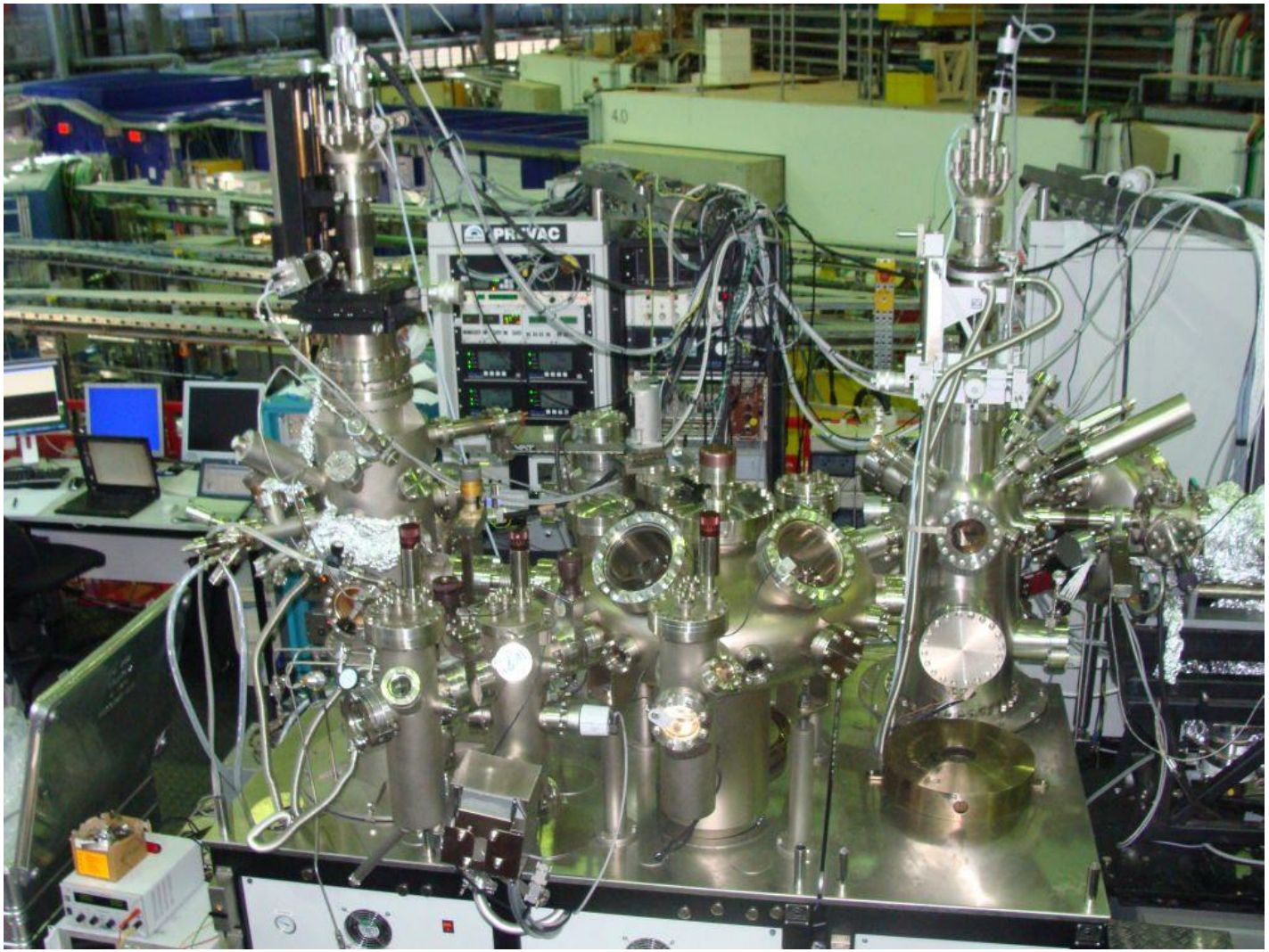
- Possible interaction of pentacene with metal substrate through graphene - ?

Presence of „surface phase“ similar to chemisorbed pentacene on Ag(111)
[*Käfer et al, CPL,* **442** (2007) 376–383]

- Additional challenge:

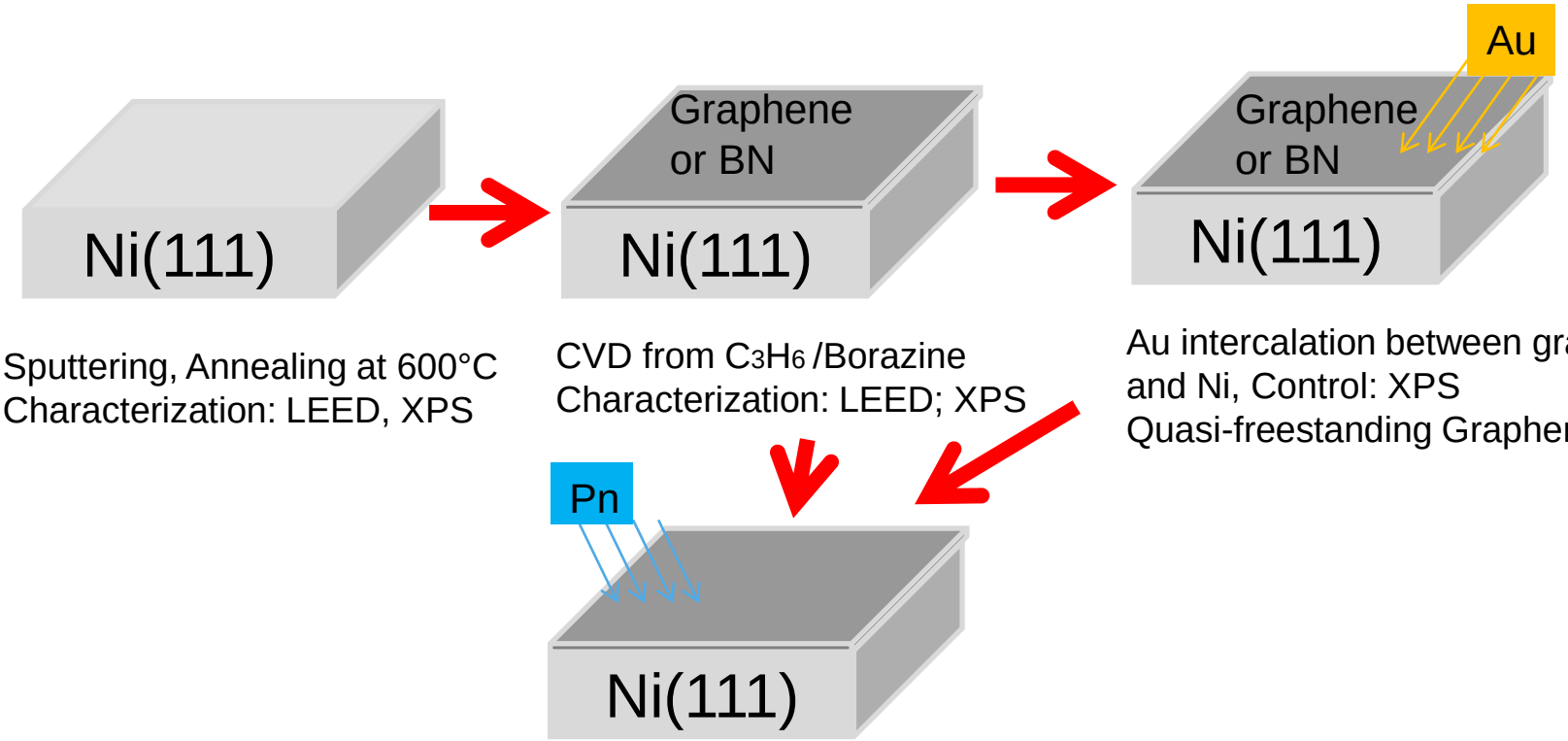
Evaluation of C *K*-edge NEXAFS spectra for organic/graphene systems

