

IHP Research Training Network Title:

Designing Inorganic/Organic DEvices

Network short title: **DIODE**

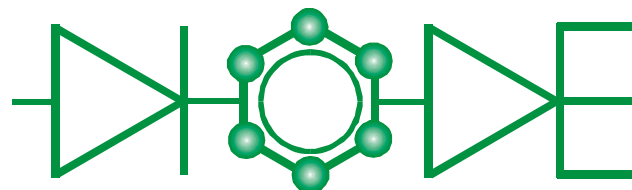
Contract No: HPRN-CT-1999-00164

Commencement date of contract: 1.2.2000

Duration of contract: 48 months



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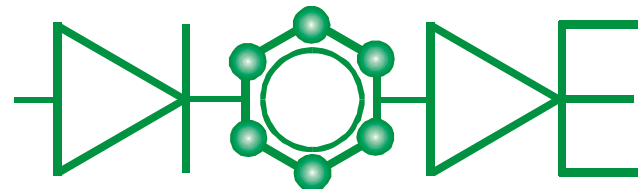
*DRTZ*

*TUC*

# Science and Networking



IHP Research Training Network



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*TUC*

# The DIODE Partners

Technische Universität Chemnitz (TUC)

Universidad Autonoma de Madrid (UAM)

Technische Universität Braunschweig (TUB)

Trinity College Dublin (TCD)

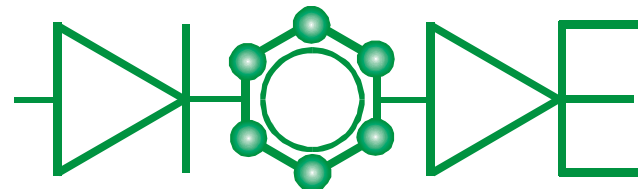
Universita degli Studi di Roma “Tor Vergata” (Rome)

University of Wales Aberystwyth (UWA)

Universität-GH Paderborn (UGHP)

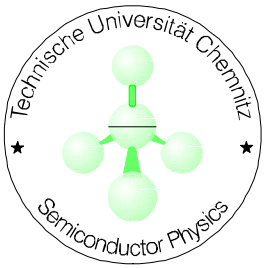


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# Molecular Control of **III-V** Diodes

**Metal/III-V Semiconductor** contacts

High frequency  
application

e.g. Mixers,  
Modulators

**Challenge:**  
lowering operating voltage.

**Organic thin interlayer**

- **Metal/organic/InP**

A. Böhrer *et al.* Mater. Sci. and Eng. B  
51 (1998) 58

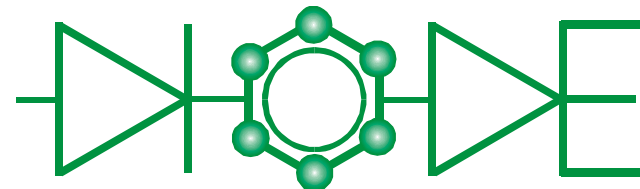
: Rectifying behavior

: Superior to commercial diode

: High frequency limit: 42 GHz



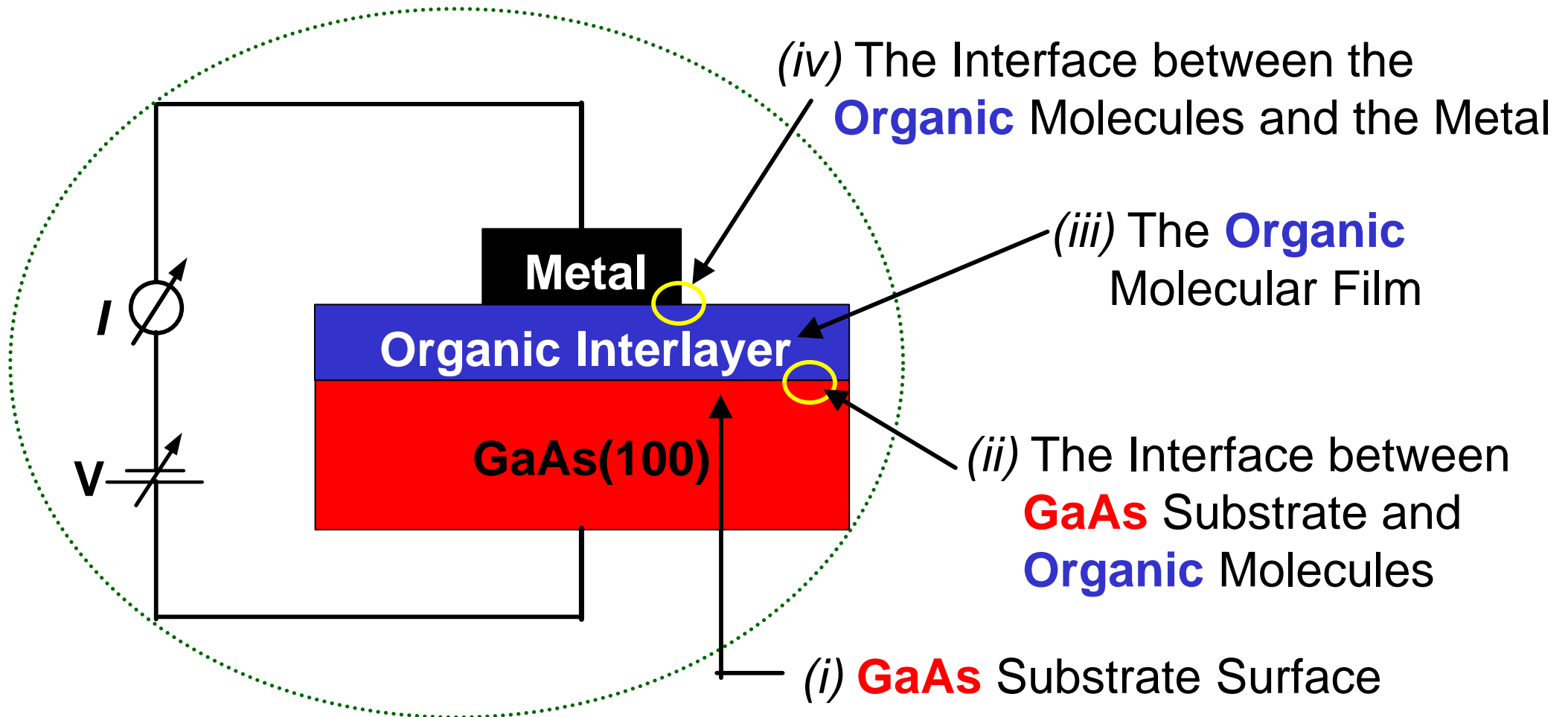
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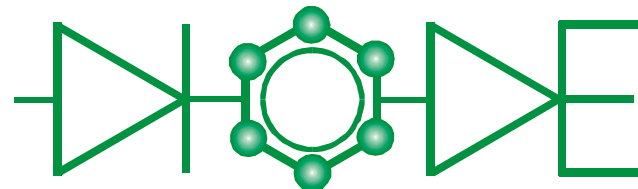
Dietrich RT Zahn,  
TU Chemnitz

# DIODE: Objectives and Work Plan

(v) The Overall Device Performance



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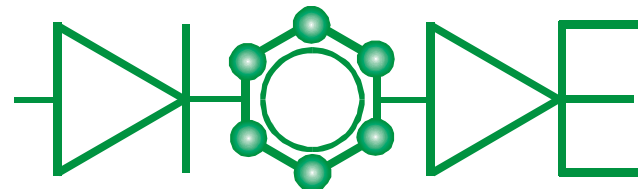
*D. R. T. Zahn,  
TU Chemnitz*

# Methods and Approach

Node	Core Expertise
TUC	Optical and electrical probes
UAM	Band line-up theory, local structure
TUB	Device fabrication and characterisation
TCD	Structural probes: Synchrotron radiation
Rome	Device simulation, theory of current transport
UWA	Chemical and electronic state probes
UGHP	Theory of molecular structure/ adsorption



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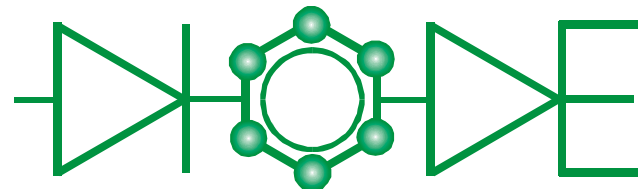


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# Milestones

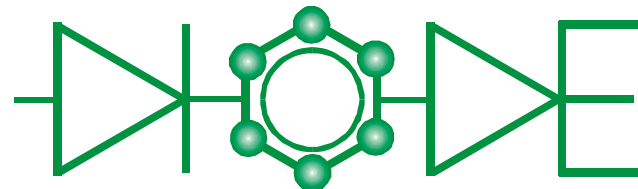
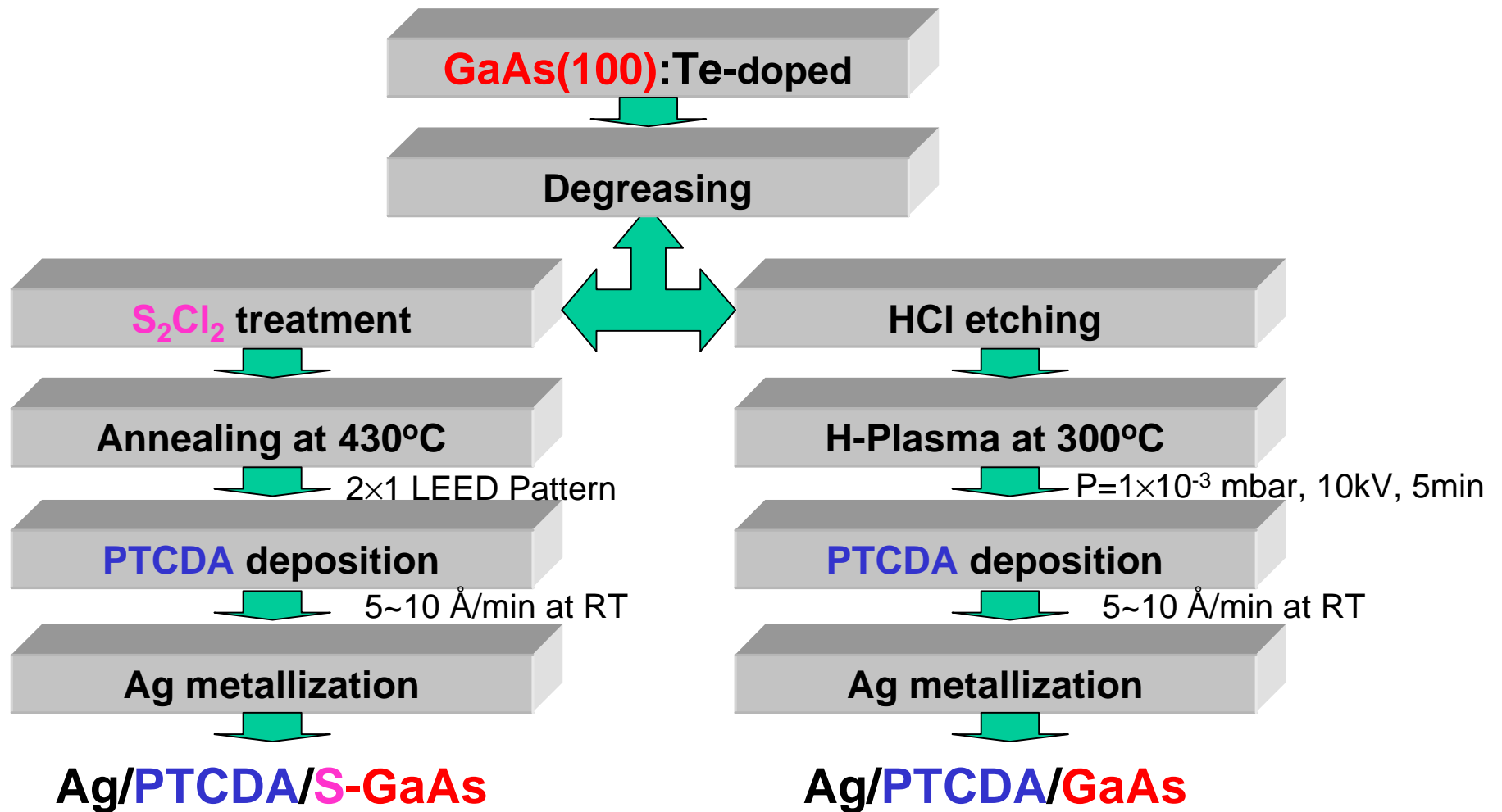


