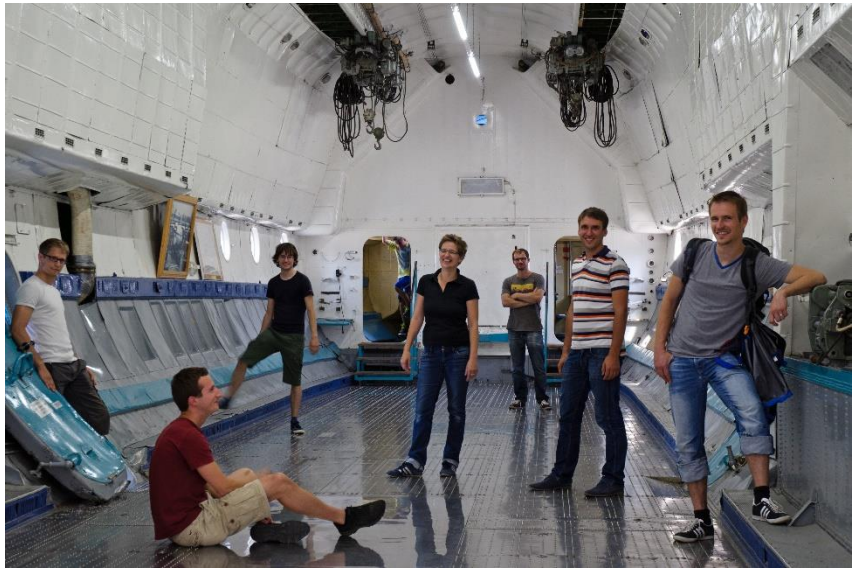
AG TEGEDER



Christopher Bronner
Lea Bogner
Alexander Broska
Sascha Feldmann
David Gerbert
Anton Haase
Sebastian Hagen
Marc Hänsel

Felix Leyssner
Friedrich Maaß
Michael Schulze
Vipilan Sivanesan
Arnulf Stein
Stephan Stremlau
Erwan Varene
Maximilian Vogtland

Molecular processes at interfaces and in thin films

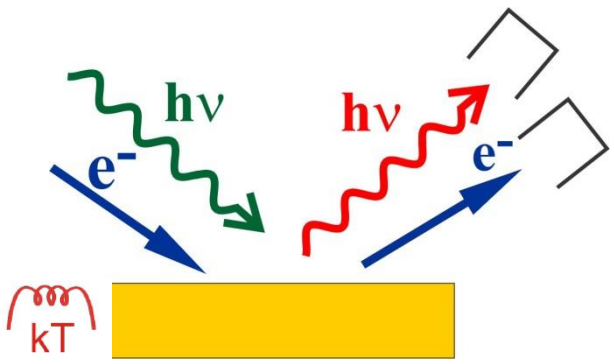
- Understanding electronically and thermally induced elementary processes in molecular ensembles

Analysis

- *Electronic structure*
- *Structural properties*
- *Dynamics of electronically excited states*

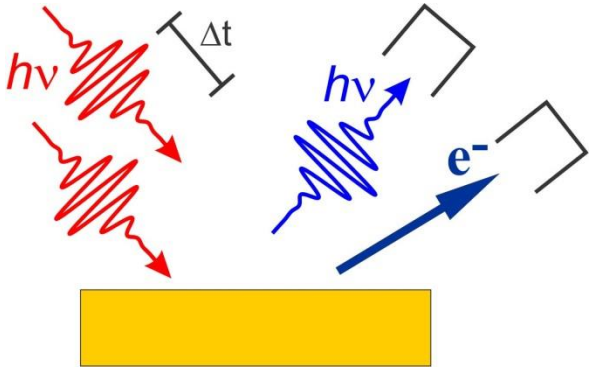
Spectroscopy

static



HREELS, UPS, 2PPE, SHG, SFG, TPD
XPS, NIXSW

dynamic

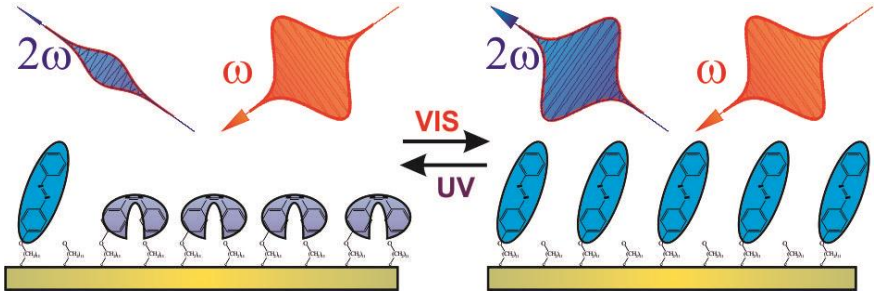


2PPE, SHG,

Overview over current research areas in our labs

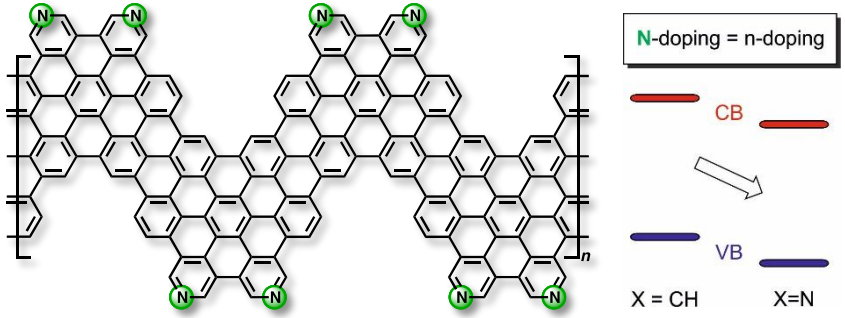
UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

Molecular switches at surfaces



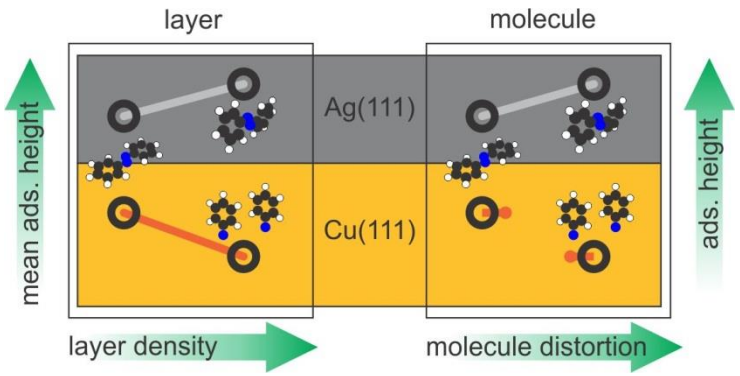
- Controlled modification of interface properties

Graphene nanoribbons



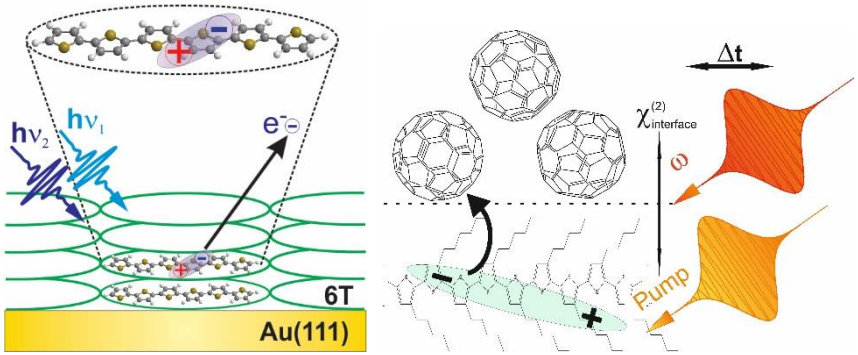
- Tuning of electronic properties

Molecule-substrate interactions



- Understanding binding properties

π-conjugated organic materials

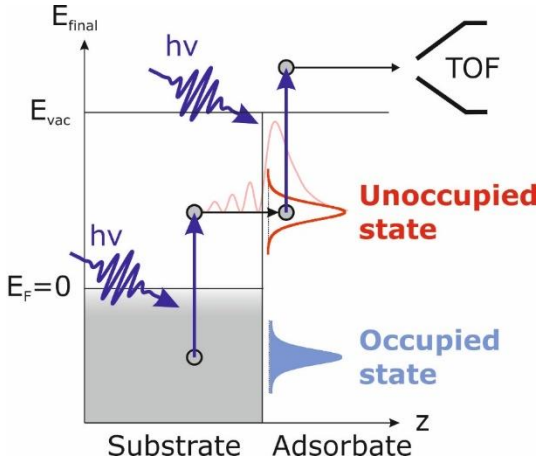


- Understanding optoelectronic properties

AGT
MOLEKULARE PROZESSE AN OBERFLÄCHEN

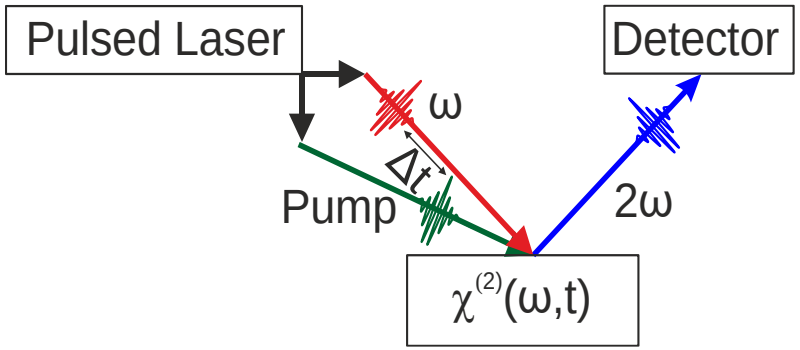
Experimental methods

Two-photon photoemission (2PPE)