XPS/NEXAFS endstation @ HESGM (BESSY II)



Sample preparation and layout of the experiment

Used systems: EG/Ni(111), EG/Au/Ni(111) and h-BN/Au/Ni(111)



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

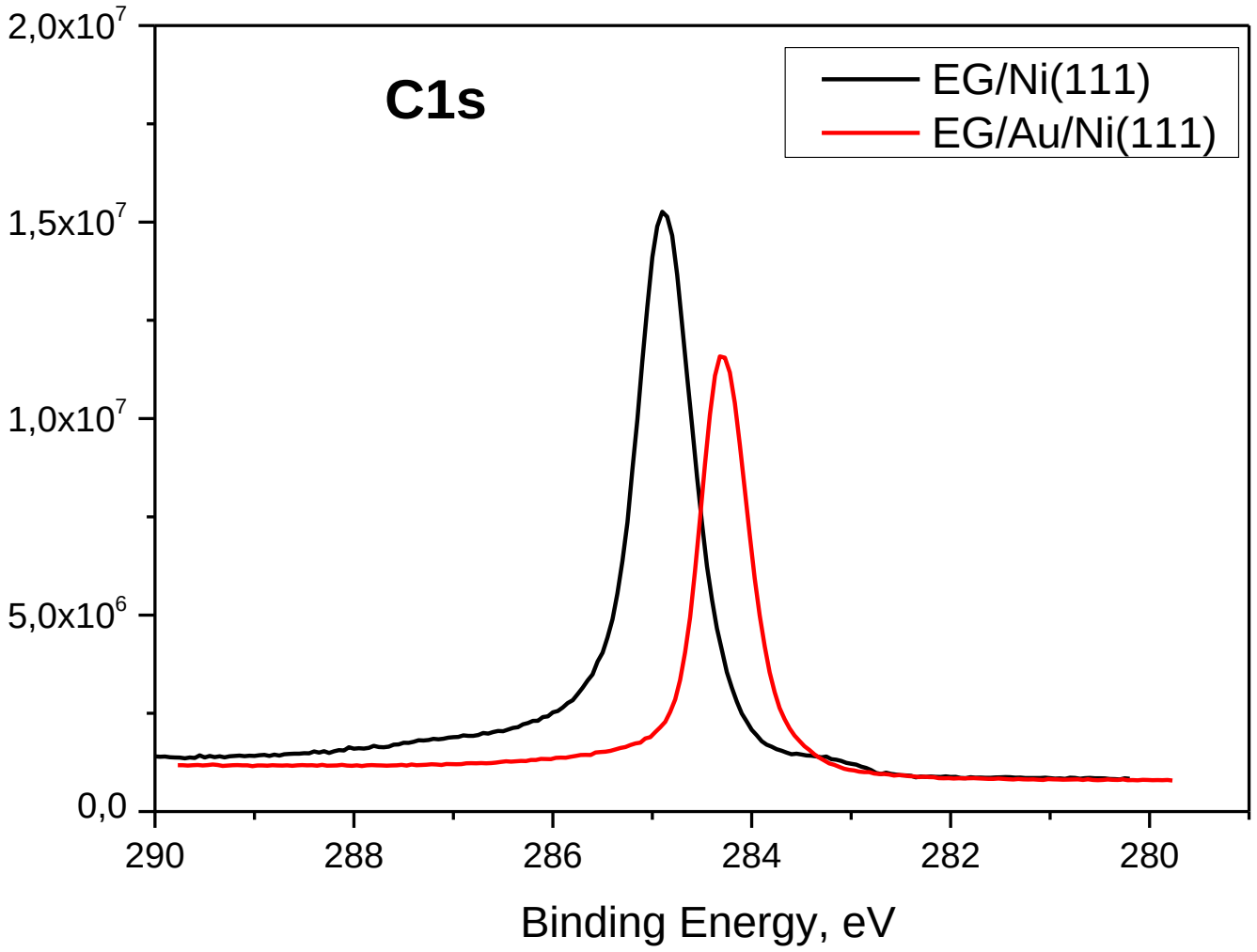
CVD from C_3H_6 /Borazine
Characterization: LEED; XPS

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

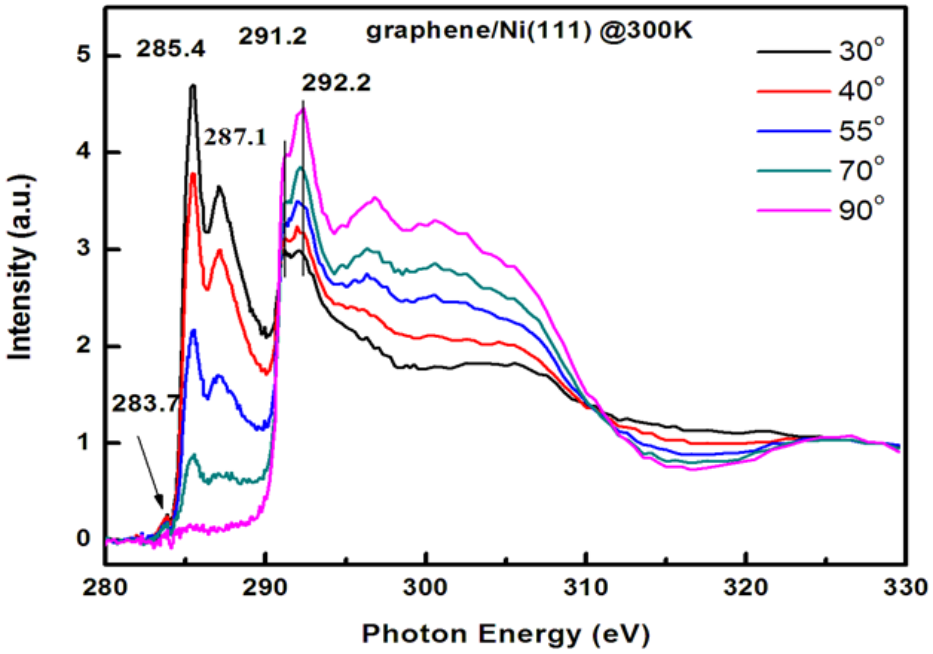
Pn deposition
Characterization: XPS, NEXAFS