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# GaAs Surface Preparation







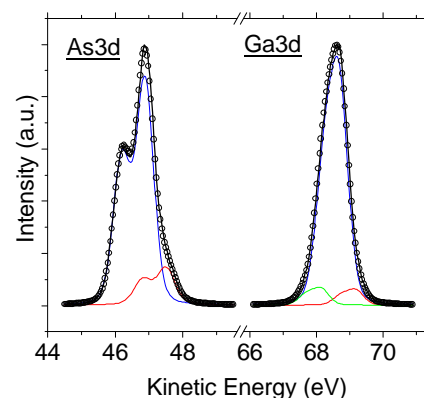
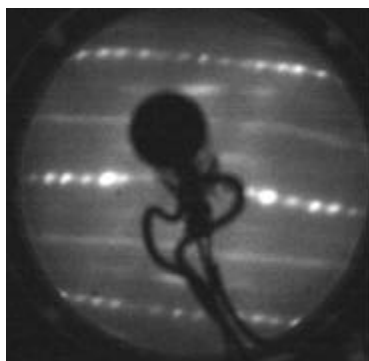
# GaAs(001) substrate preparation



The TCD group is investigating a range of substrate preparation methods, by a combination of LEED and SXPS.

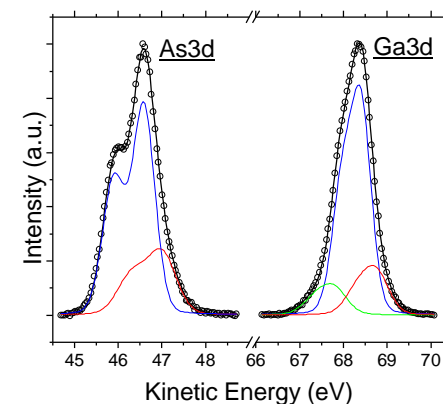
- **Argon sputtered GaAs(100)-1x6:**

Sample sputtered for one hour at 500eV at room temperature, argon pressure of  $7 \times 10^{-5}$  mbar, sample current of 2.5  $\mu$ A. Annealed at 500°C for 20 minutes and cooling rate of 20°C/min.

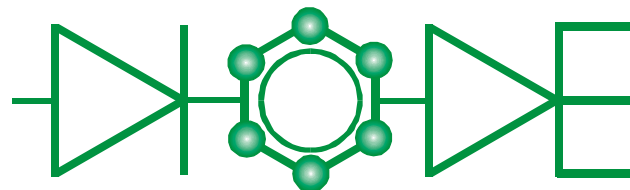


- **Atomic hydrogen cleaned GaAs(100)-2x1:**

two cycles of 30000 L (equivalent to 25 mins exposure @  $2.6 \times 10^{-5}$  mbar) of atomic hydrogen, one at room temperature, the second at 300°C). The room temperature treatment removes the Group V oxides while the high temperature cycle removes the Group III oxides.



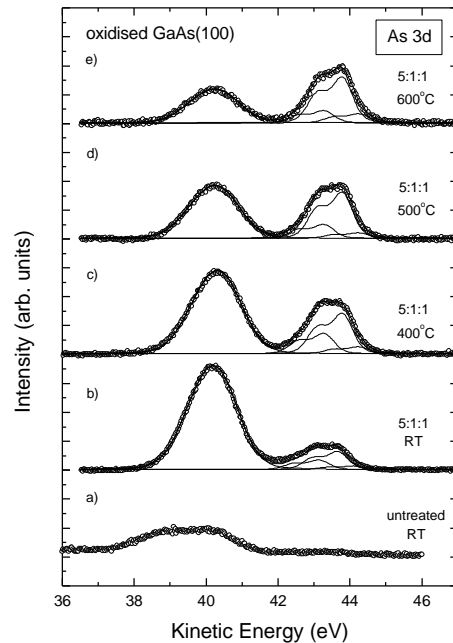
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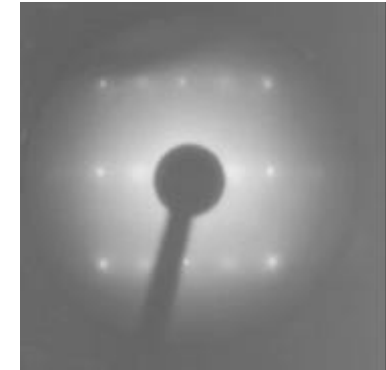
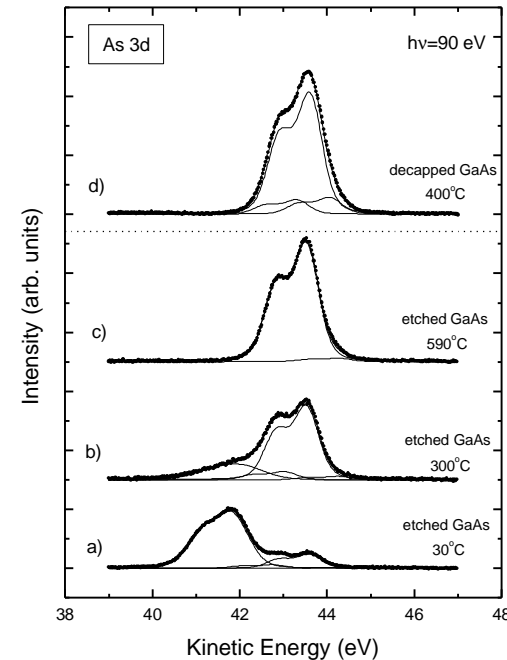
Gregory Cabailh  
TrinityCollege  
Dublin

# The GaAs Surface

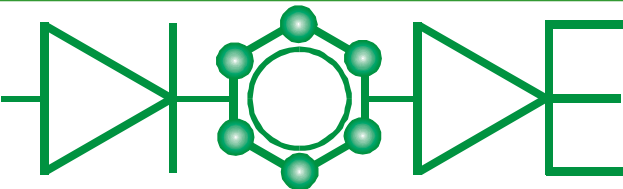
## Oxide-terminated



## Sulfide-terminated



- As and Ga oxides – thermally stable
- Surface is not ordered
- As-S desorbed at 500°C
- Surface is ordered – 2x1



# UAM: Se-induced Surface Reconstruction

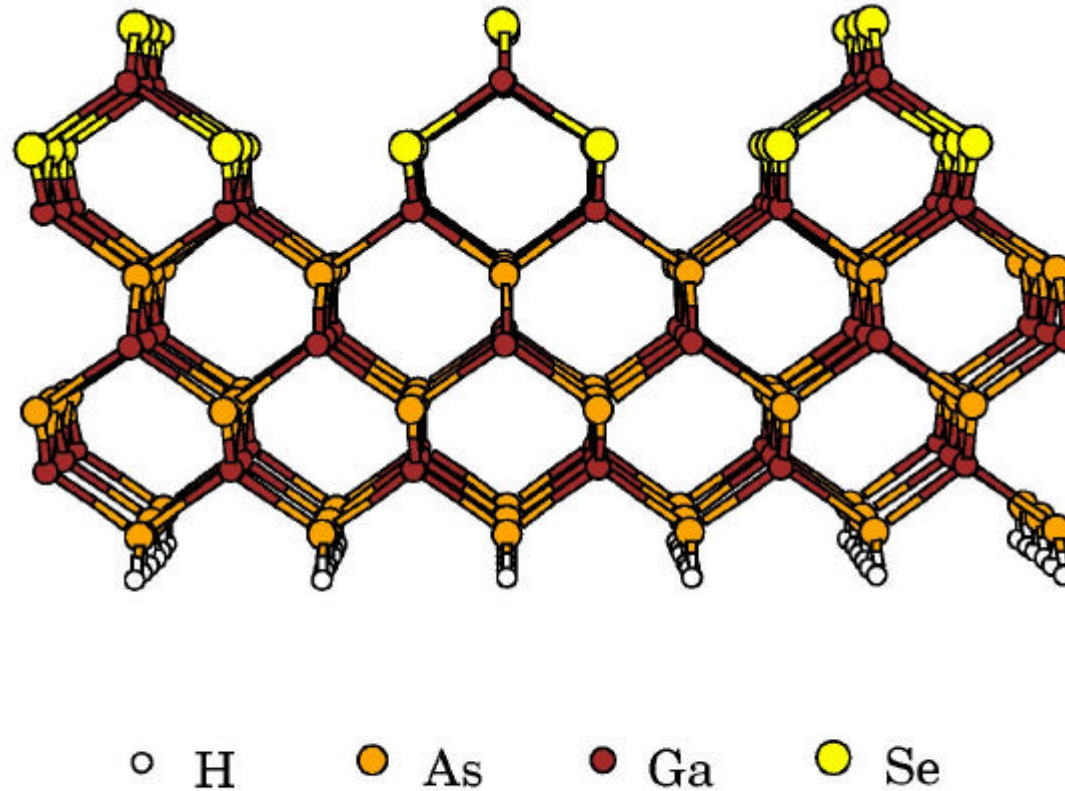
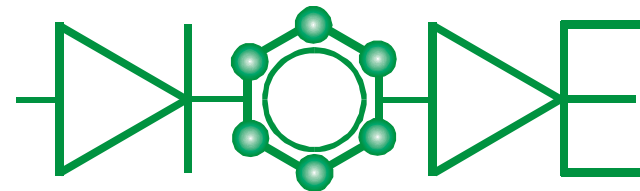


Figure 1: Lateral view of the Se-passivated GaAs(100)-surface.