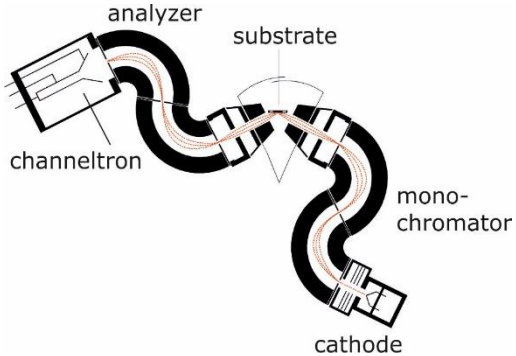
- electronic structure, dynamics, dispersion

Second harmonic generation (SHG)



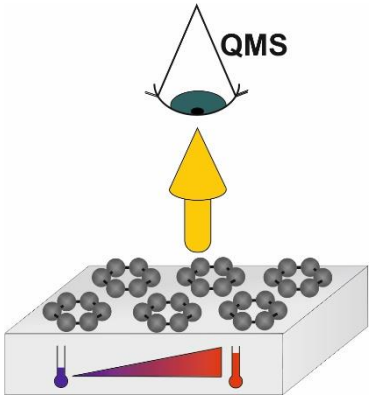
- electronic properties, dynamics

High-resolution electron energy loss spectroscopy (HREELS)



- Vibrational & electronic properties

Temperature programmed desorption (TPD)