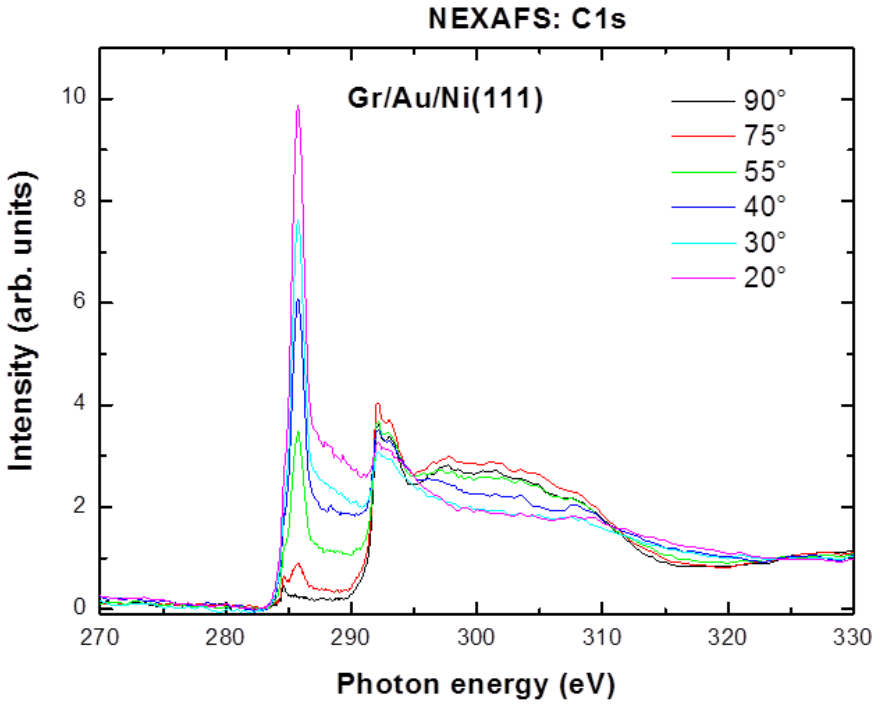
Pn thickness calibration with QCM

XPS: Shift of C1s line after Au intercallation



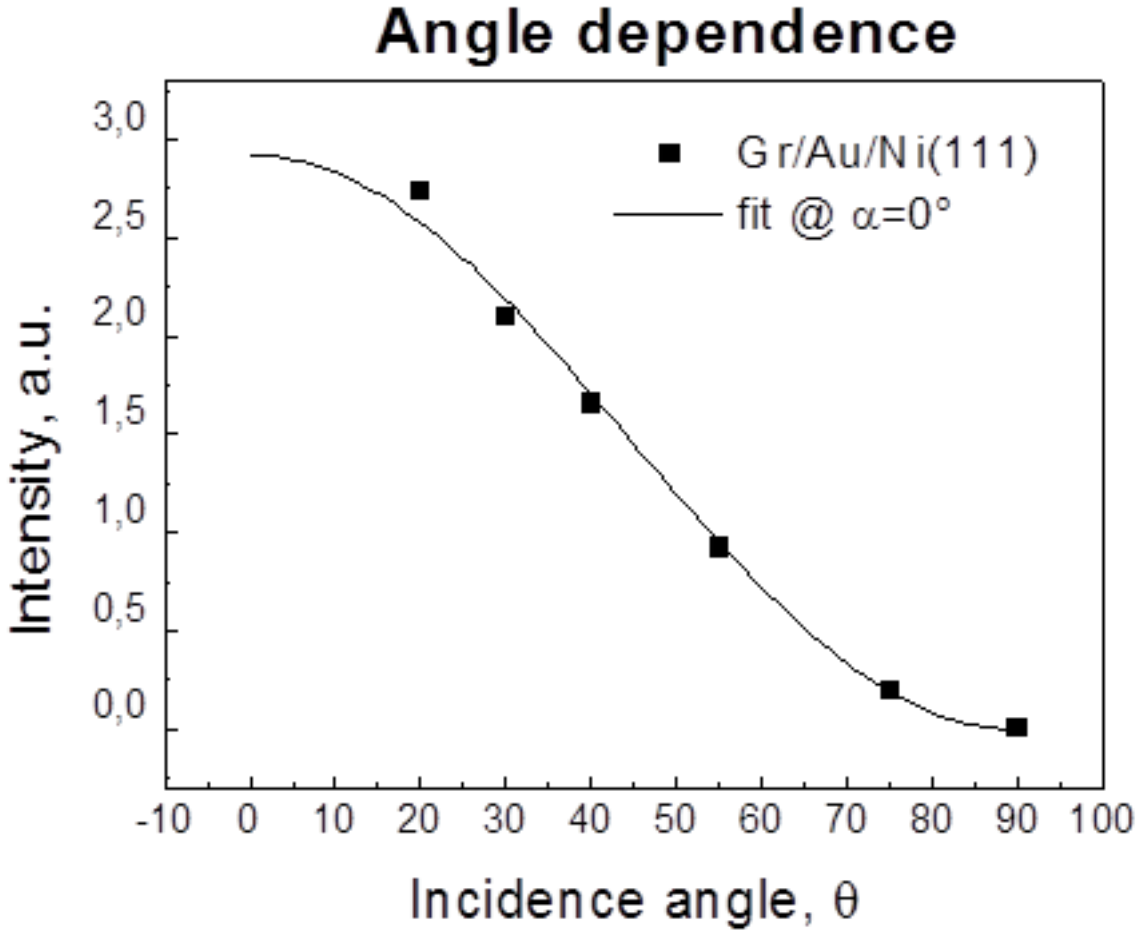
NEXAFS: Comparison of EG/Ni and EG/Au/Ni