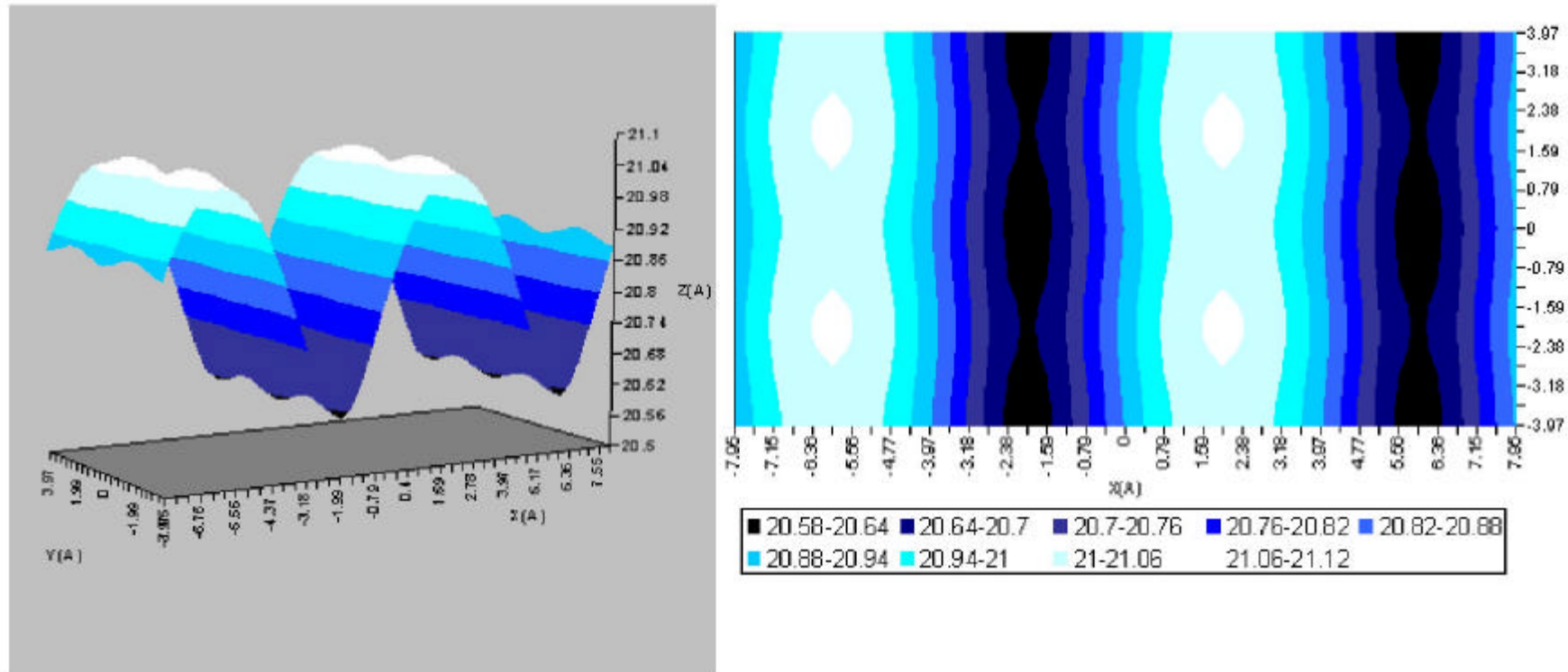


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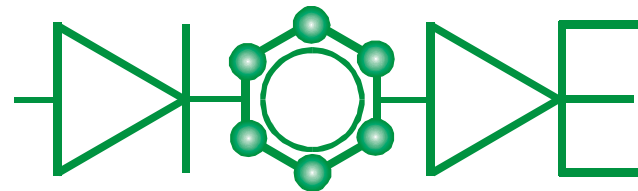


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# UAM: Calculated STM Images



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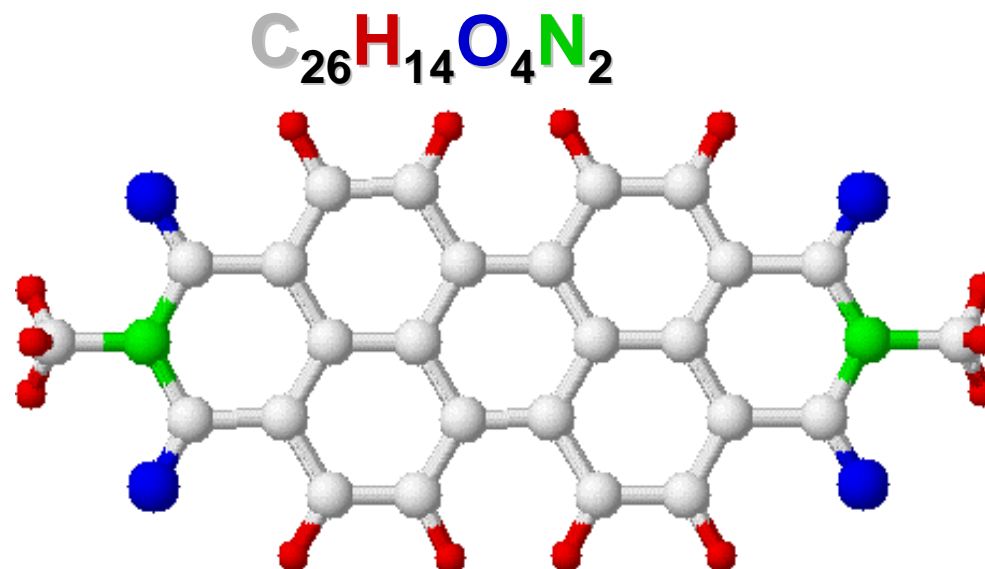
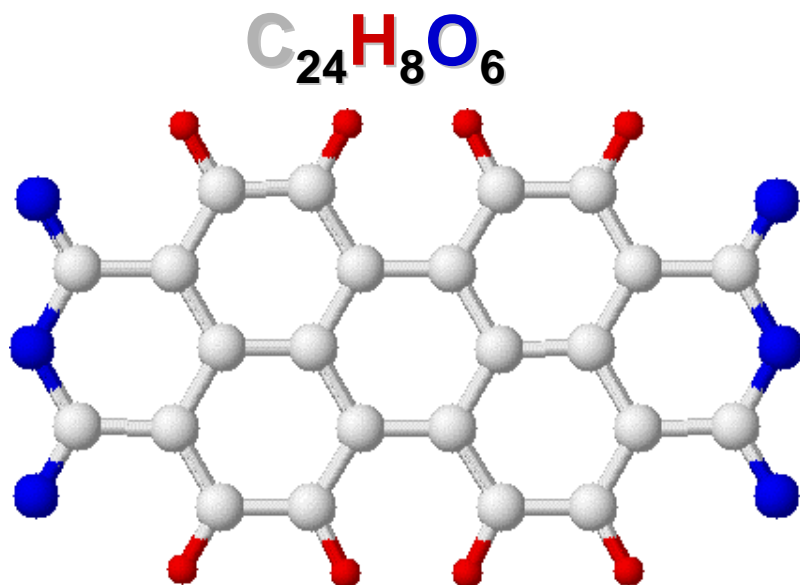


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# Perylene derivatives

**PTCDA**: 3,4,9,10- Perylenetetracarboxylic dianhydride

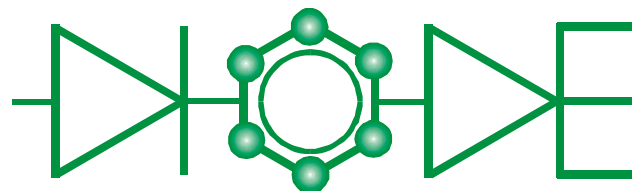
**DiMe-PTCDI**: 3,4,9,10- Perylenetetracarboxylic diimide



+ Phthalocyanines at UWA



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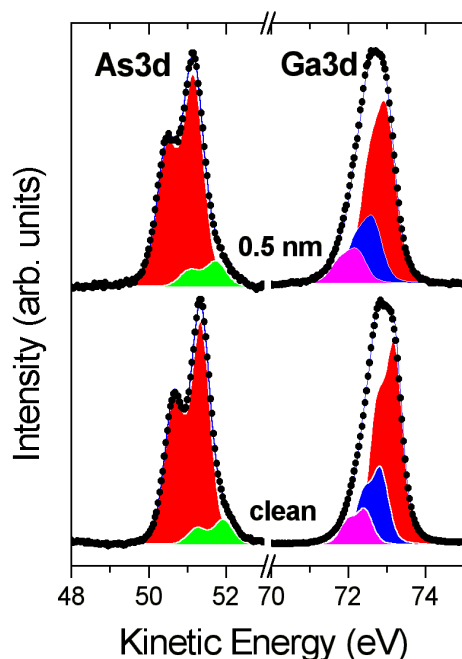


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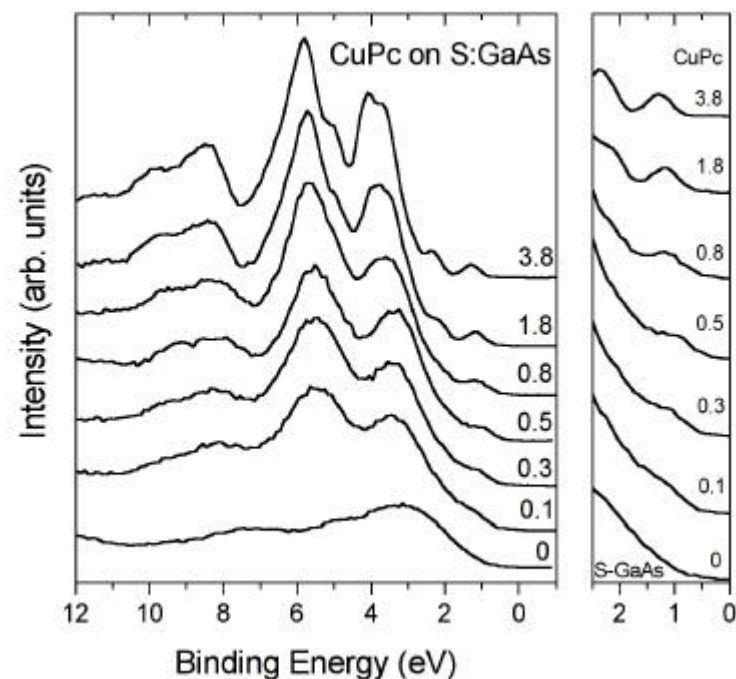
# Organic layers