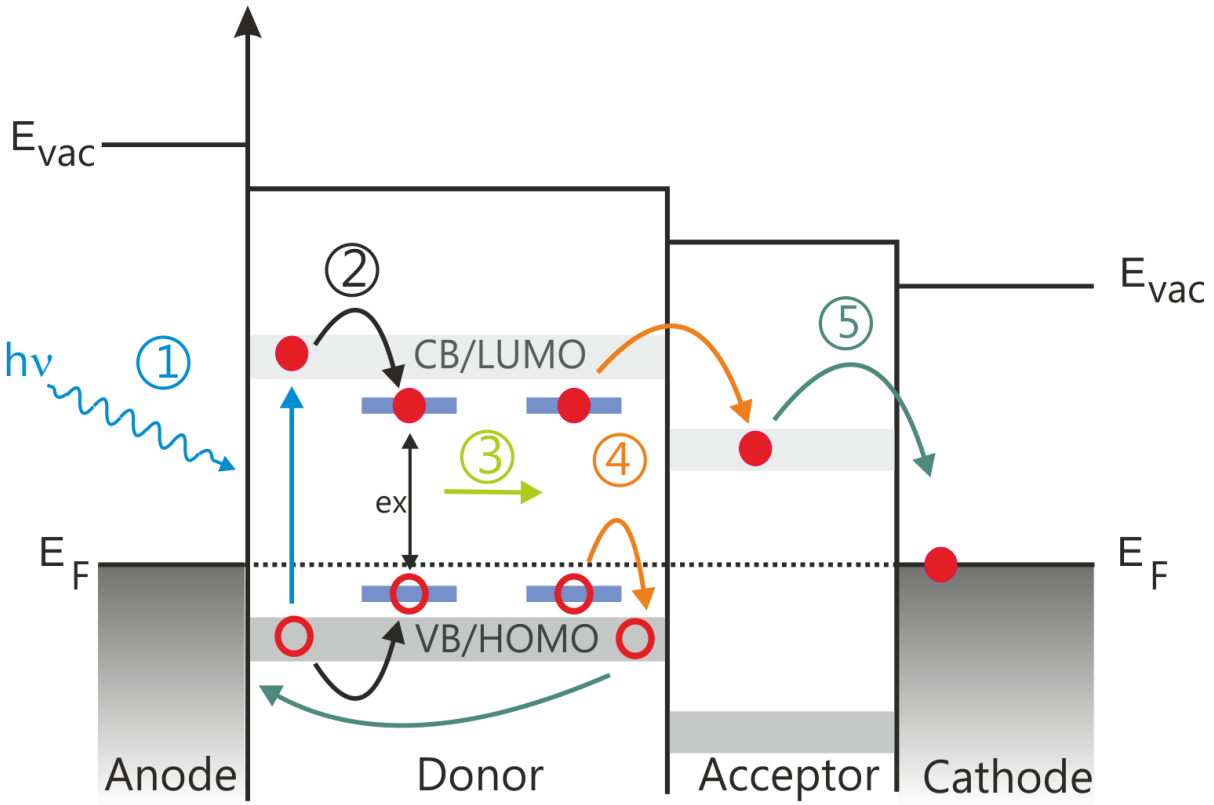


- Coverage & binding energies

Motivation

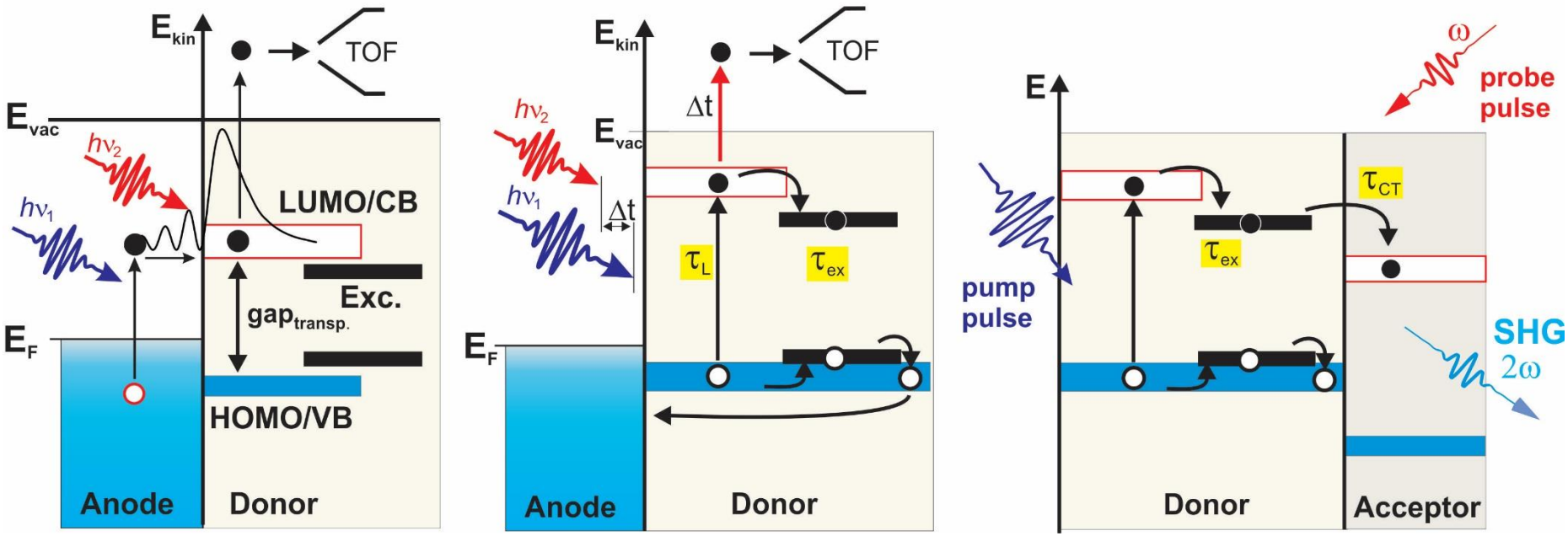
Optoelectronic devices

Organic photovoltaic cells



1. Light absorption
2. Exciton generation
3. Exciton separation
4. Charge transport
5. Charge extraction

Goal

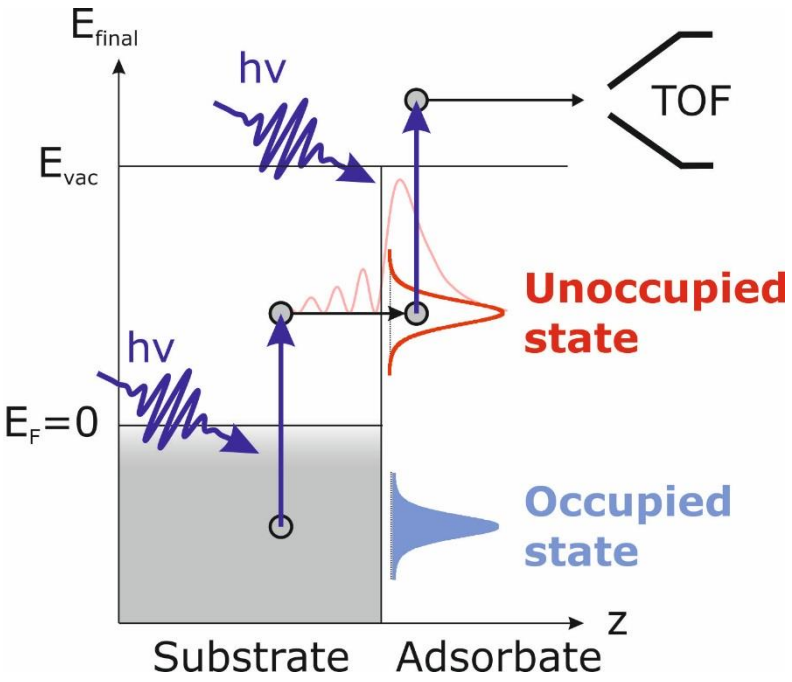


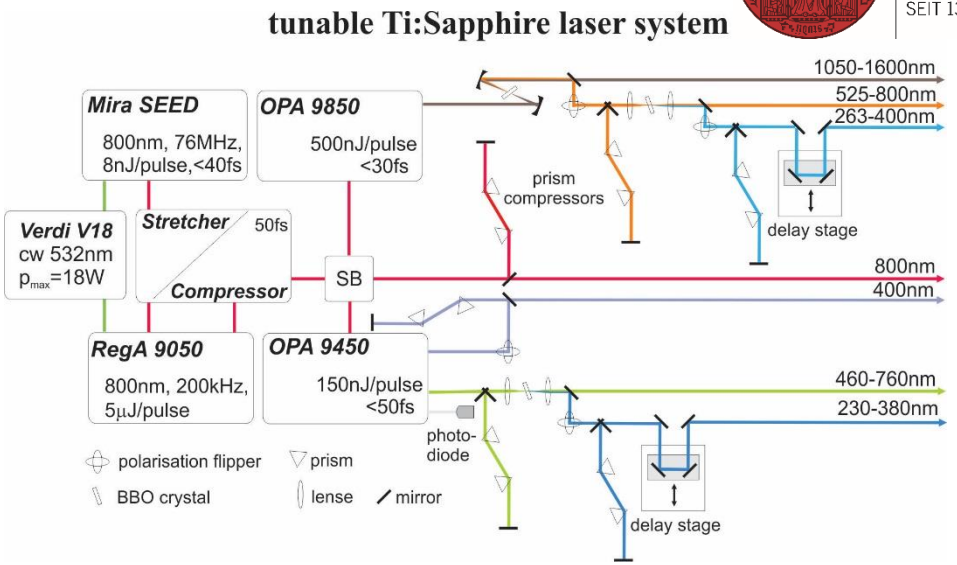
⇨ Energy level alignment (electron/hole injection barriers)

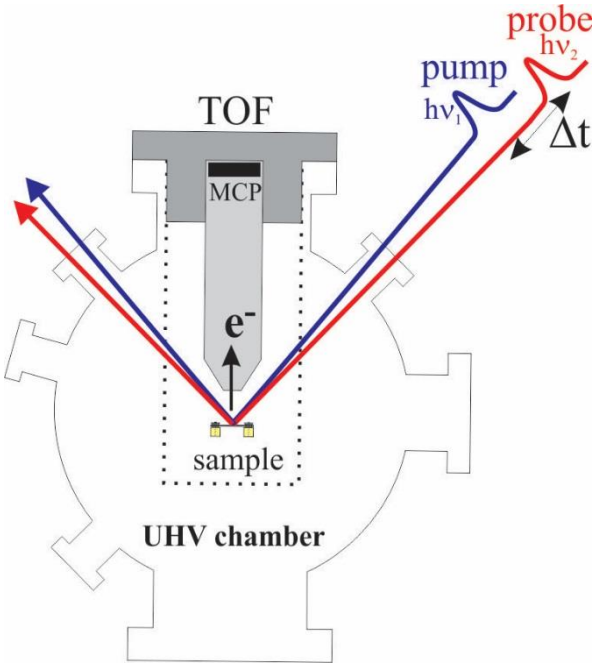
⇨ Charge carrier and exciton dynamics at the interface and within the film

⇨ Correlation between the electronic structure as well as dynamics (lifetimes) of the excited states and the energy conversion efficiency

Two-photon photoemission (2PPE)





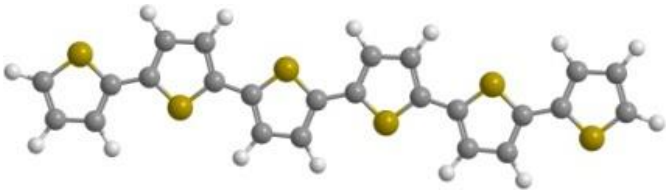


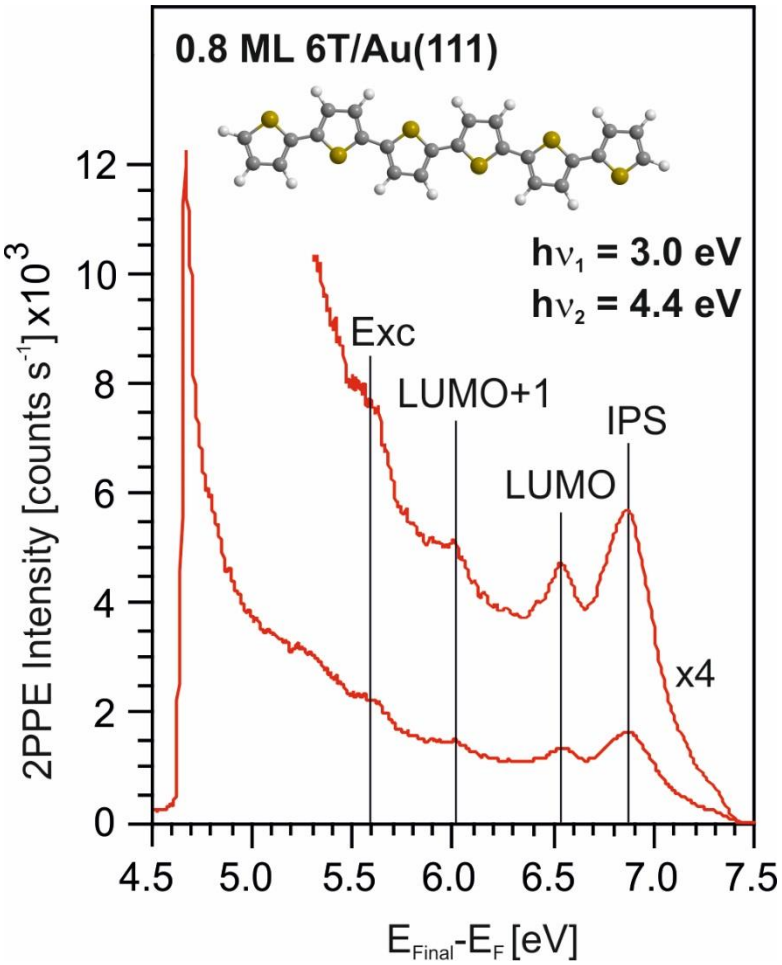
- electronic structure
- occupied and unoccupied states
- time-resolved: lifetimes
- angle-resolved: dispersion