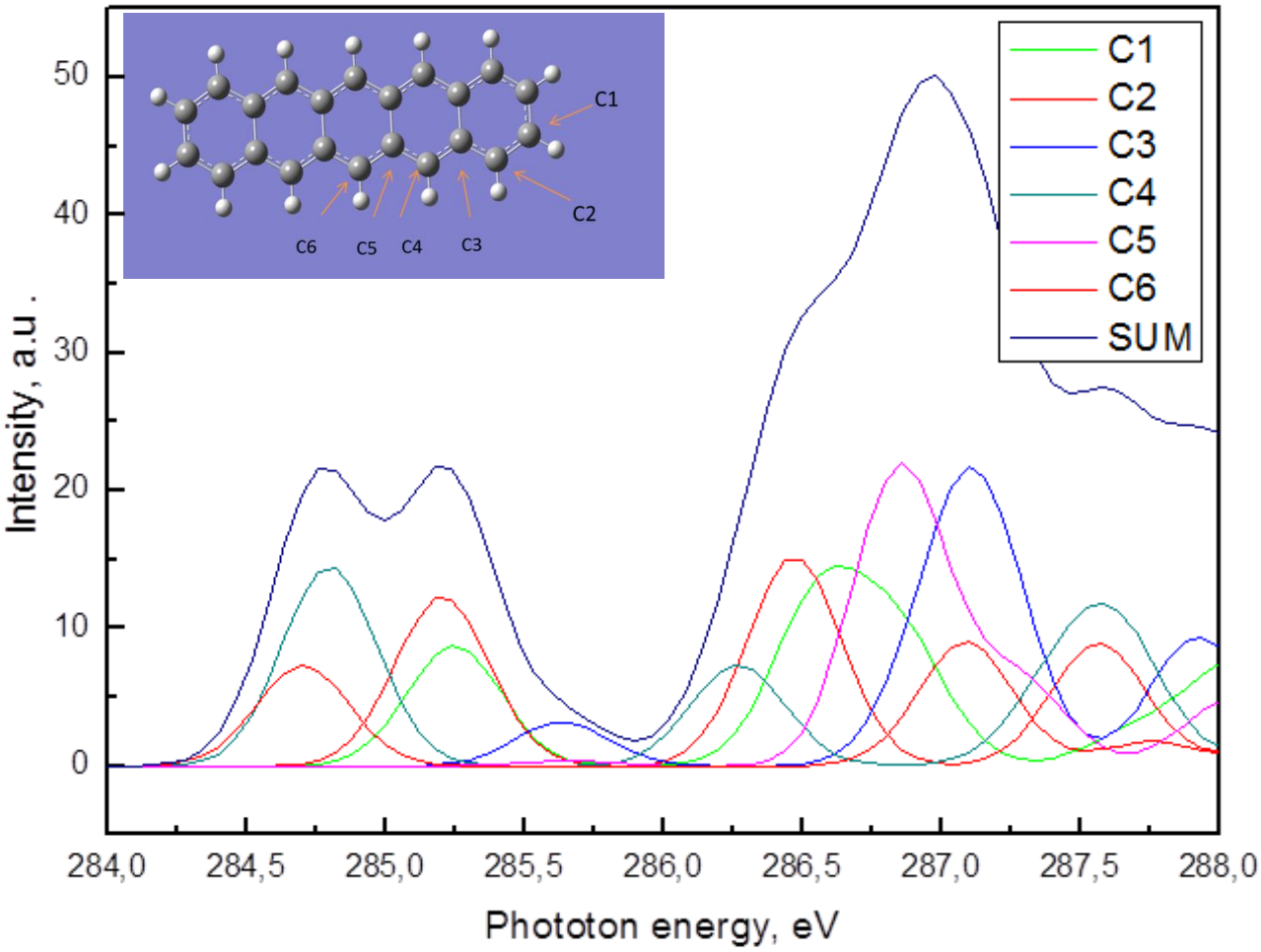
„Strong“

„Weak“

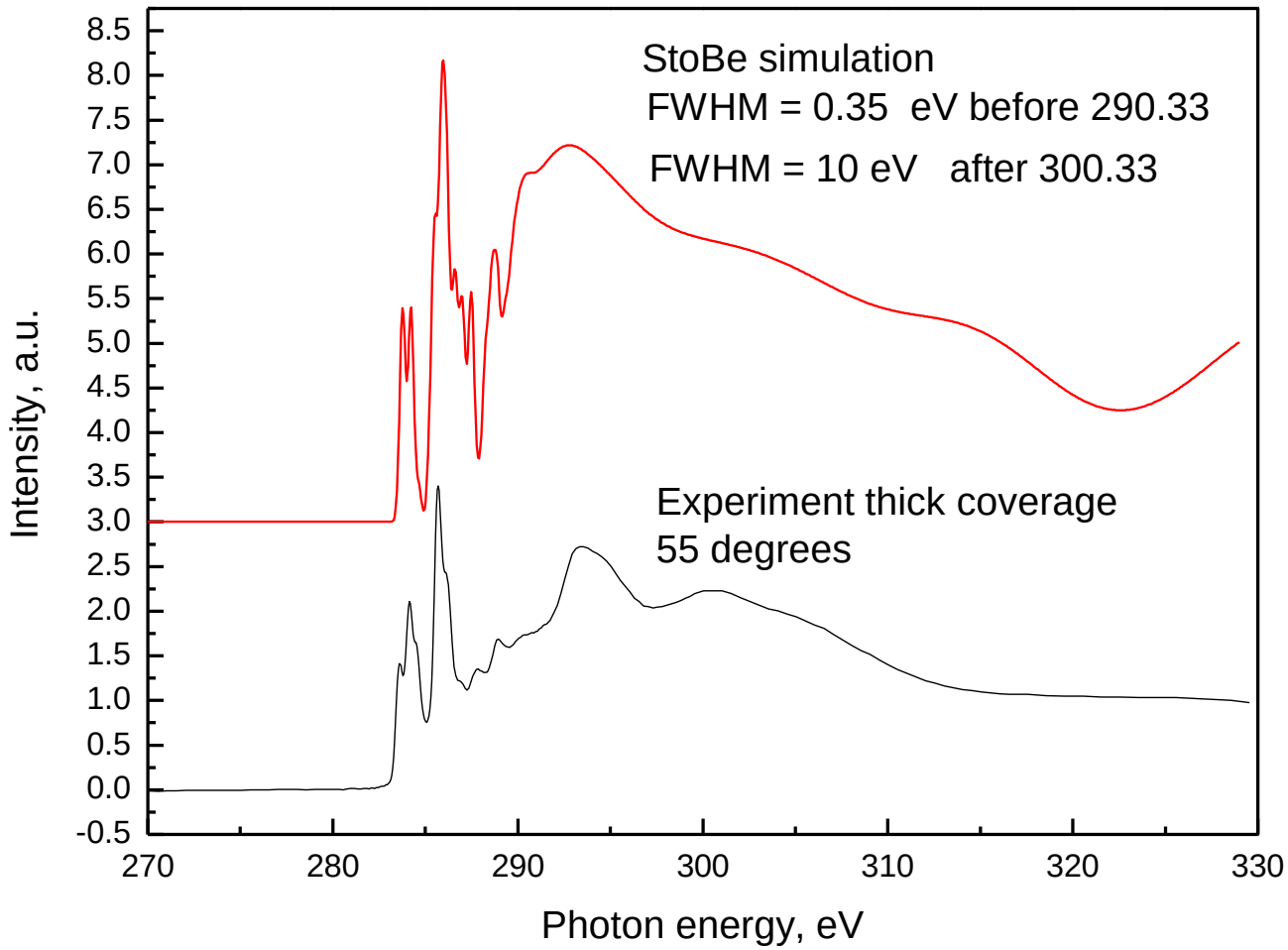


$$I(\alpha,\theta) = A\{P(1/3)[1 + (1/2)(3\cos^2\theta - 1)(3\cos^2\alpha - 1)] + (1 - P)(1/2)\sin^2\alpha\}$$

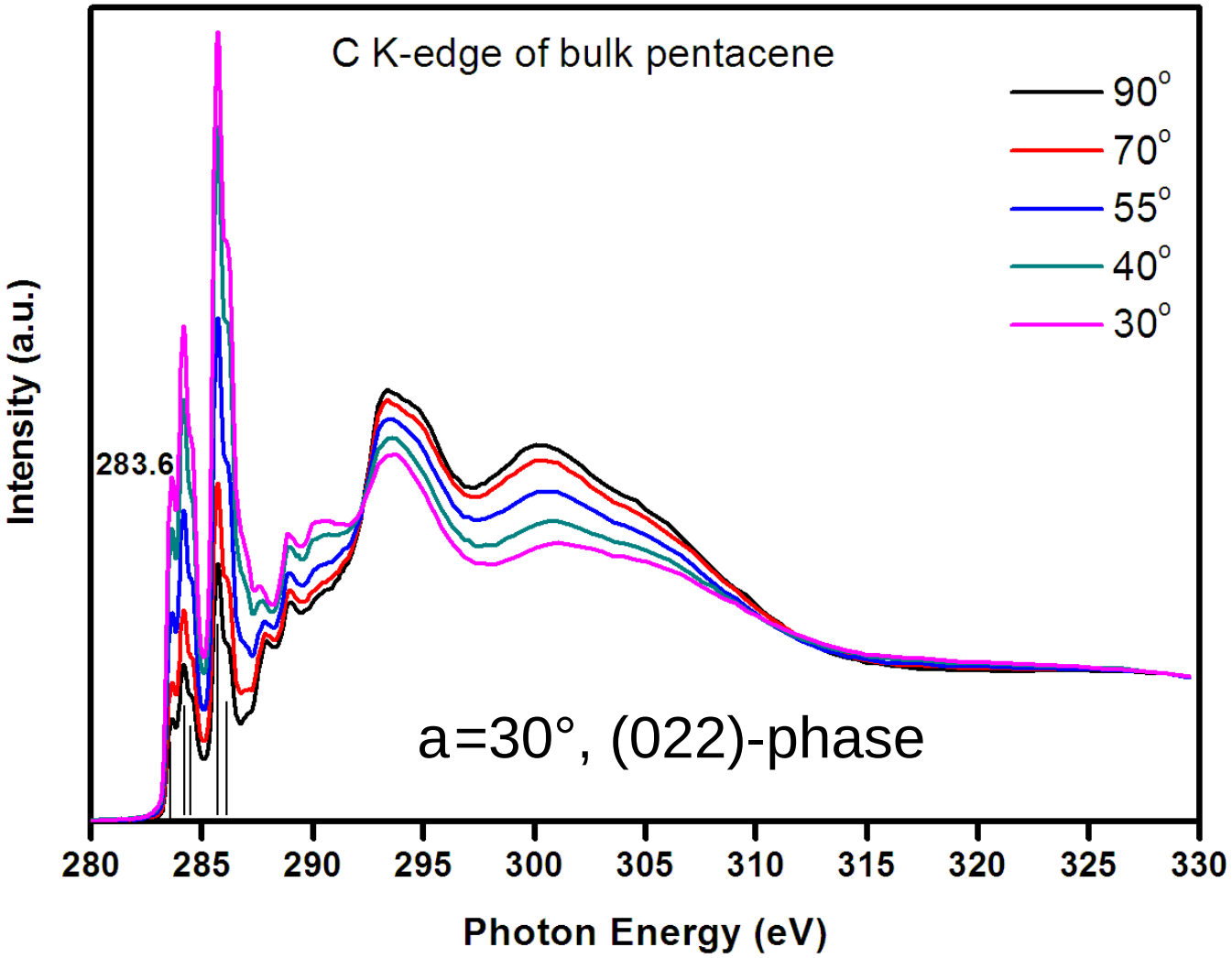
Simulation of NEXAFS spectra of Pn molecule (in gas phase)