## Interface Bonding

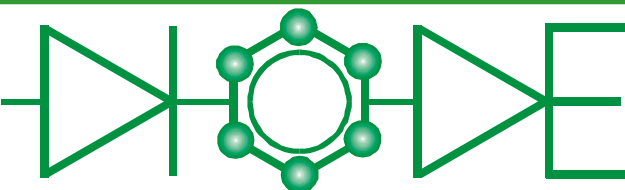


- CuPc on GaAs – core level SXPS
- Very weak interface bonding

## Occupied electronic states



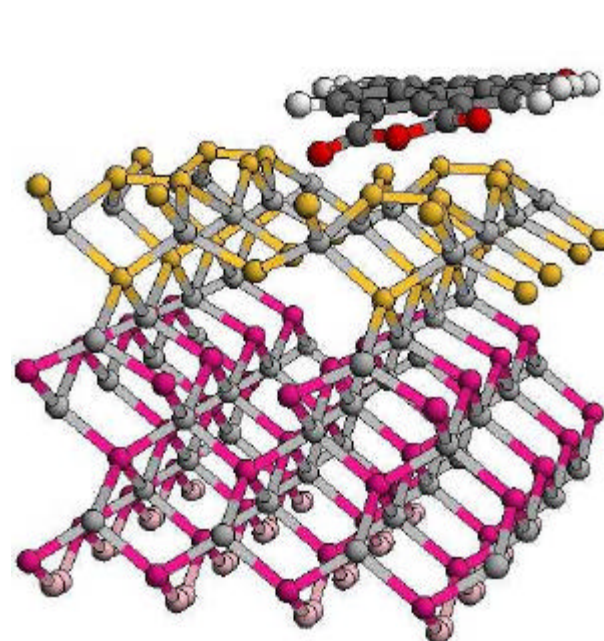
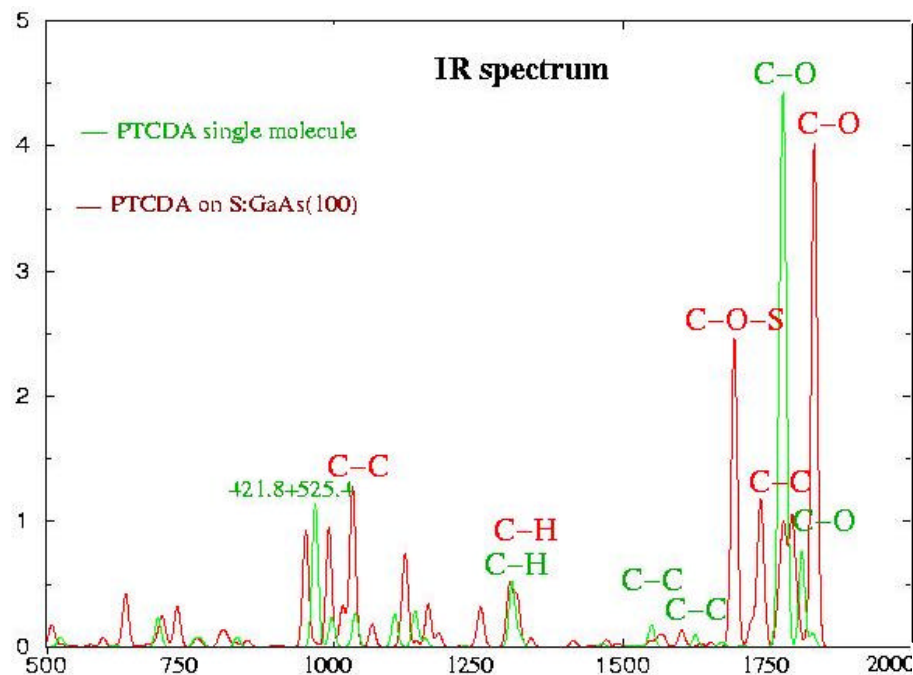
- CuPc on GaAs - valence level SXPS
- Development of CuPc MO states



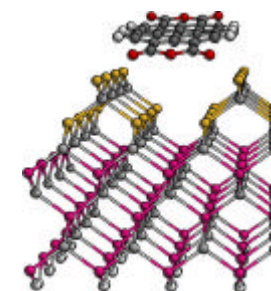




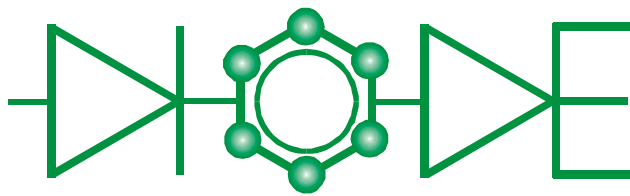
# Single PTCDA molecule on S:GaAs



- The most stable position of one PTCDA molecule on the *b* reconstructed S:GaAs
- In the IR spectrum of the adsorbed molecule the C-O peak splits
- Interaction between the surface S and the O of the PTCDA
- Right, the most stable position of one PTCDA molecule on the *i* reconstruction
- Further analysis of monolayers and a realistic interface follows



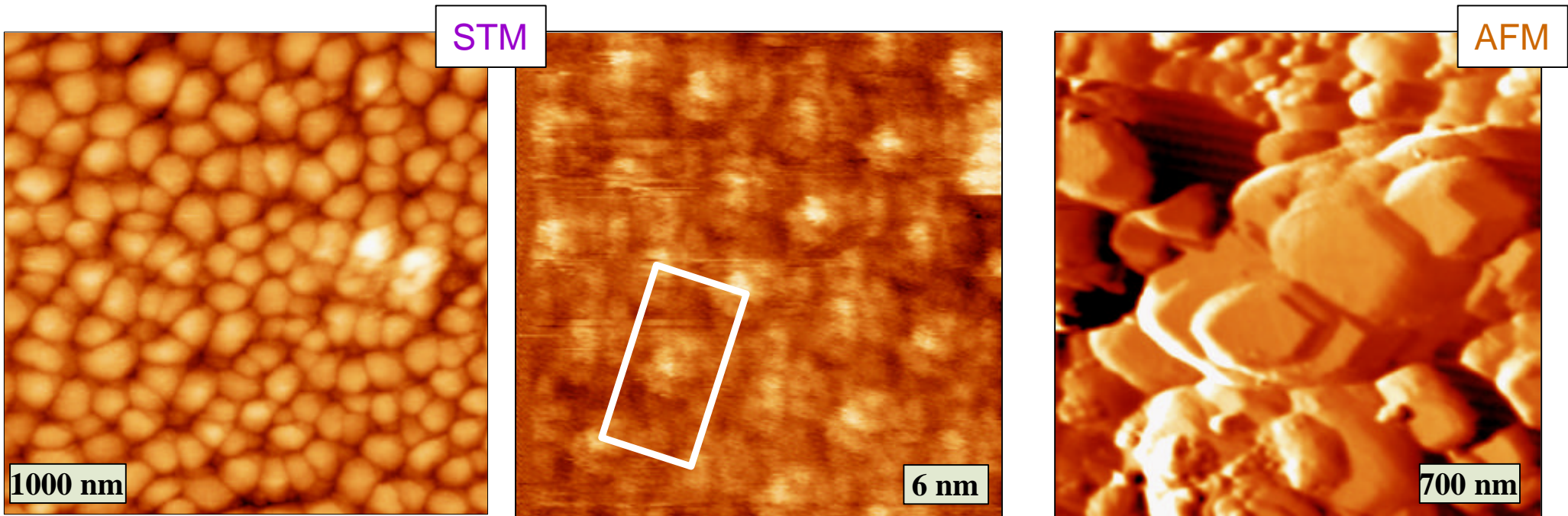
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Szucs Bernadett,  
Paderborn

# UAM: STM and AFM

*PTCDA /S-GaAs(100)*

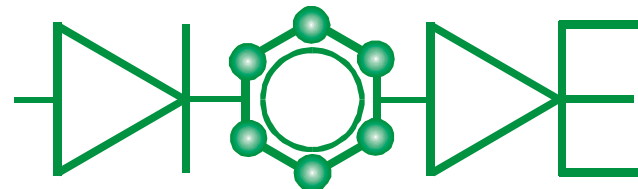


- Growth of the organic layer
  - Molecular resolution
  - Bulk unit cell

- Growth of Organic Crystals

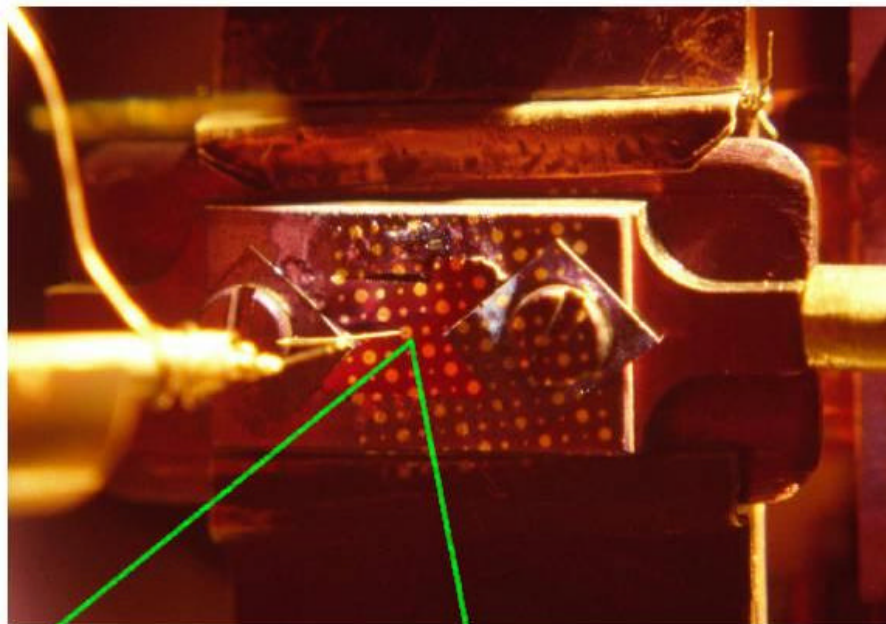


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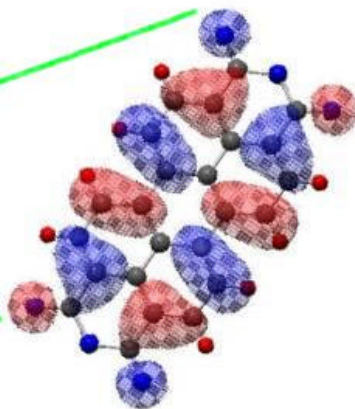
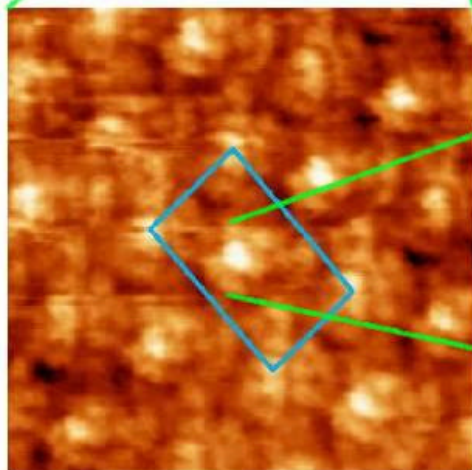


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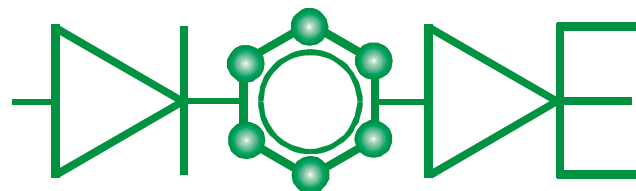