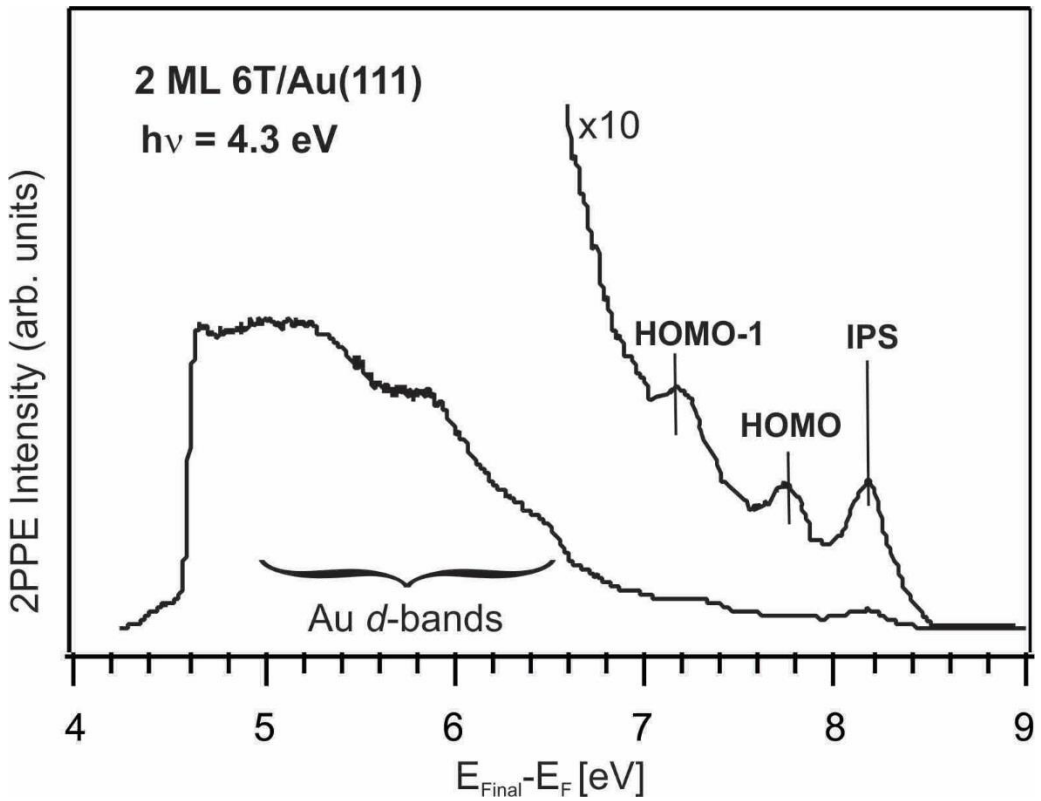
Electronic structure and exciton dynamics: 6T

UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

Electronic structure: 6T/Au(111)



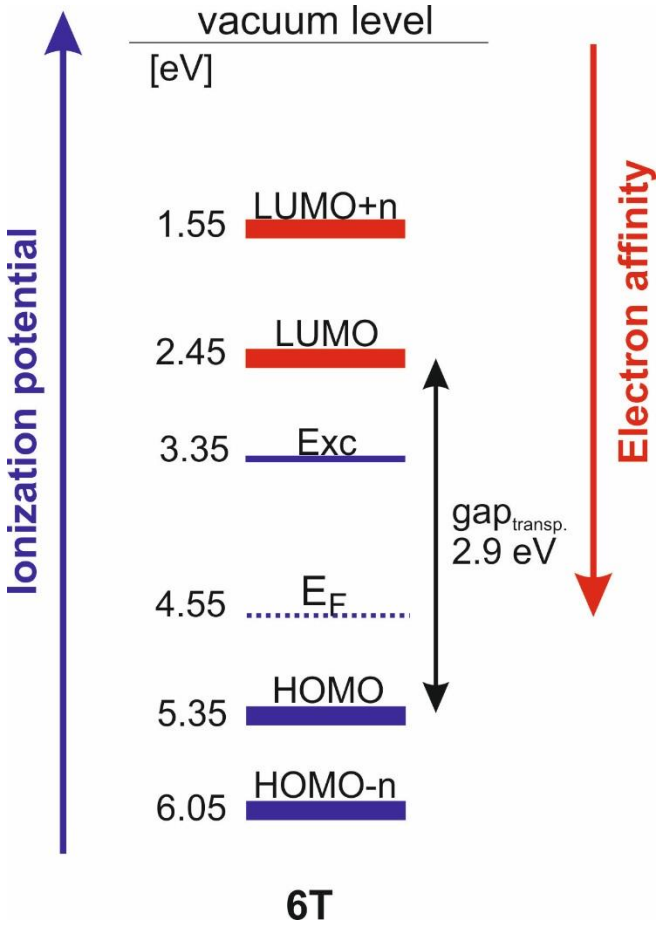




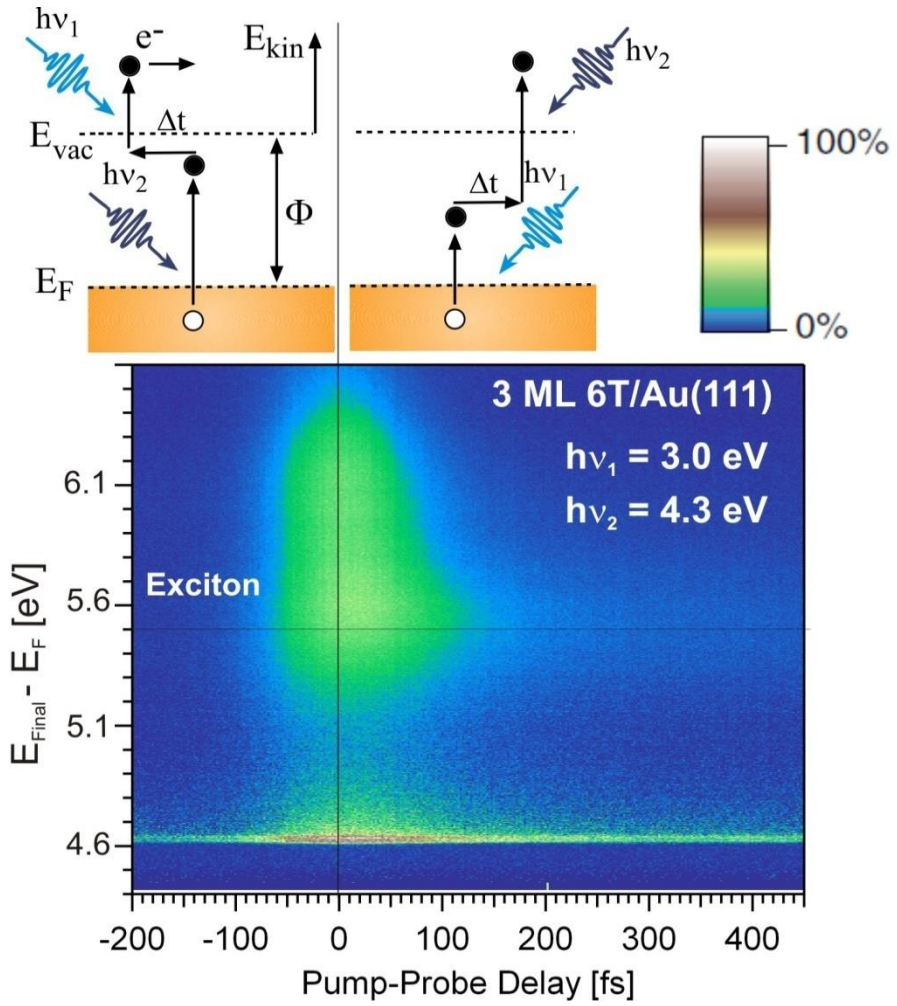
Electronic structure and exciton dynamics: 6T/Au(111)

UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

Electronic structure



Exciton dynamics

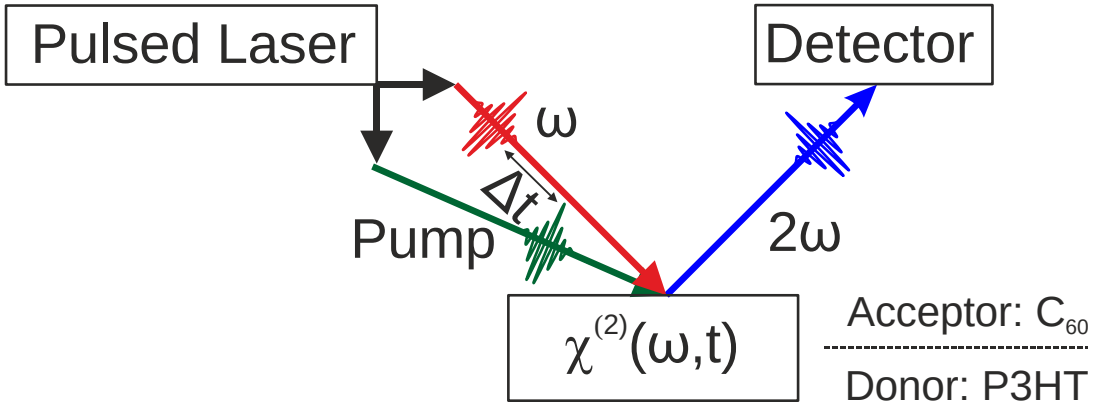


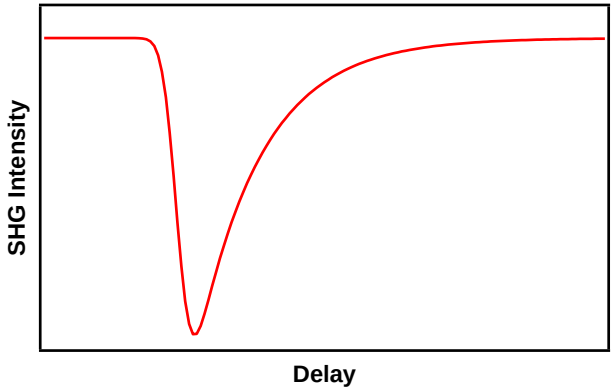
→ Exciton binding energy: 0.9 eV

→ Transport (HOMO-LUMO) gap: 2.9 eV

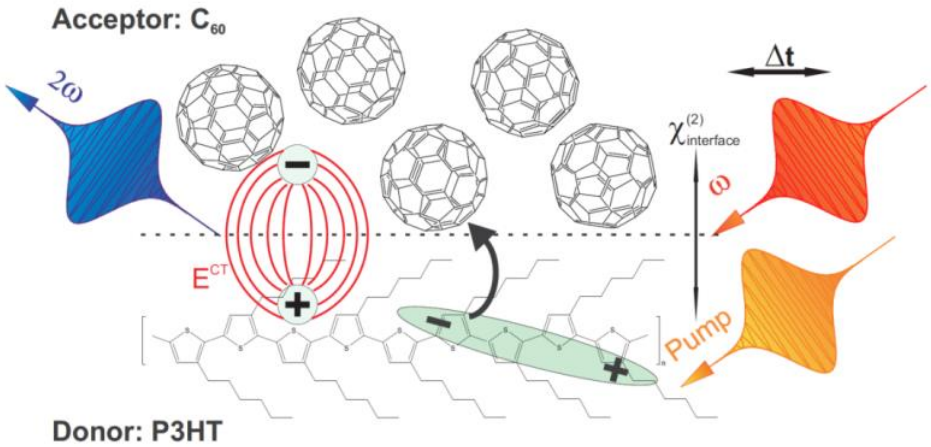
Charge separation at P3HT/C_{60} interface

Time-Resolved Second Harmonic Generation (TR-SHG)





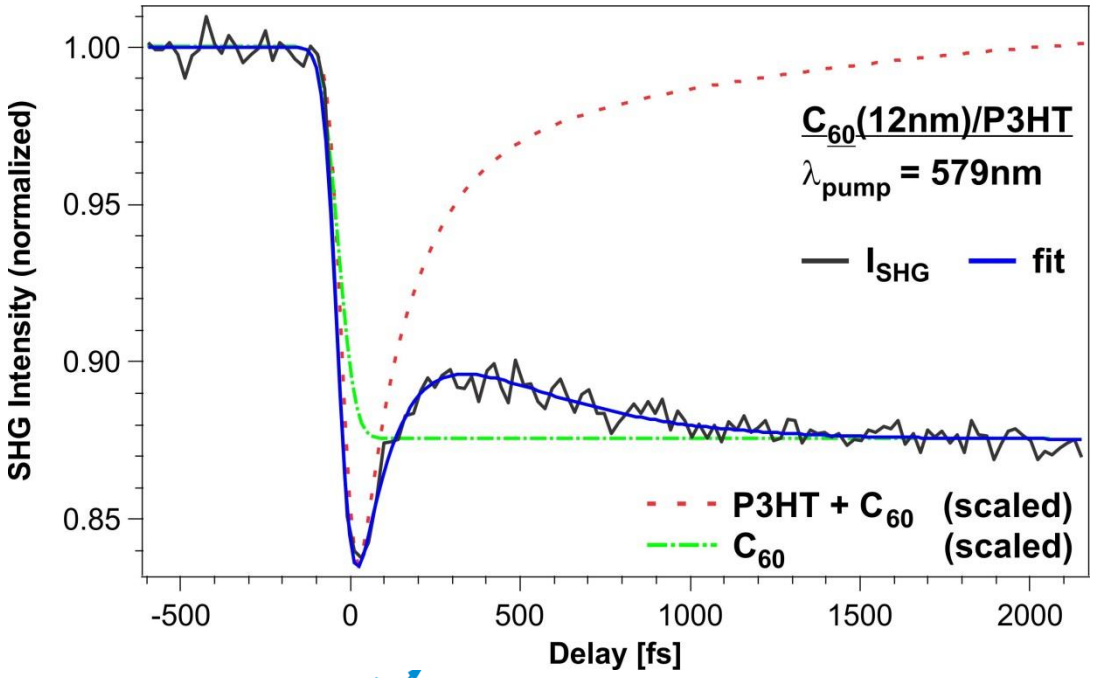
- Interface sensitive
- Time-resolved (femtosecond)
- Energy-resolved
- Polarisation-resolved

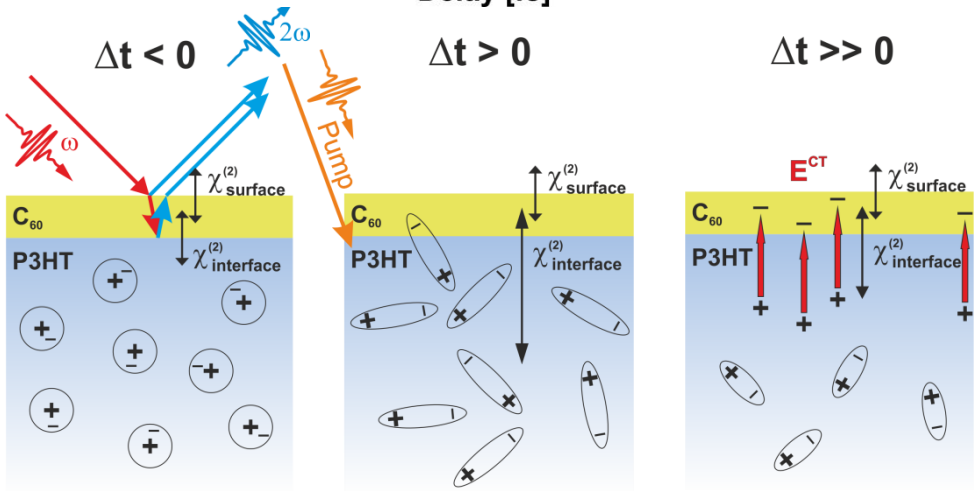


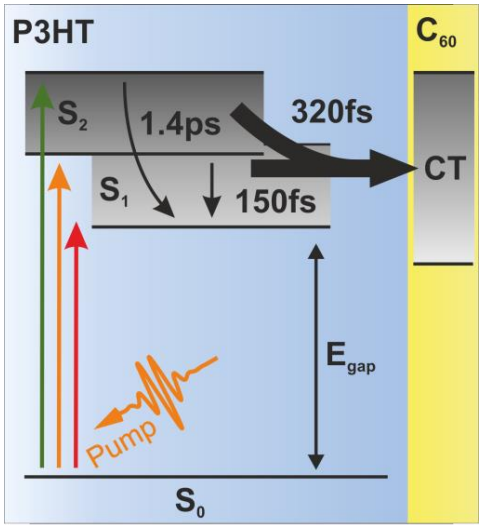
➢ Charge transfer (CT): located at the interface, electric-field-induced SHG (EFISH)