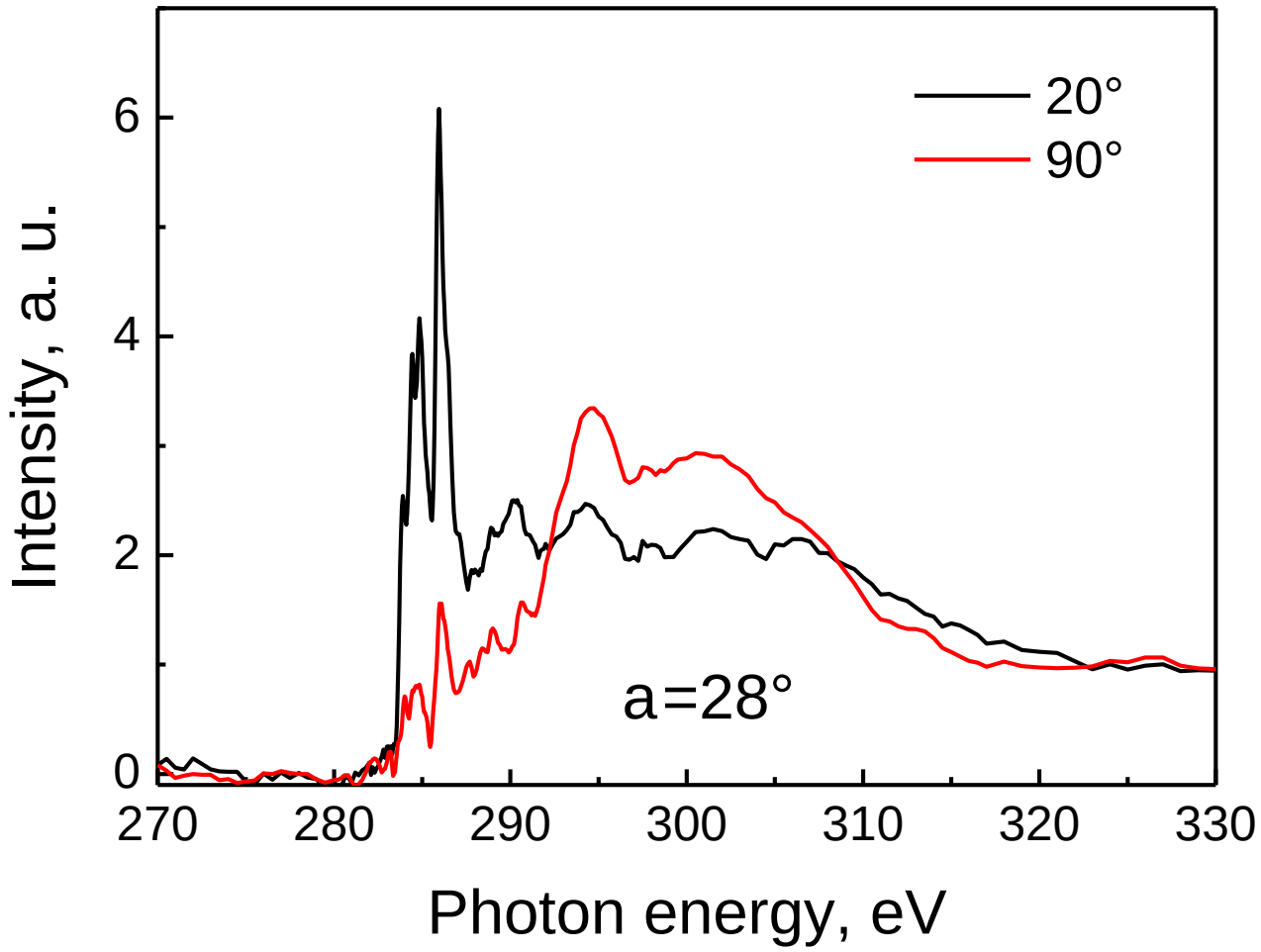
Comparison: simulation vs. experiment



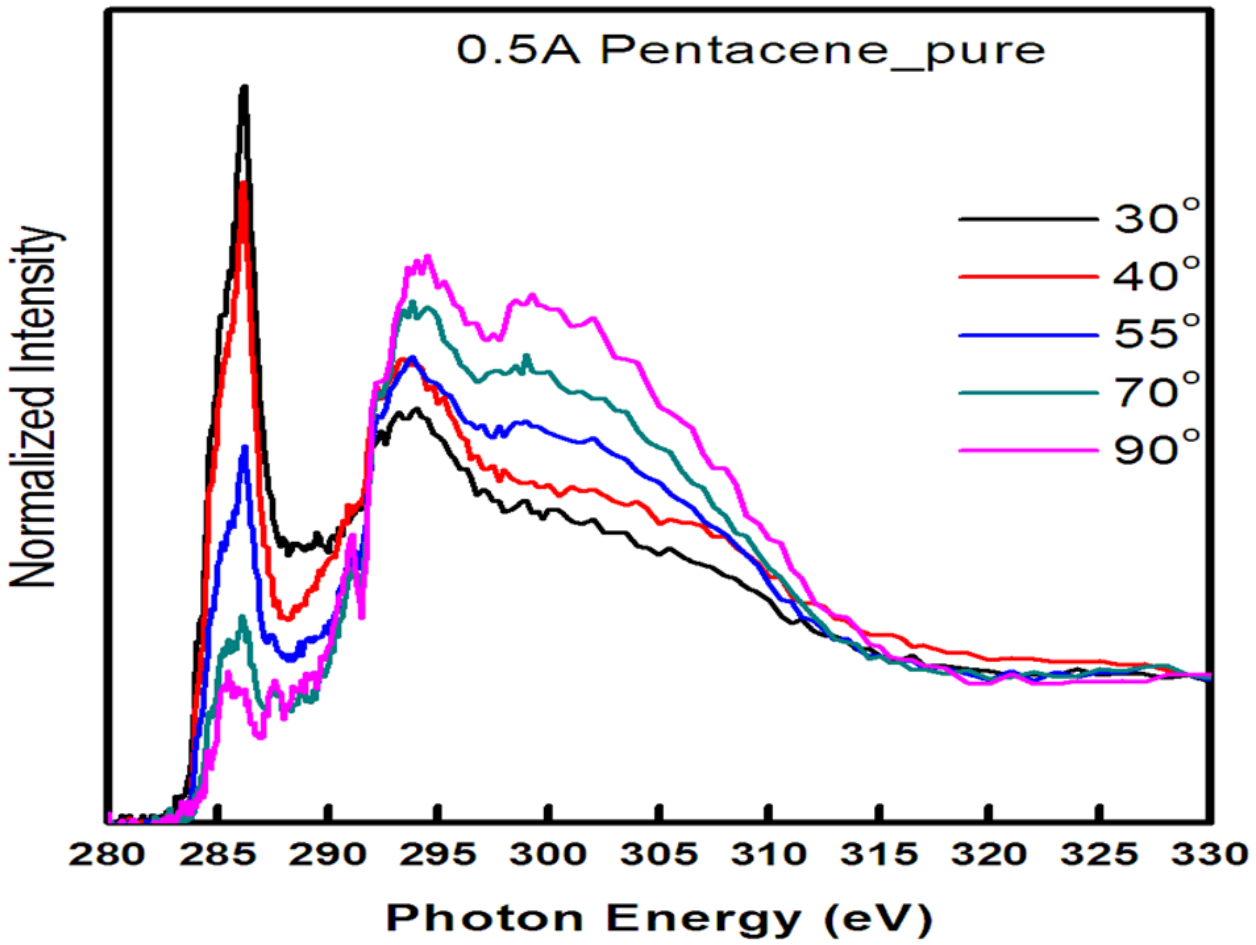
Pentacene on graphene: multilayer



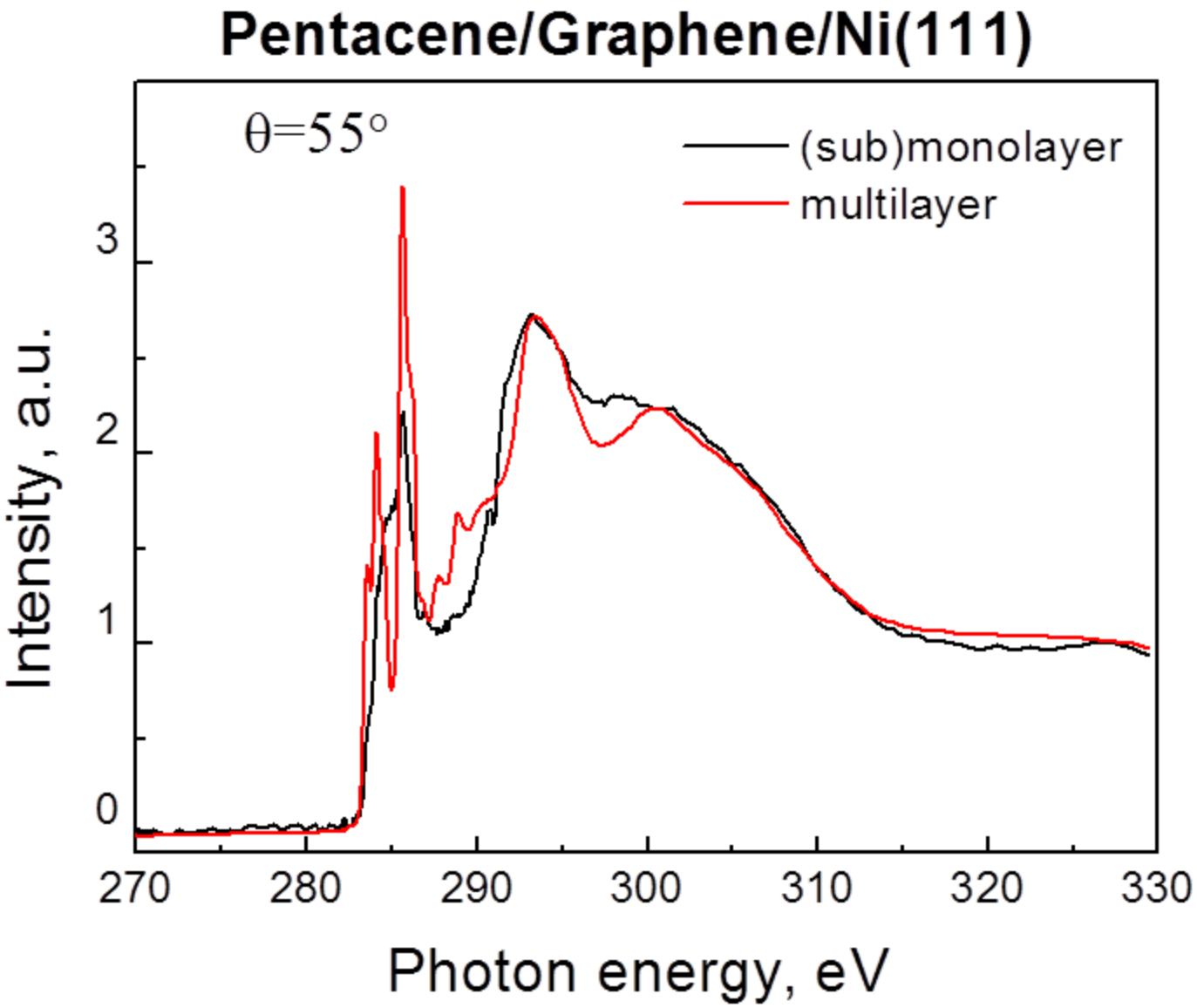
Pentacene on h-BN: multilayer

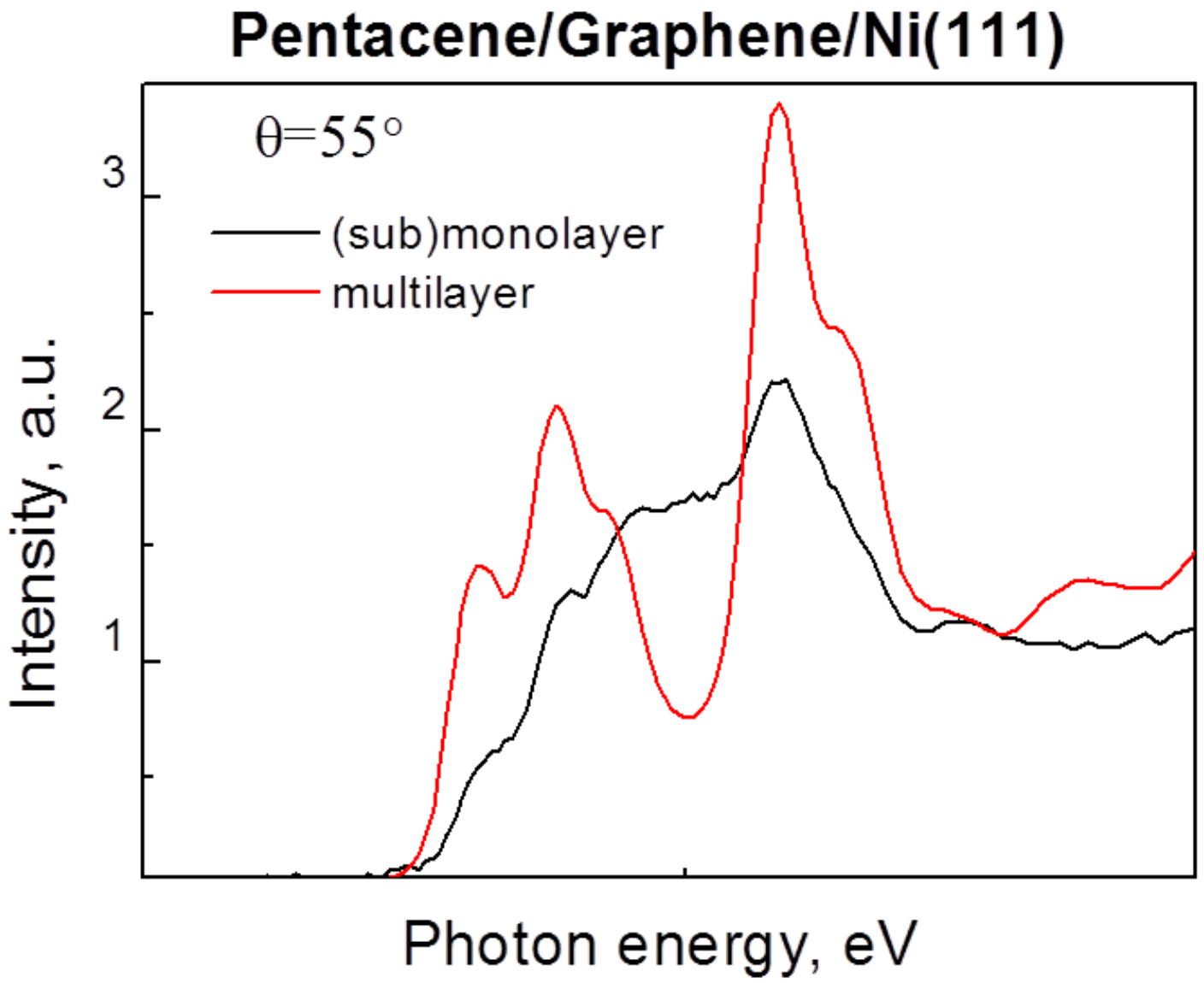