*In situ* IV probing of  
Ag/PTCDA/GaAs  
diodes

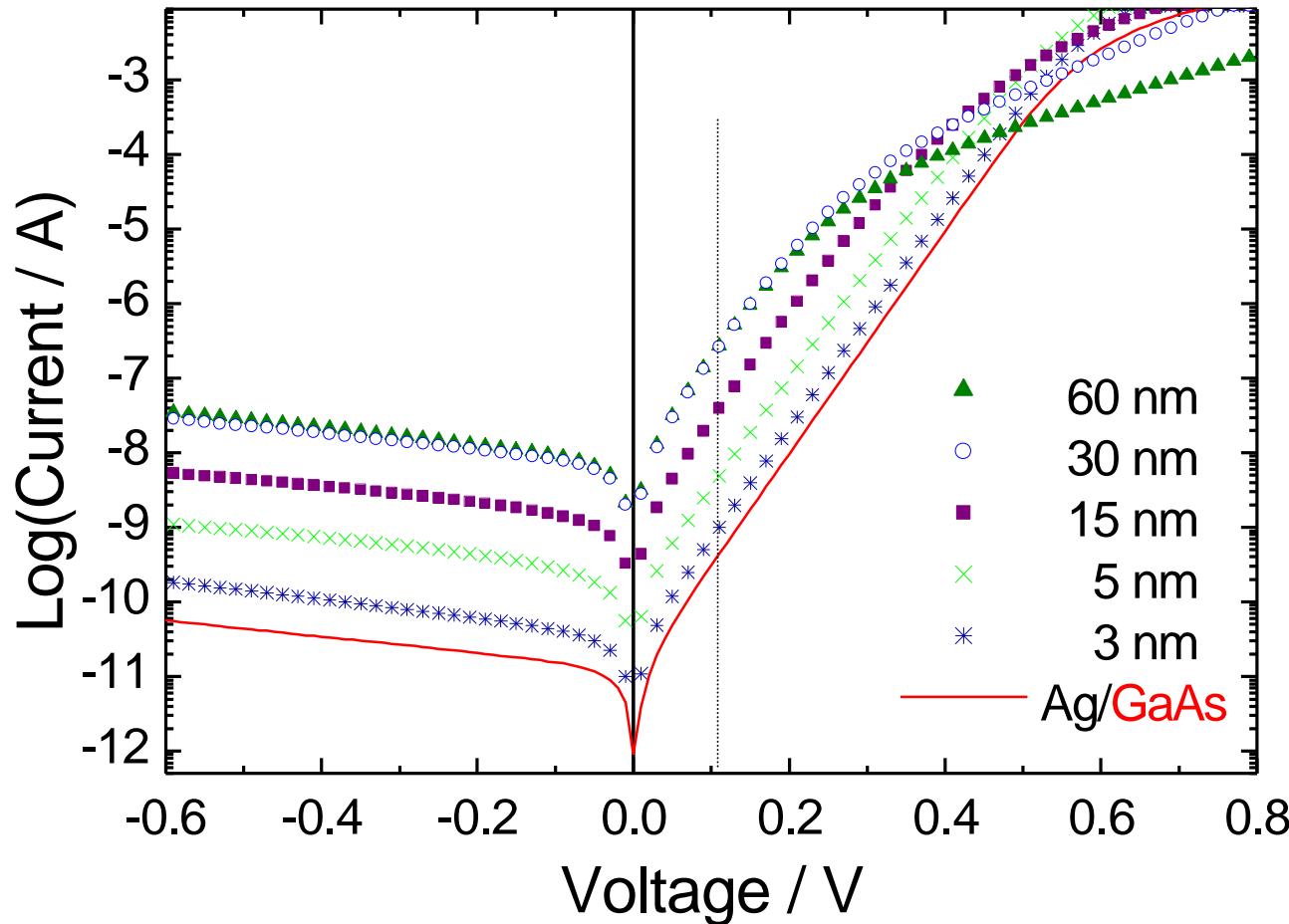


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# IV Characteristics of **Ag/PTCDA/GaAs(100) Diodes**



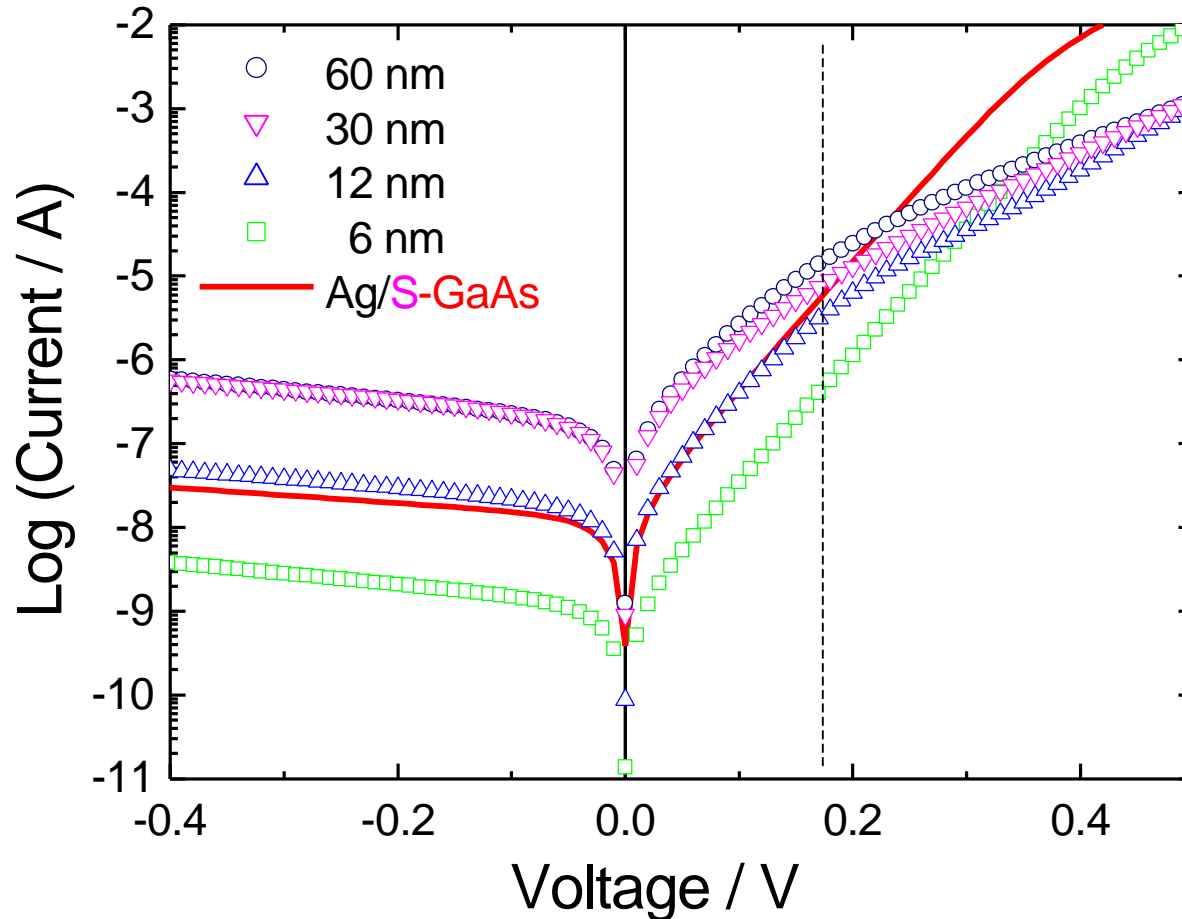
## Low injection region:

- Current  $I$  **increases** with layer thickness  $d$ .
- Current can be described by **thermionic emission**.

## High injection region:

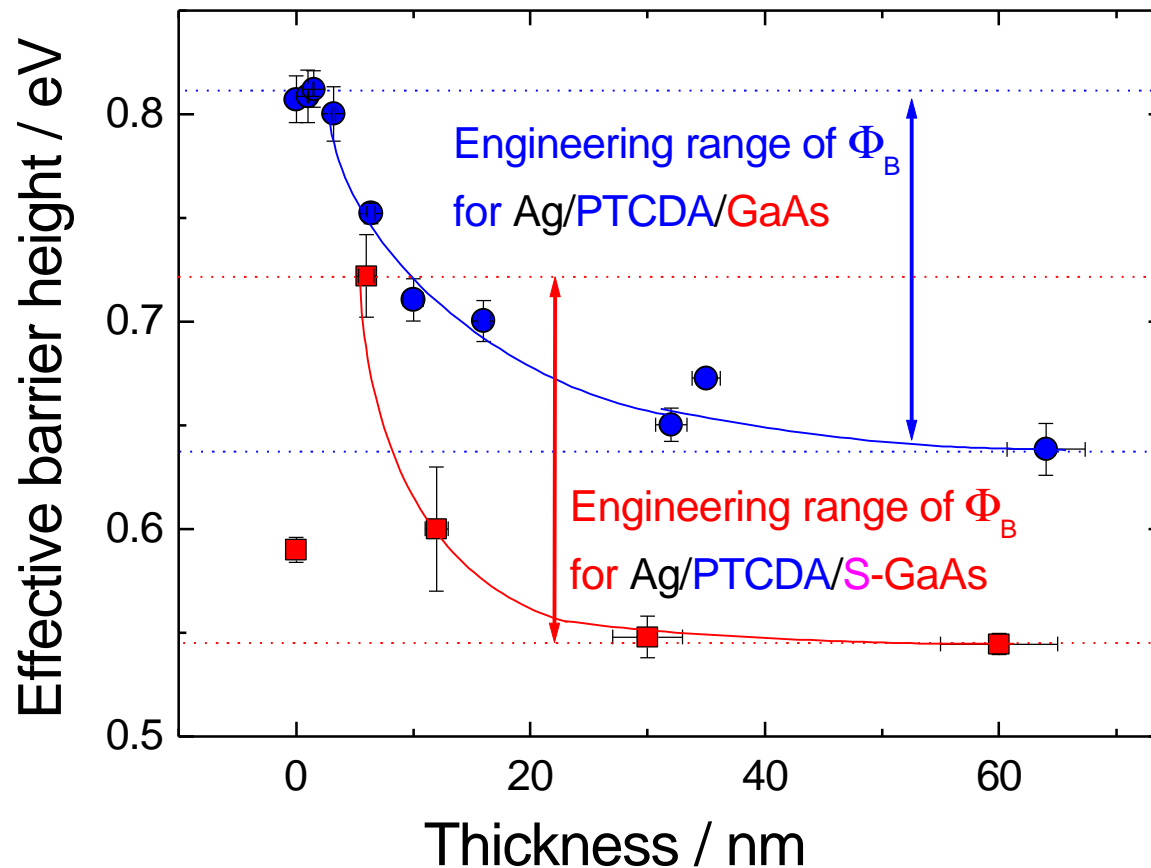
- Current  $I$  **decreases** with layer thickness  $d$ .
- **Space charge effects** govern the transport behaviour.