Charge separation at P3HT/C_{60} interface

C_{60}/P3HT Layer



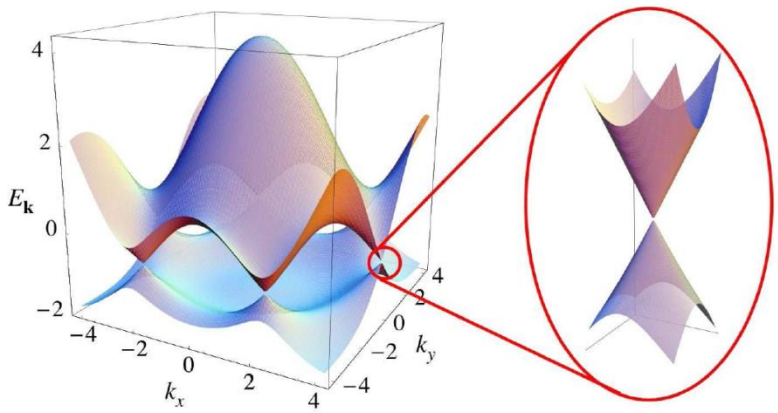


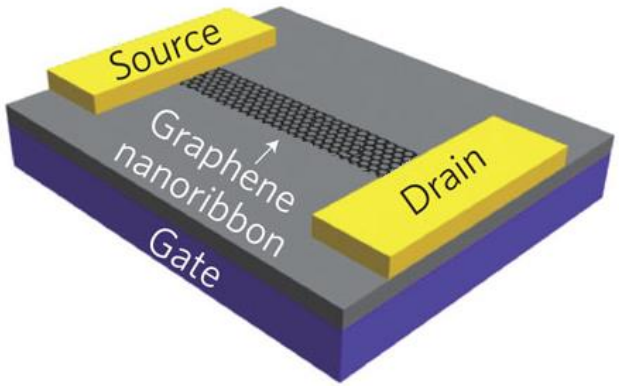


Graphene Nanoribbons (GNR)

Graphene

A. H. Castro Neto *et al.*, Rev. Mod. Phys. **81**, 109 (2009)

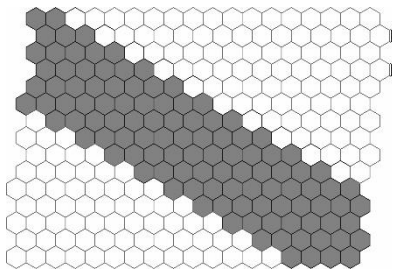




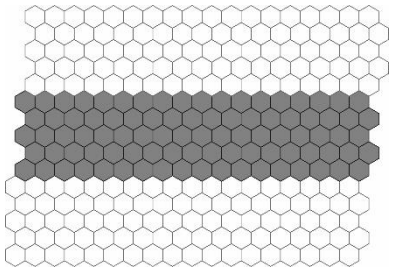
adapted from: J. Bai *et al.*, Nature Nanotechnology **5**, 655 (2010)

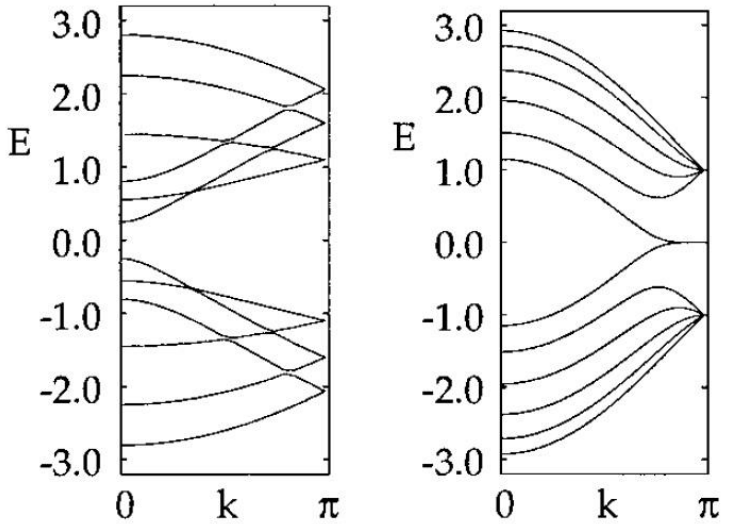
GNR

Armchair



Zigzag





K. Nakada *et al.*, Phys. Rev. B **54**, 17954 (1996)

Top-down GNR fabrication techniques

- **Lithographic patterning**

  (etch mask formed in electron beam)

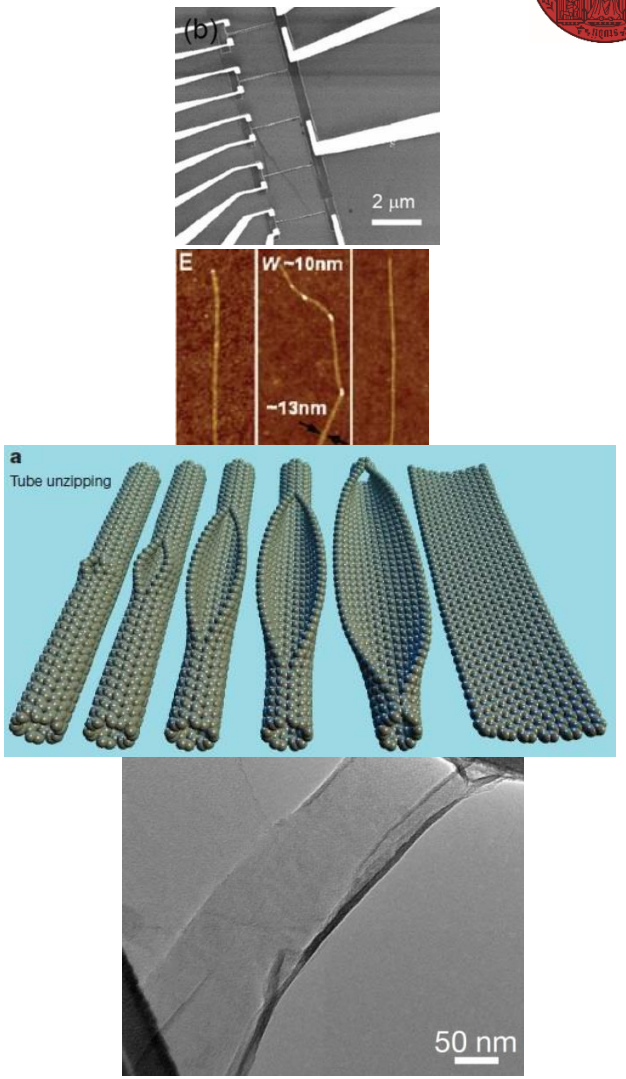
- **Exfoliating graphene**

  (annealing graphite in hydrogen gas)

- **Unzipping carbon nanotubes**

  (using $KMnO_4$)

- **<u>Problem:</u>**
  - Edges‘ quality is unclear
  - Relatively wide GNRs
  - Defects (Chemical preparation)



M. Y. Han *et al.*, Phys. Rev. Lett. **98**, 206805 (2007)
X. Li *et al.*, Science **319**, 1229 (2008)
D. V. Kosynkin *et al.*, Nature **458**, 872 (2009)