Pn/EG/Ni(111): Submonolayer

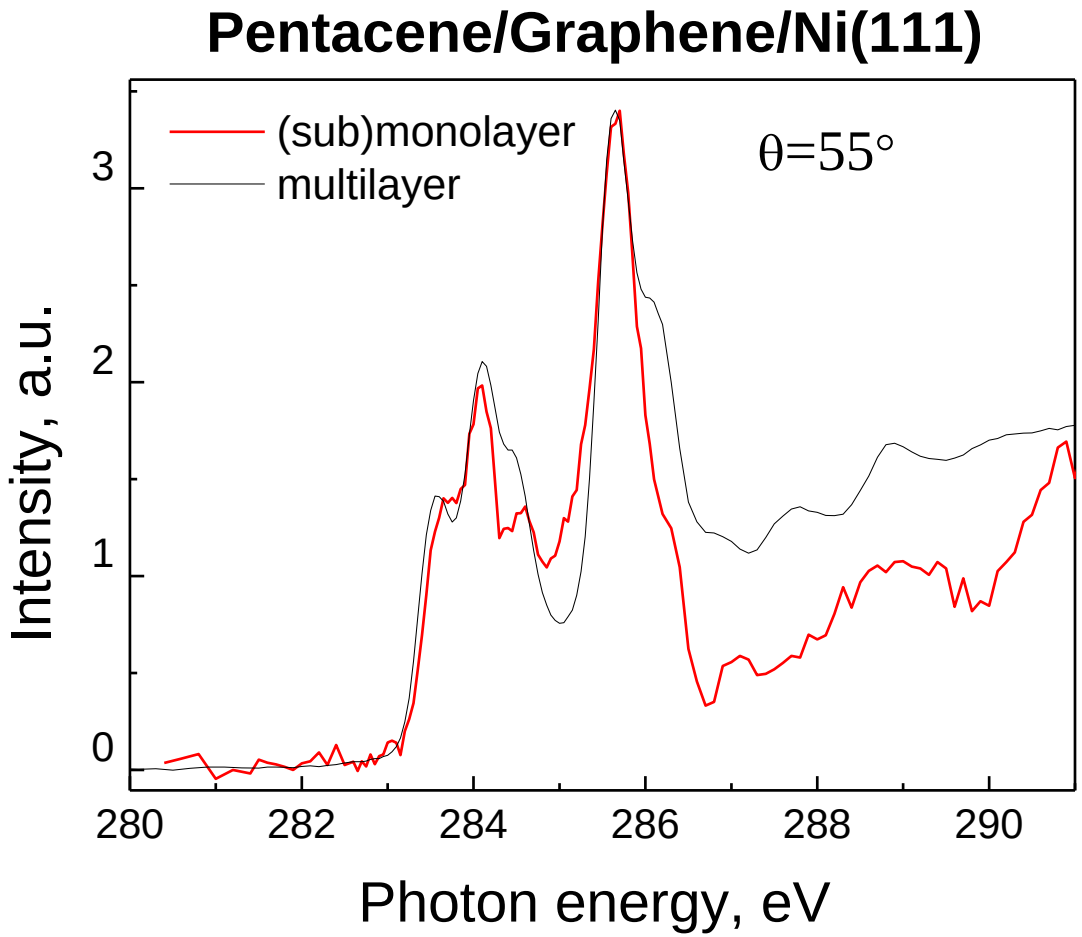


Broadening – hybridization – „strong“ interaction?
Or some additional contribution?


Pentacene/Graphene/Ni(111)
θ=55°
(sub)monolayer
multilayer
Intensity, a.u.
0
1
2
3
270
280
290
300
310
320
330