# IV Characteristics for **Ag/PTCDA/S-GaAs(100)**



- **Low injection region:**
  - Initial decrease in current, then increase
  - Saturation above 30 nm.
- **High injection region:**
  - Dominated by **SCLC**

# Effective Barrier Height for Ag/PTCDA/GaAs(100) Diodes

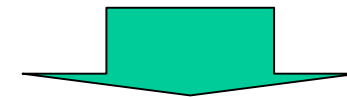


- Ag/PTCDA/GaAs

$\Phi_B = 0.64 \sim 0.81$  eV

- Ag/PTCDA/S-GaAs

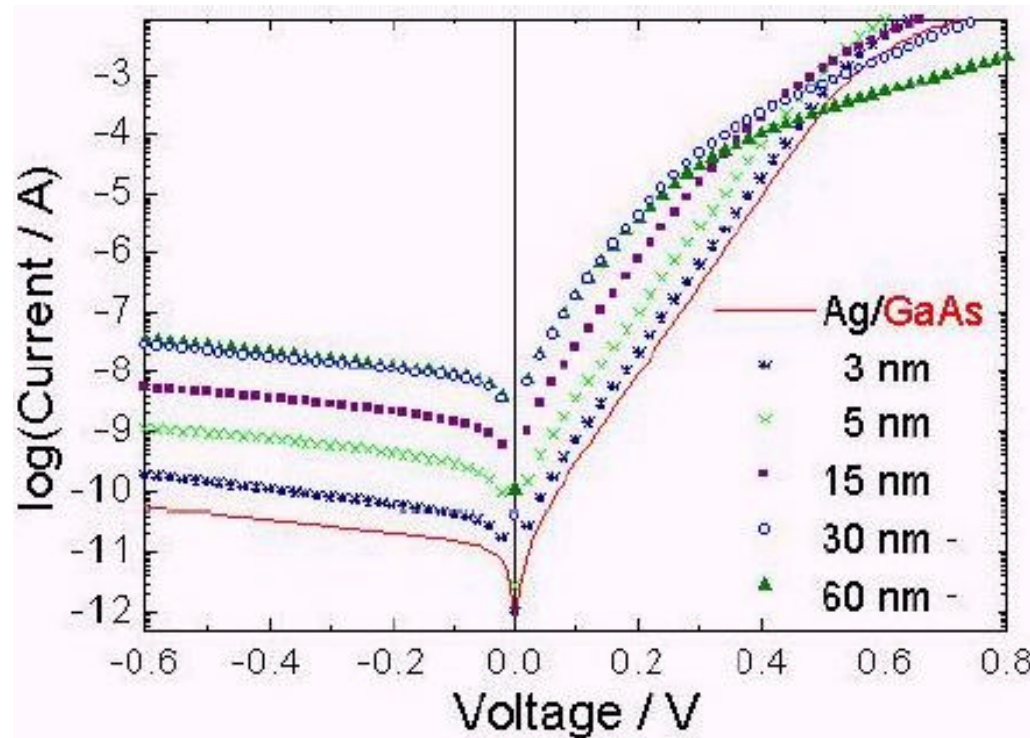
$\Phi_B = 0.54 \sim 0.73$  eV



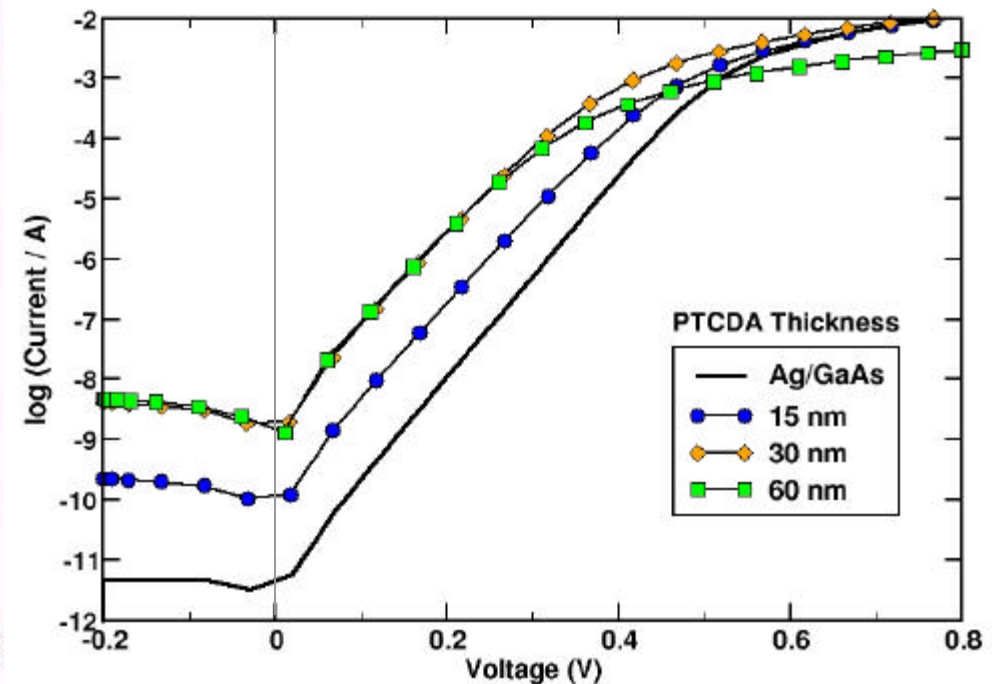
The effective barrier height can be tuned by different surface treatments and by the organic modification.

# Comparison Experiment and Simulation

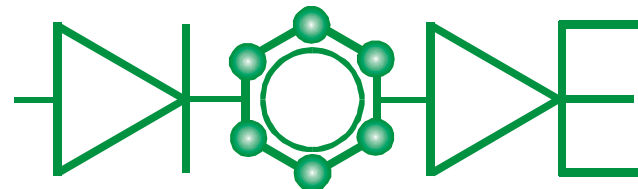
TUC



Rome



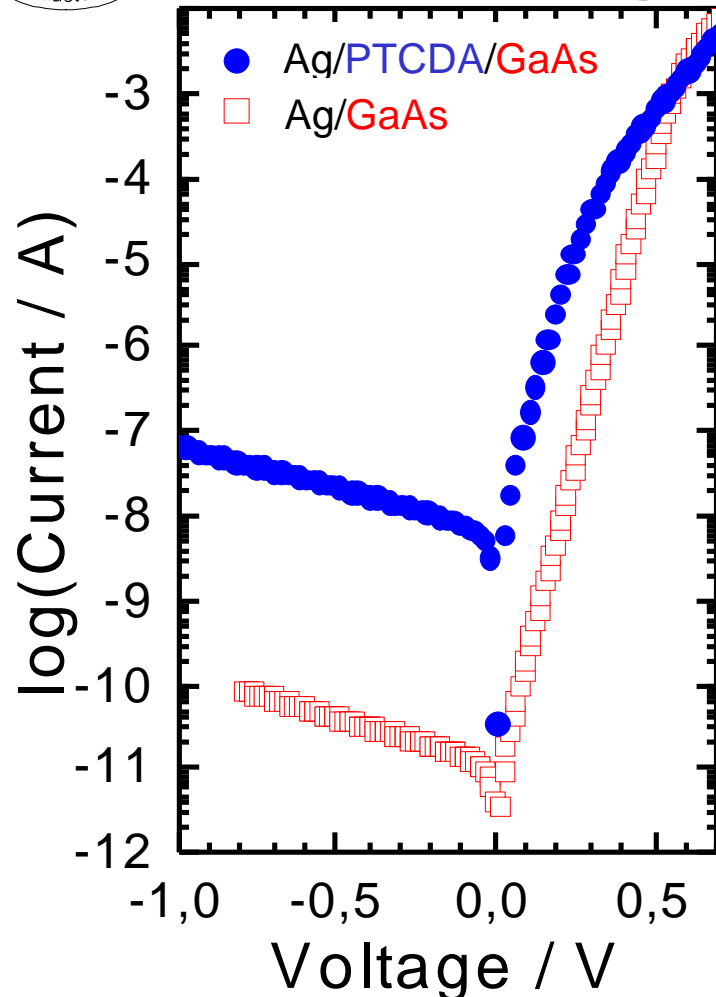
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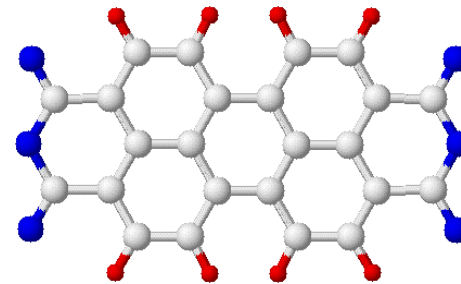
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*TUC*



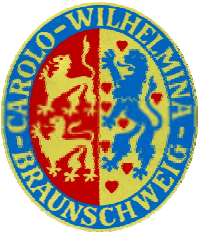
# ***PTCDA modified Ag/GaAs(100)*** **Schottky Contacts**



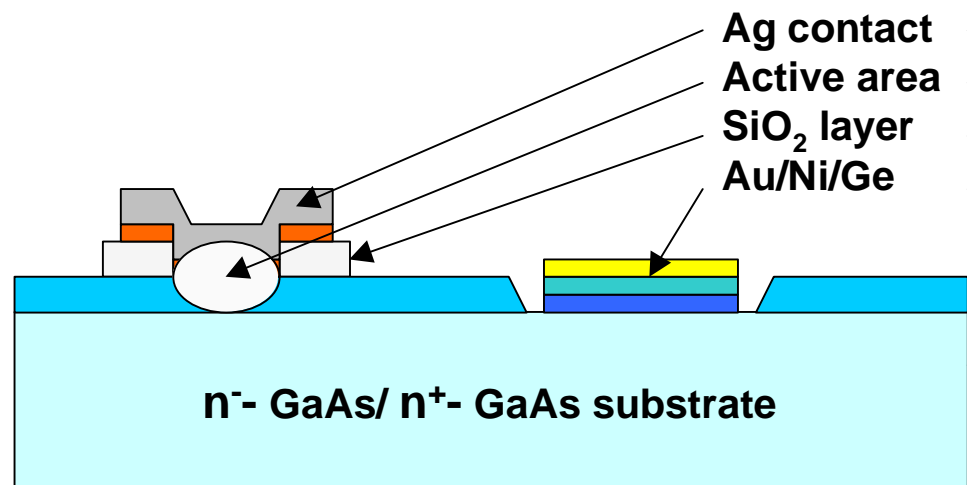
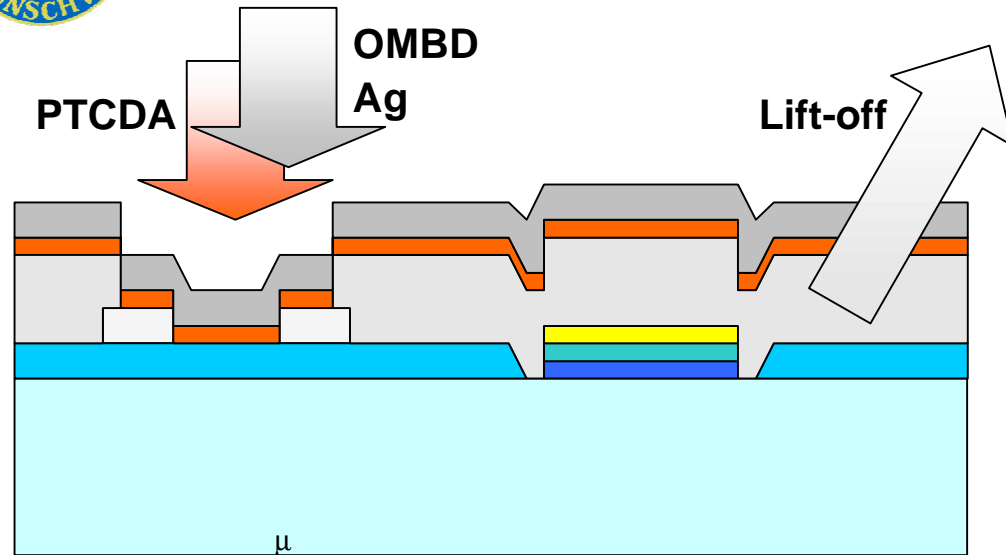
- 30 nm **PTCDA** interlayer.
- **Reverse bias/Low forward bias**  
Increase in current ( $\times 1000$ )  
Decrease in barrier height ( -150 meV)
- **High forward bias**  
Deviation from **thermionic emission**.