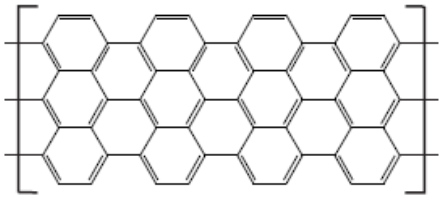
Surface-assisted bottom-up fabrication

Precursor

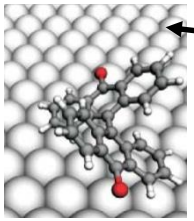
T_s=470 K:
C-C coupling

Polymer

T_s=670 K:
Cyclodehydrogenation

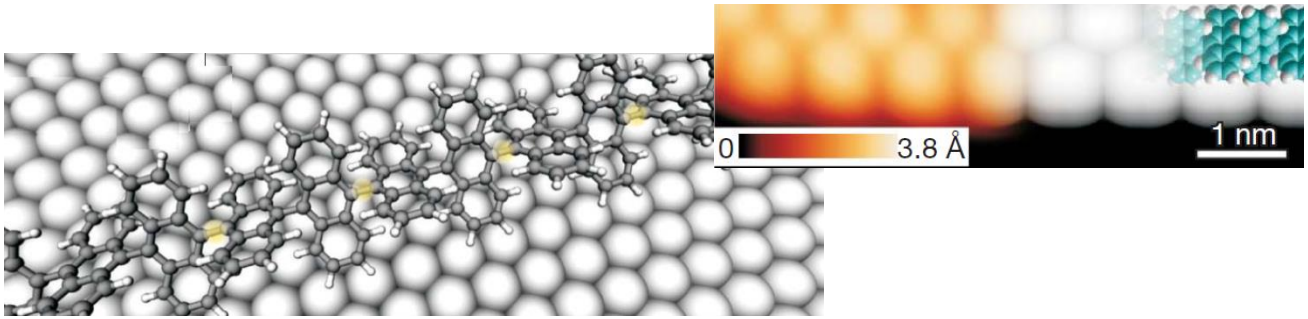


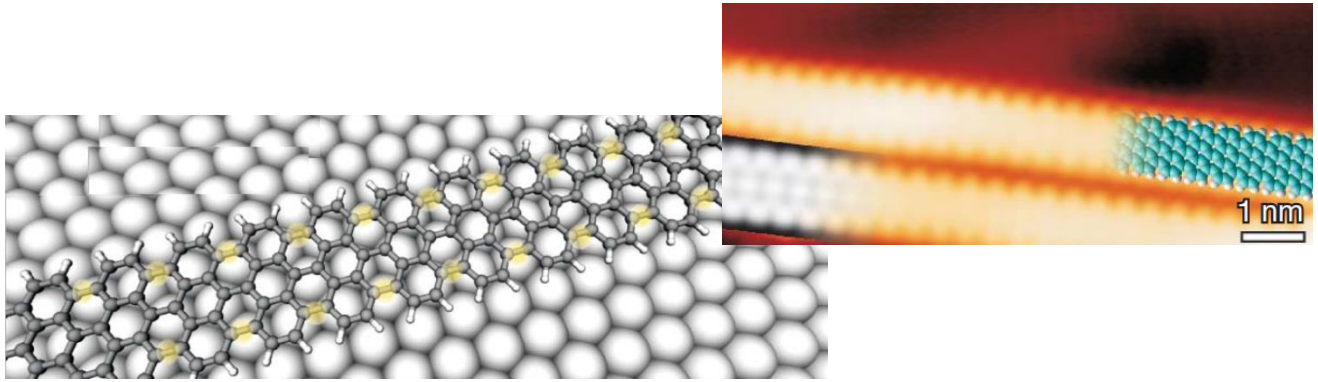
Graphene nanoribbon



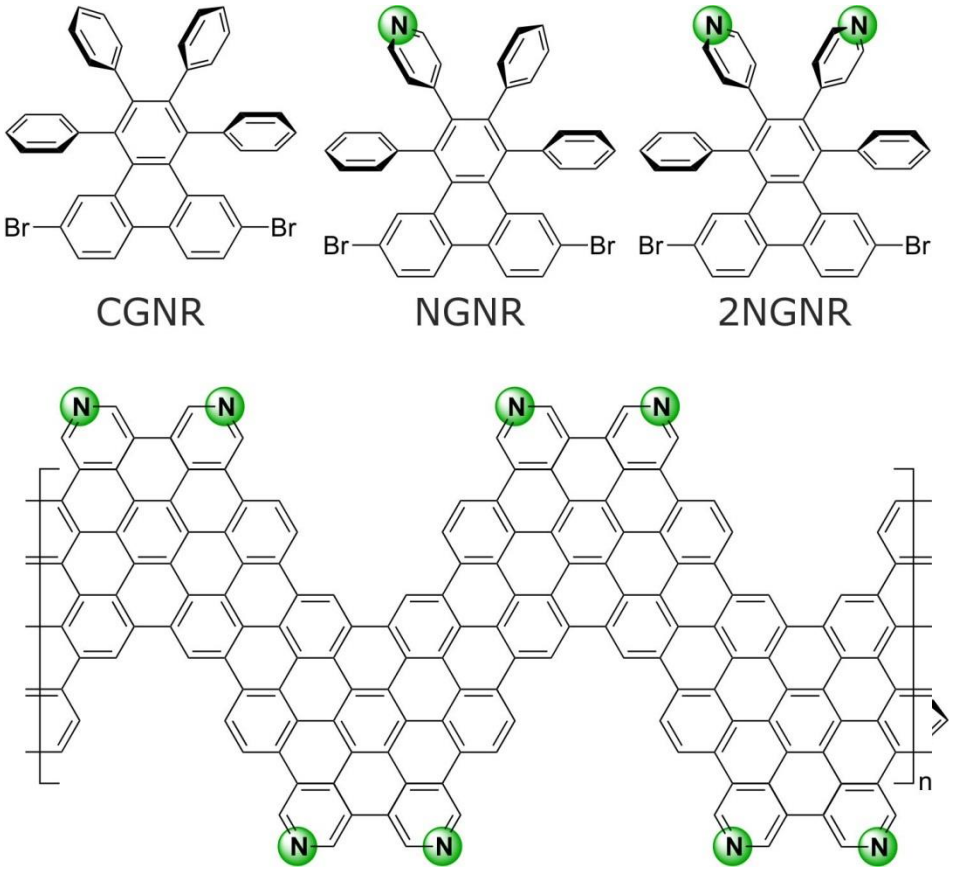
Au(111) surface

J. Cai *et al.*, Nature **466**, 470 (2010)



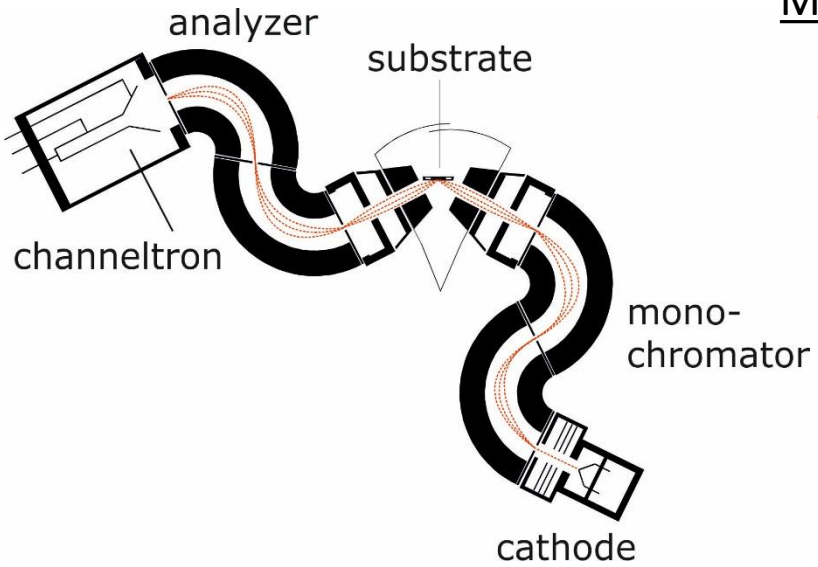


Synthesis of Doped Chevron-Type GNR on Au(111)



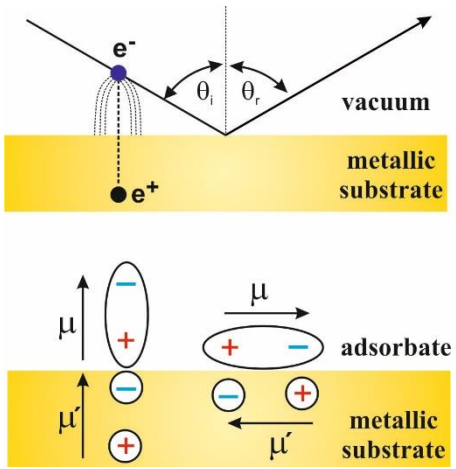
Following GNR formation with HREELS

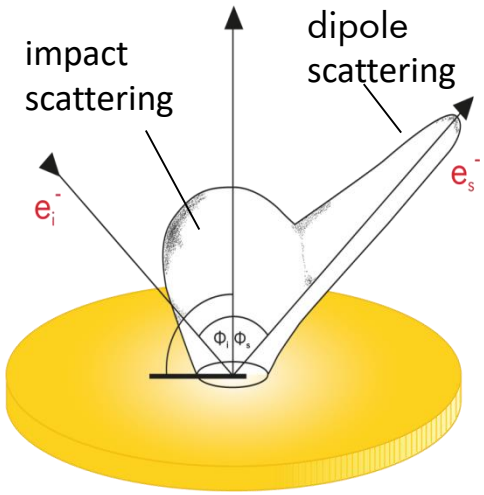
High-resolution electron energy loss spectroscopy (HREELS)