Photon energy, eV


Pentacene/Graphene/Ni(111)
θ=55°
(sub)monolayer
multilayer
Intensity, a.u.
1
2
3
Photon energy, eV

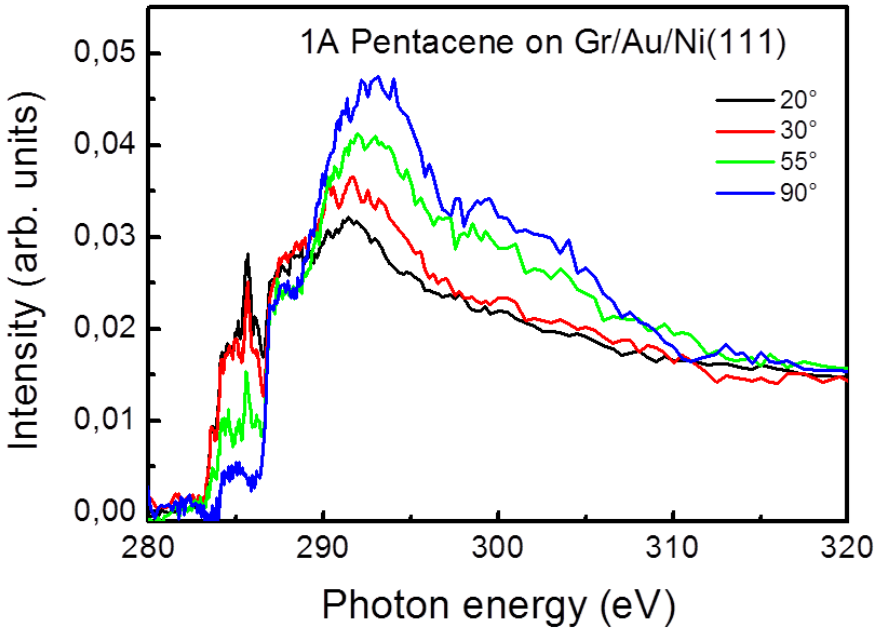
Correction of Graphene contribution

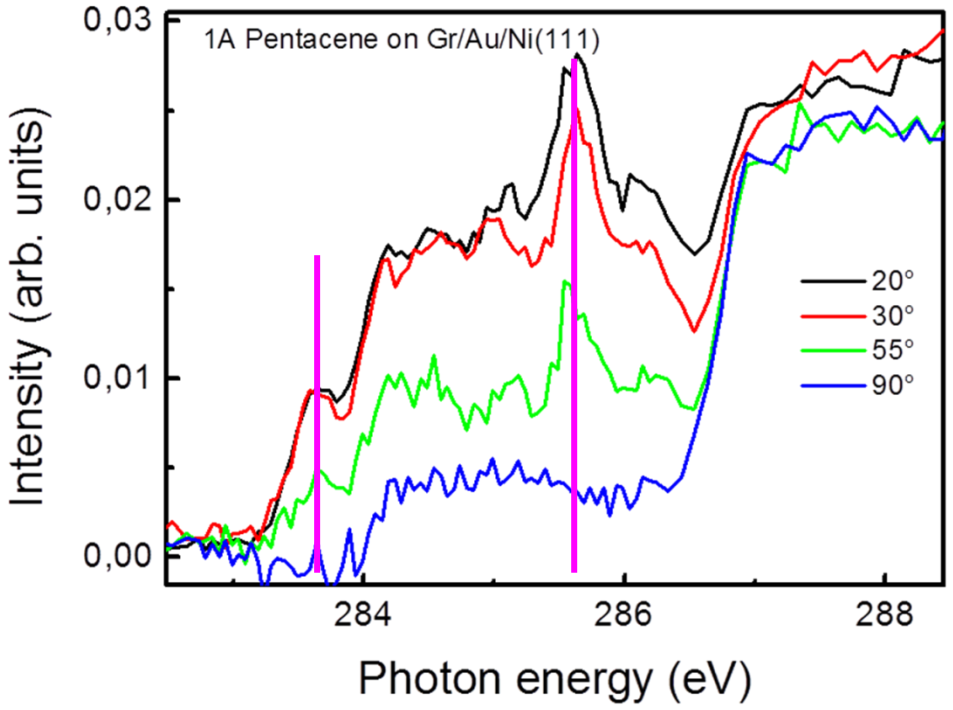


No hybridization – „weak“ interaction!