3,4,9,10-**P**erylene**t**etra**c**arboxylic **d**ianhydride (  $\text{C}_{24}\text{H}_8\text{O}_6$  )



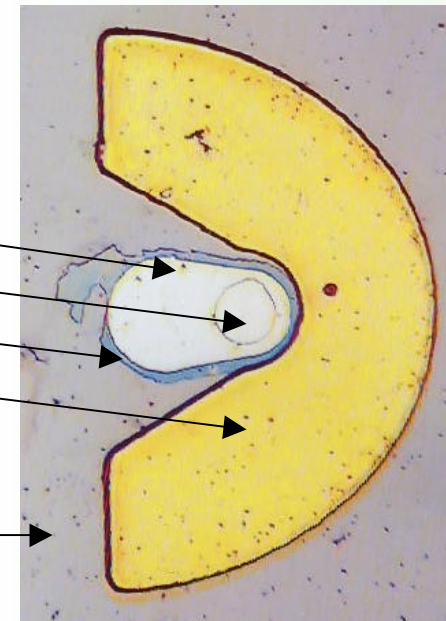
# Technology



## OMBD

- PTCDA(10nm)
- Ag(200nm)

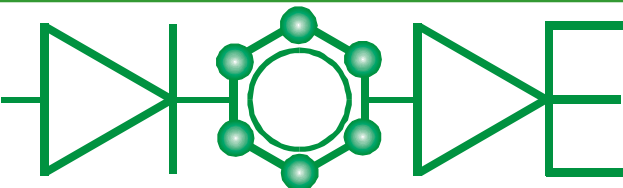
Lift-off in 20%NaOH



100  $\mu\text{m}$

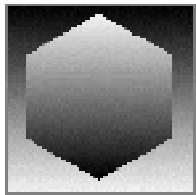


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**TU Braunschweig**

# Connections to Industry



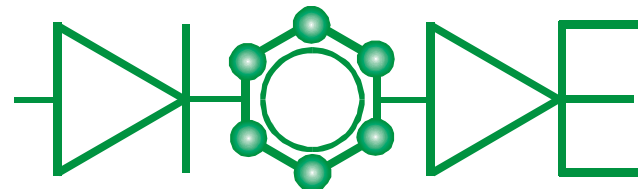
**SYNTEC**

Chemistry and Technology  
of Information Recording

**united  
monolithic  
semiconductors**



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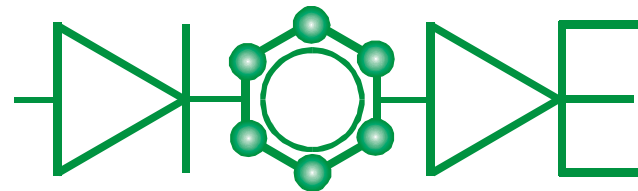
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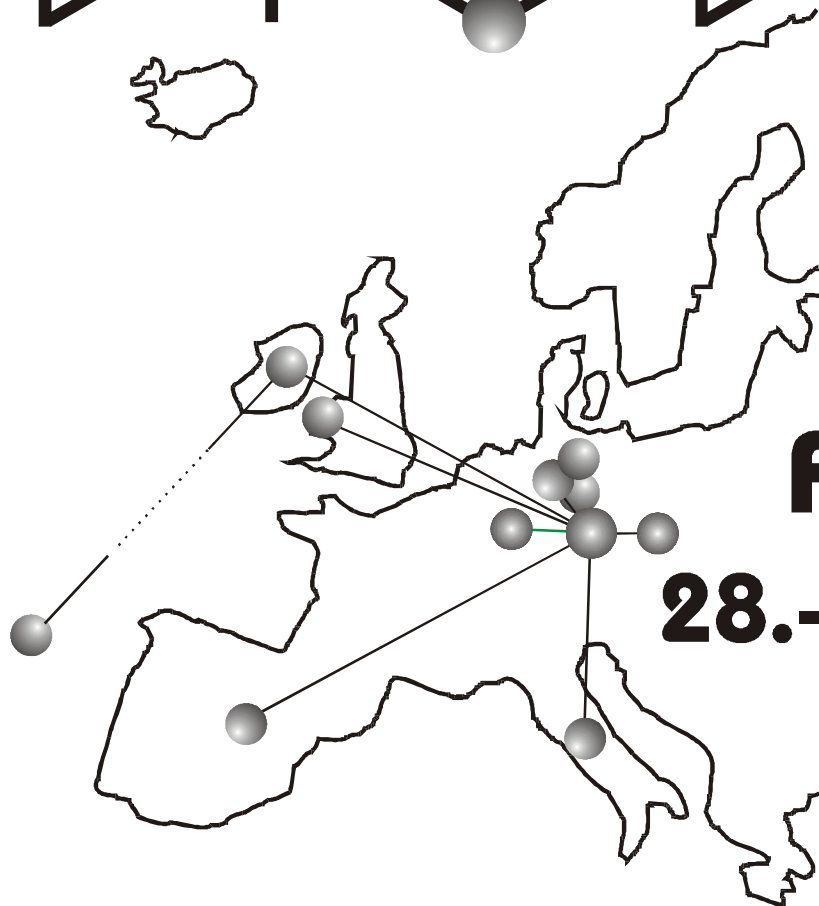
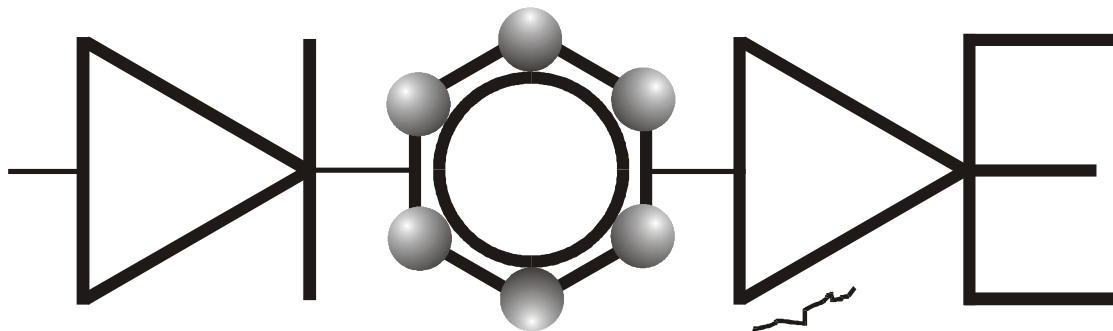
# Training



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# Franken

## 28.-30.09.2000

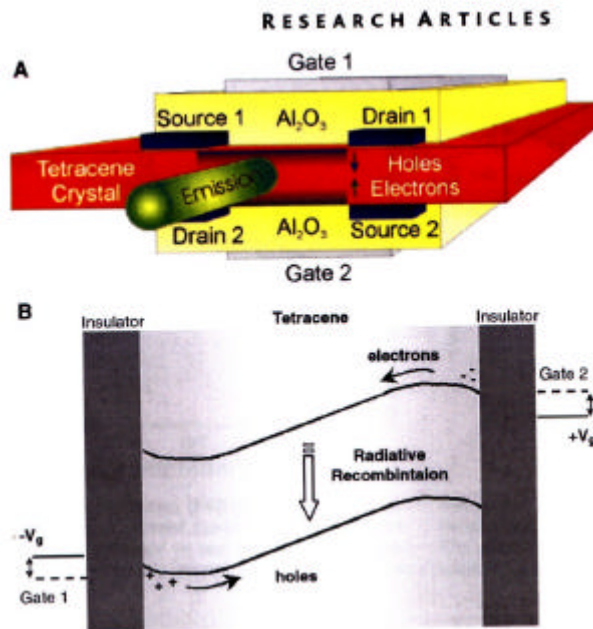
Supported by:

**Edgar-Heinemann-Stiftung an der Technischen Universität  
Chemnitz**

**Freiberger Compound Materials GmbH**

**Graduiertenkolleg Dünne Schichten und Nichtkristalline  
Materialien**

**Institut für Physik der Technischen Universität Chemnitz**



# Symposium

## Organic Solids

at the March meeting of the Germany Physical Society (DPG), Hamburg March 26-30, 2001

### Organization:

W. Brütting (Bayreuth), N. Karl (Stuttgart), K. Leo (Dresden), M. Sokolowski (Bonn)

### Objective:

The intention is to focus contributions about the electronic, structural and optical properties of organic thin films and crystals into a one-day symposium, giving an overview about this rapidly developing field.

### Presentations:

Besides invited talks [confirmed speakers: B. Batlogg (Lucent Technologies/ETH Zürich), A. Kahn (Princeton University), D. Bradley (Sheffield University)], further oral and poster sessions are planned. The symposium will be held in English language.

### Submissions:

For submitting contributions, use the website <http://www.dpg-tagungen.de>

Deadline: December 15, 2000.