Mechanisms: dipole and impact scattering

surface-selection rule



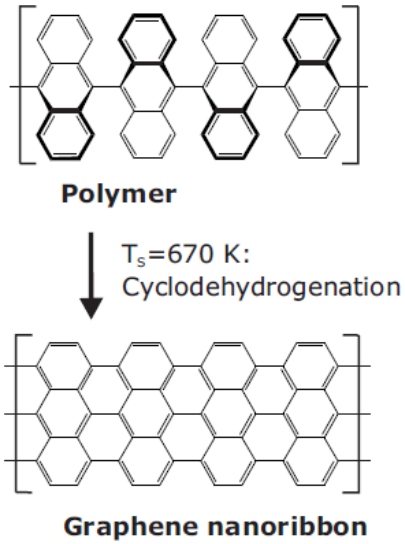


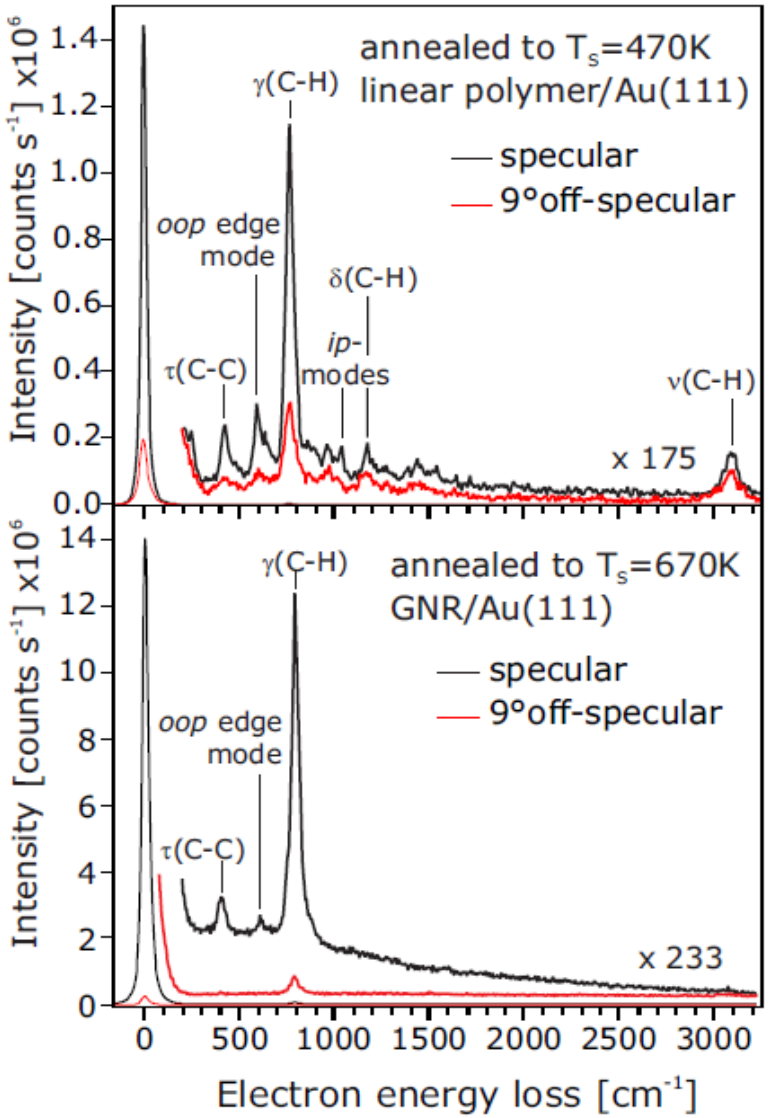
- Vibrational spectroscopy: molecular orientation
- Electronic transitions: optical gap, optically forbidden transitions

Two scattering regimes

- Specular geometry $\Phi_i=\Phi_r$
- Off-specular geometry $\Phi_i\neq\Phi_r$

Following GNR formation with HREELS

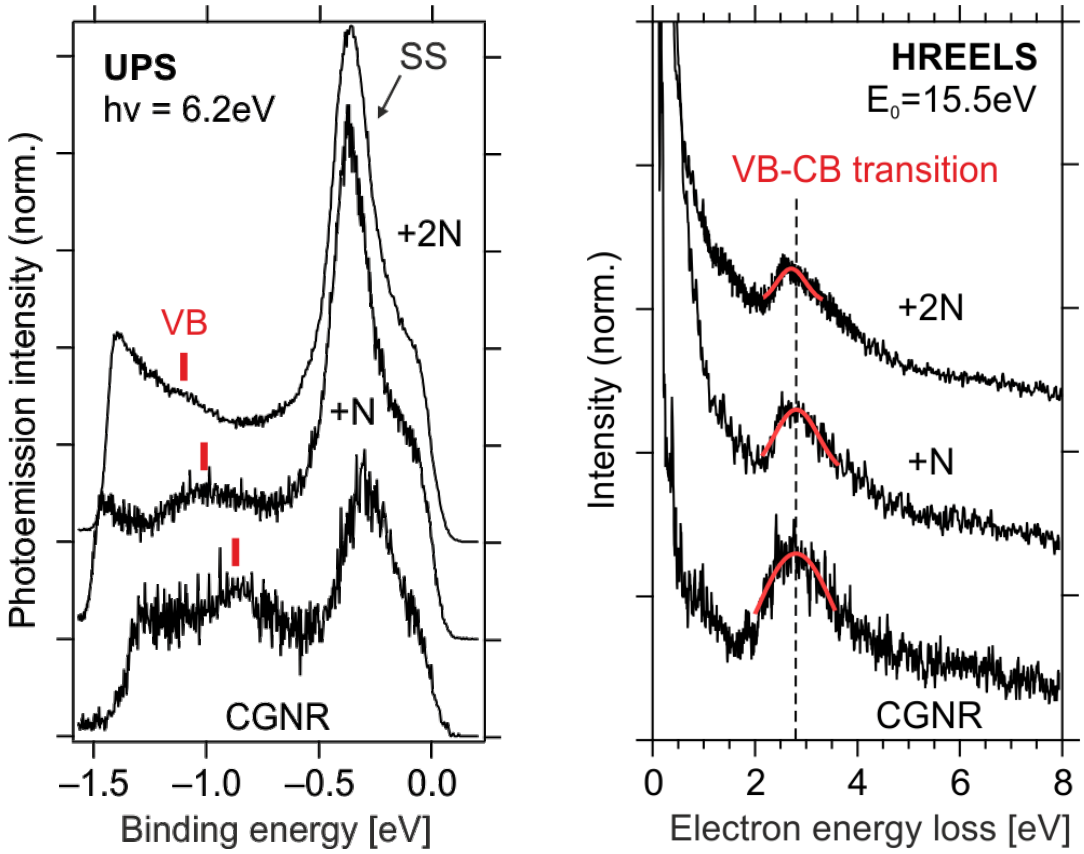




Pronounced changes

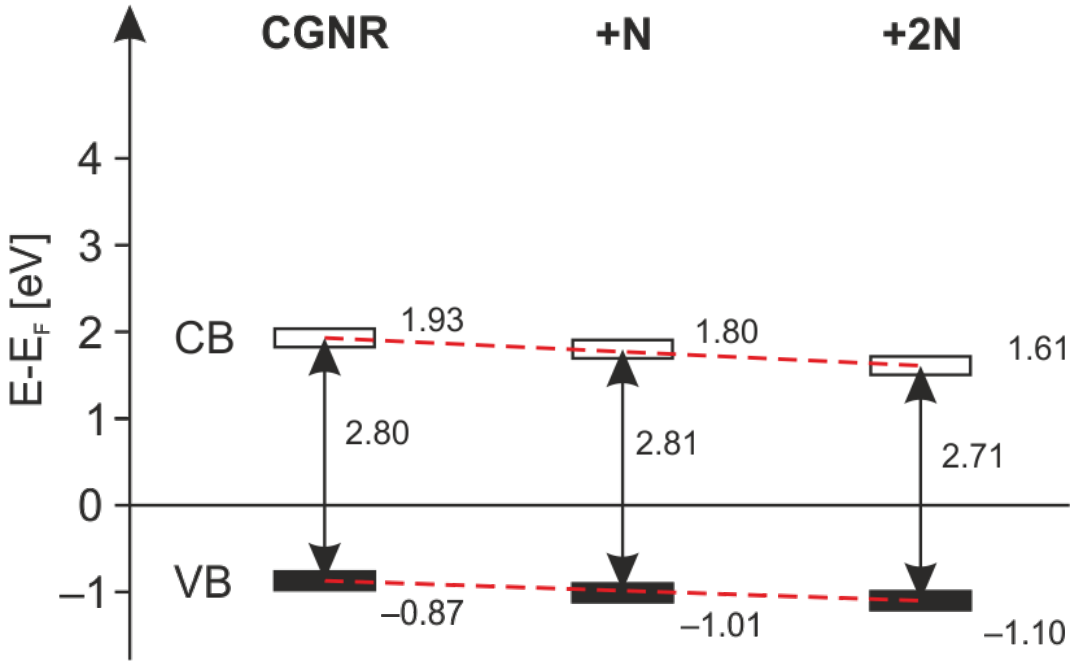
- Higher elastic peak
- Less modes
- Increased dipole-activity of bending mode

Band Structure of the Doped GNR



- VB shifts to lower energies
- Band gap of 2.8eV independent of doping

Effect of Doping on the Electronic Structure



- **Shift** of approx. 0.1 eV/N to lower energies
- Band gap **size** remains unaffected
- Atomcially **precise** dopant concentration and position
- Does not interfere with bottom-up **synthesis**

Bachelor-, Master- & PhD – positions available!!