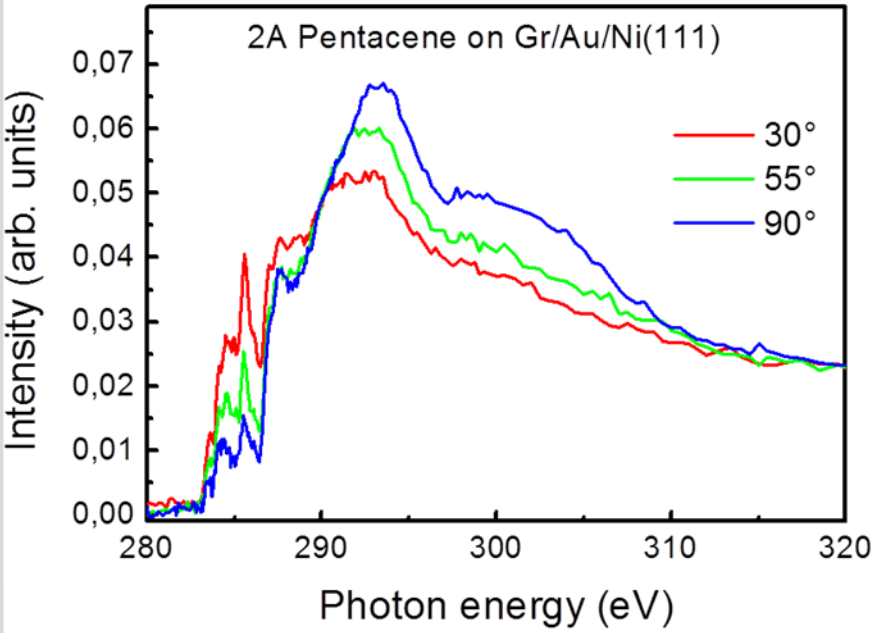
Flat orientation of the first Pn layer!

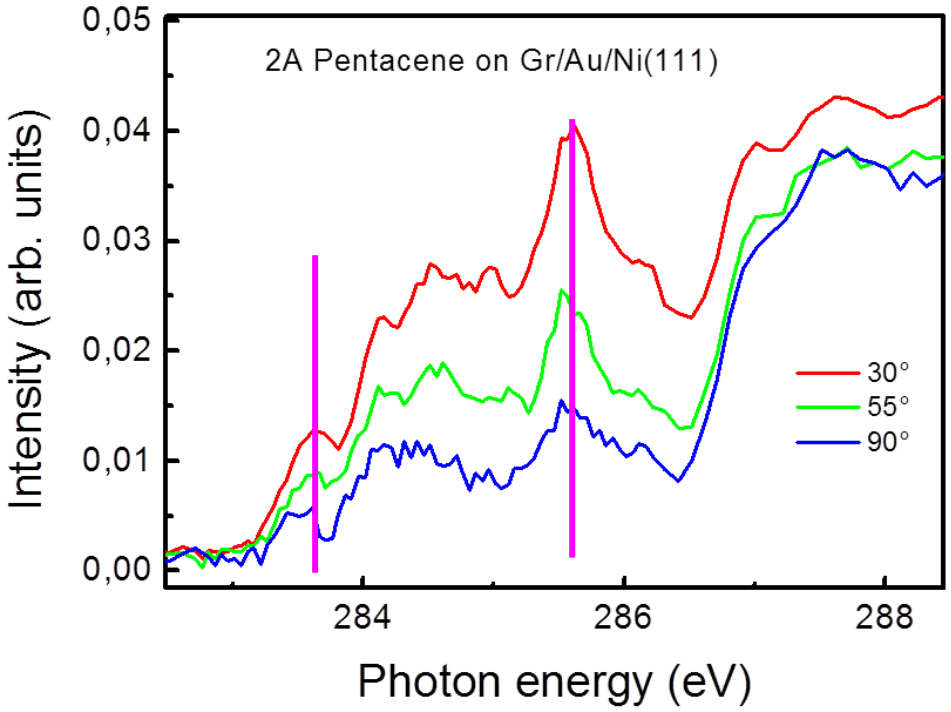
EG/Au/Ni(111): Submonolayer



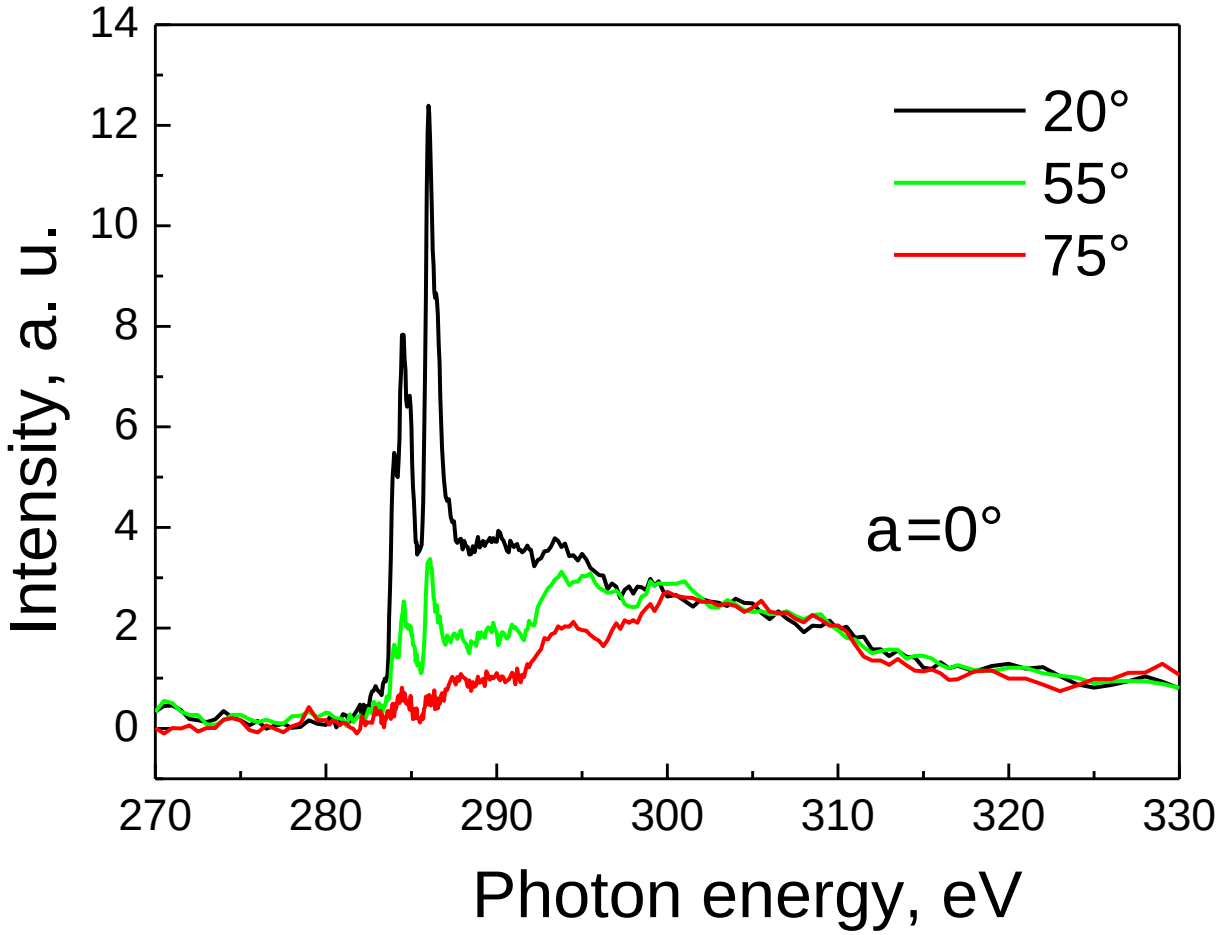


EG/Au/Ni(111): growth of the second layer





Pentacene on h-BN: (sub)monolayer



Conclusions

1. Flat orientation of pentacene at submonolayer coverages – independent on substrate configuration
2. Direct growth of tilted phase already for the second layer
3. Weak interaction between pentacene and graphene
4. No „surface phase“ was observed – no interaction with metal substrate through EG layer

Thank you for attention!