### Further Information:

Contact Prof. K. Leo, TU Dresden, +49-351-463-7533/Fax -7065, [leo@iapp.de](mailto:leo@iapp.de)



supported by



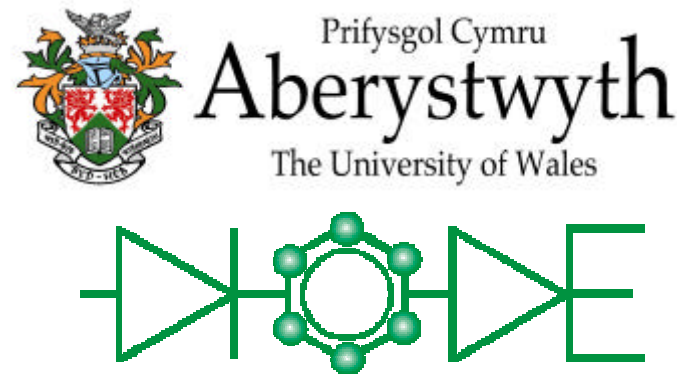
## **DIODE Symposium during the DPG Spring Meeting in Hamburg** **Monday, 26.3.2001, 14.00 – 17.30, Room S11, Congress Centrum Hamburg** **Tiergartenstr. 2, 20355 Hamburg**

- 14.00 Dietrich RT Zahn                      Welcome and Introduction
- 14.15 Georgeta Salvan (YR, Technische Universität Chemnitz)  
             Optical and Electrical Characterization of Ag/PTCDA/GaAs Diodes
- 14.30 Rafal Oszwaldowski (YR, Universidad Autonoma de Madrid)  
             Orbital Occupancy Approach for DFT Calculations
- 14.45 Eike Becker (Technische Universität Braunschweig)  
             Characterisation of Organic/Inorganic Heterostructures by UPS and Photoelectric Measurements
- 15.00 Gregory Cabailh (YR, Trinity College Dublin)  
             LEED Studies of PTCDA Deposited on GaAs (100) Surfaces
- 15.15 Marieta Gheorghe (YR, Universita degli Studi di Roma "Tor Vergata")  
             Tunneling in Organic Materials
- 15.30 Hans Joachim Steiner (YR, University of Wales Aberystwyth)  
             Electronic Properties of CuPc-Films on III-V Semiconductor Surfaces
- 15.45 Michael Sternberg (Universität-GH Paderborn)  
             DFTB Transfer-Matrix Formulation for Calculating Electronic Properties of Inorganic/Organic Device Structures
- 16.00 Coffee Break
- 16.15 [\*\*Antoine Kahn \(Princeton University\)\*\*](#)  
             Electronic Structures of Interfaces between Organic Molecular Thin Films and Metals, Organic Molecular Films, and Inorganic Semiconductors: a Summary

# DIODE Workshop II – July 19<sup>th</sup> – 21<sup>st</sup>, 2001

## *Organic Layers on Semiconductors*

### Final Programme



**Thursday, July 19<sup>th</sup>**

Arrive at Aberystwyth – Penbryn Hall, U.W.A.

**Friday, July 20<sup>th</sup>**

0800

Breakfast (Branwen's, Penbryn)

0900

Welcome (Room A12)

Dietz Zahn (co-ordinator)

Andy Evans (local organisor)

0910

Prof. [Steven Forrest, Dept. of Electrical Engineering, Princeton University](#), USA

(invited)

*Growth of Organic Thin Films By Organic Vapor Phase Deposition*

1000

Eike Becker, Technische Universität, Braunschweig, Germany

*Microwave applications and characterisation of organic-inorganic diodes*

1025

Marieta Gheorghe, Universita` di Roma "Tor Vergata", Italy

*Development of simulation tools for carrier transport in organic structures*

1050

Coffee (Branwen's Penbryn)

1110

Georgeta Salvan, Technische Universität, Chemnitz, Germany

*Electrical and Optical Characterization of the Ag/PTCDA/GaAs System*

1135

Joachim Steiner, University of Wales, Aberystwyth, Wales

*Energy band lineup at III-V – metal phthalocyanine interfaces*

1200

Greg Cabailh, Trinity College Dublin, Ireland

*GaAs surface preparation for organic thin film growth*

1225

Lunch (Upper Dining Hall, Penbryn)

1345

Dr. Ian Hill, Sarnoff Corporation, New Jersey, USA (invited)

*Organic TFT active matrix LCD displays*

1435

Dr. Jose Ortega, Universidad Autonoma de Madrid, Spain

*Metallisation and Schottky-barrier formation for Se-passivated GaAs(100)-surfaces*

1500

Prof. Thomas Frauenheim, Universität Gesamthochschule Paderborn, Germany

*Theoretical approach to dynamics and function of molecular systems.*

1525

Tea (Branwen's, Penbryn)

1545

Prof. Tim Jones, Imperial College, London, England (invited)

*Growth and properties of ordered organic thin films on III-V semiconductor surfaces.*

1635

Dr. Javier Mendez, Universidad Autonoma de Madrid, Spain

*Scanning Tunnelling Microscopy and Spectroscopy of PTCDA on semiconductors surfaces*

1700-1830

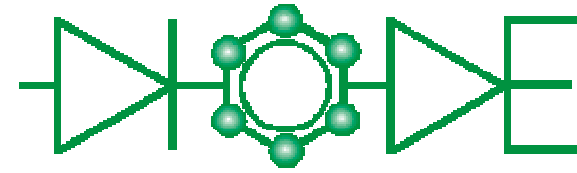
Posters ; sponsored by the Institute of Physics-Wales (prizes for best young researcher posters)

1930

Dinner (Belle Vue Royal Hotel, Aberystwyth)



Universidad Autónoma de Madrid



# DIODE-Training Workshop - Madrid April 2002

*STM, AFM and Theoretical Simulations*

To be held in Madrid, 22th - 26th April 2002

For DIODE-granted students and related young researchers.

## Program:

- **STM** (2 days)
  - **Introduction** (talk) *Dr. Julio Gómez-Herrero (UAM)*
  - **Theory STM and STS** (talk) *Dr. Jose M. Gómez-Rodríguez (UAM)*
  - **Experimental overview** *Dr. Javier Méndez (UWA-UAM) and Nicoleta Nicoara (UAM)*
  - **UHV Techniques**
    - **Sample preparation**
    - **STM**
    - **STS**
- AFM** (2 days)
  - **Introduction** (talk) *Dr. Jaime Colchero (UM)*
  - **Theory** (talk) *Dr. Rubén Pérez (UAM)*
  - **Experimental overview** *Cristina Gómez-Navarro (UAM) and Iván Cerrillo (UWA)*
  - **AFM**
- ♦ **Theoretical Simulations** (1 day)
  - **Introduction** (talk) *Dr. José Ortega (UAM)*
  - **Simulations** *Dr. Rafal Oszwaldowski (UAM) and Héctor Vázquez (UAM)*

Organizer: Javier Méndez

[javier.mendez@uam.es](mailto:javier.mendez@uam.es)

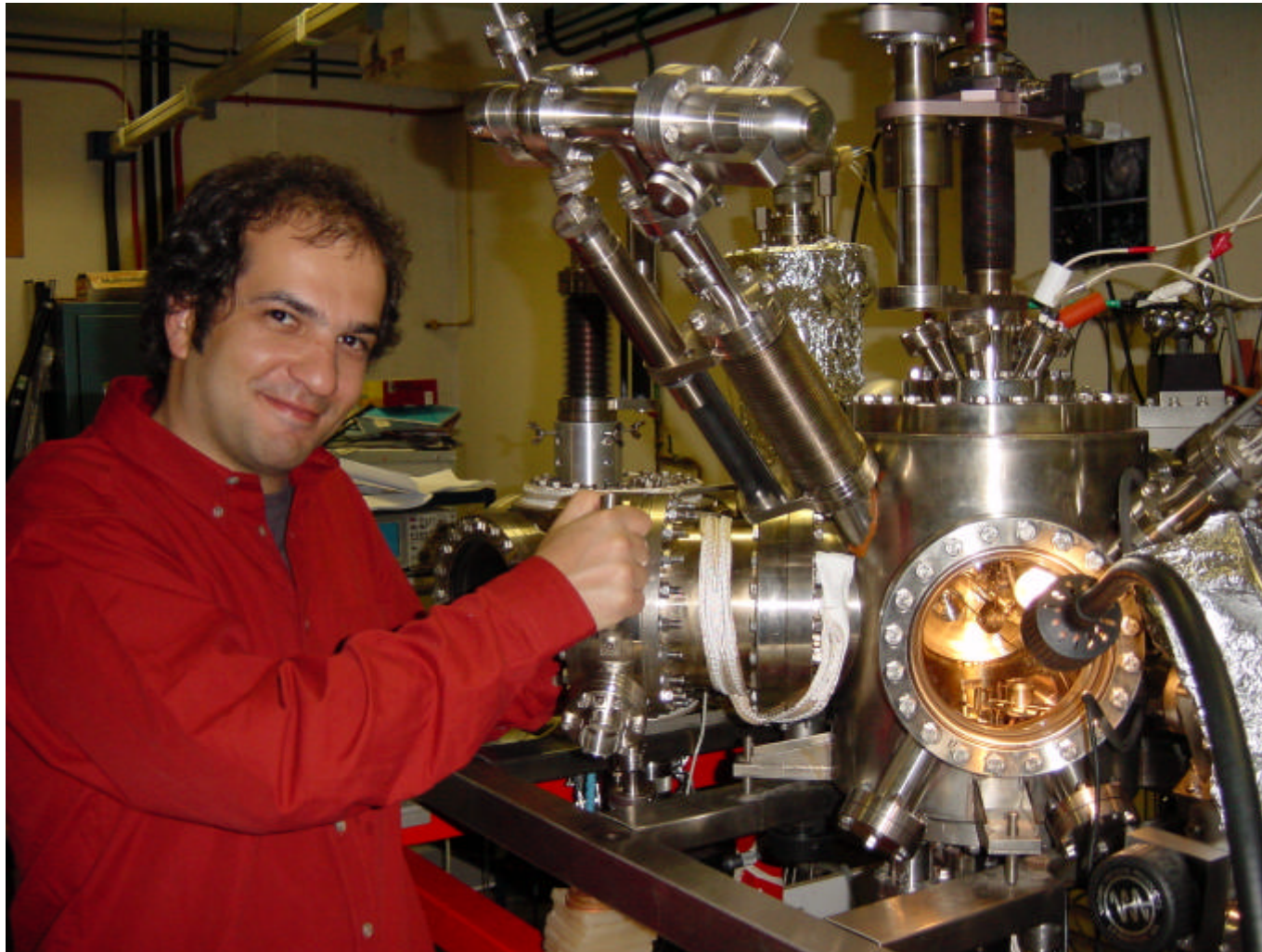
UAM: Universidad Autónoma de Madrid

UWA: University Wales Aberystwyth

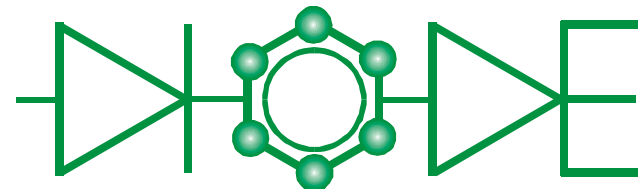
UM: Universidad de Murcia



# The STM/AFM-Workshop Organizer



IHP Research Training Network



*DRTZ*  
*TUC*



EU funded IHP Research Training Network  
Coordinator: Prof. Dr. Dietrich RT Zahn

supported by

Freiberger  Freiberger Compound Materials GmbH

 SYNTEC  
Chemistry and Technology  
of Information Recording

united   
monolithic  
semiconductors

# Newsletter no. 2

Dear DIODE members,

It is already two months ago since we all met in Franken. We are very grateful to all of you for coming and making the 1. DIODE workshop a very successful event.

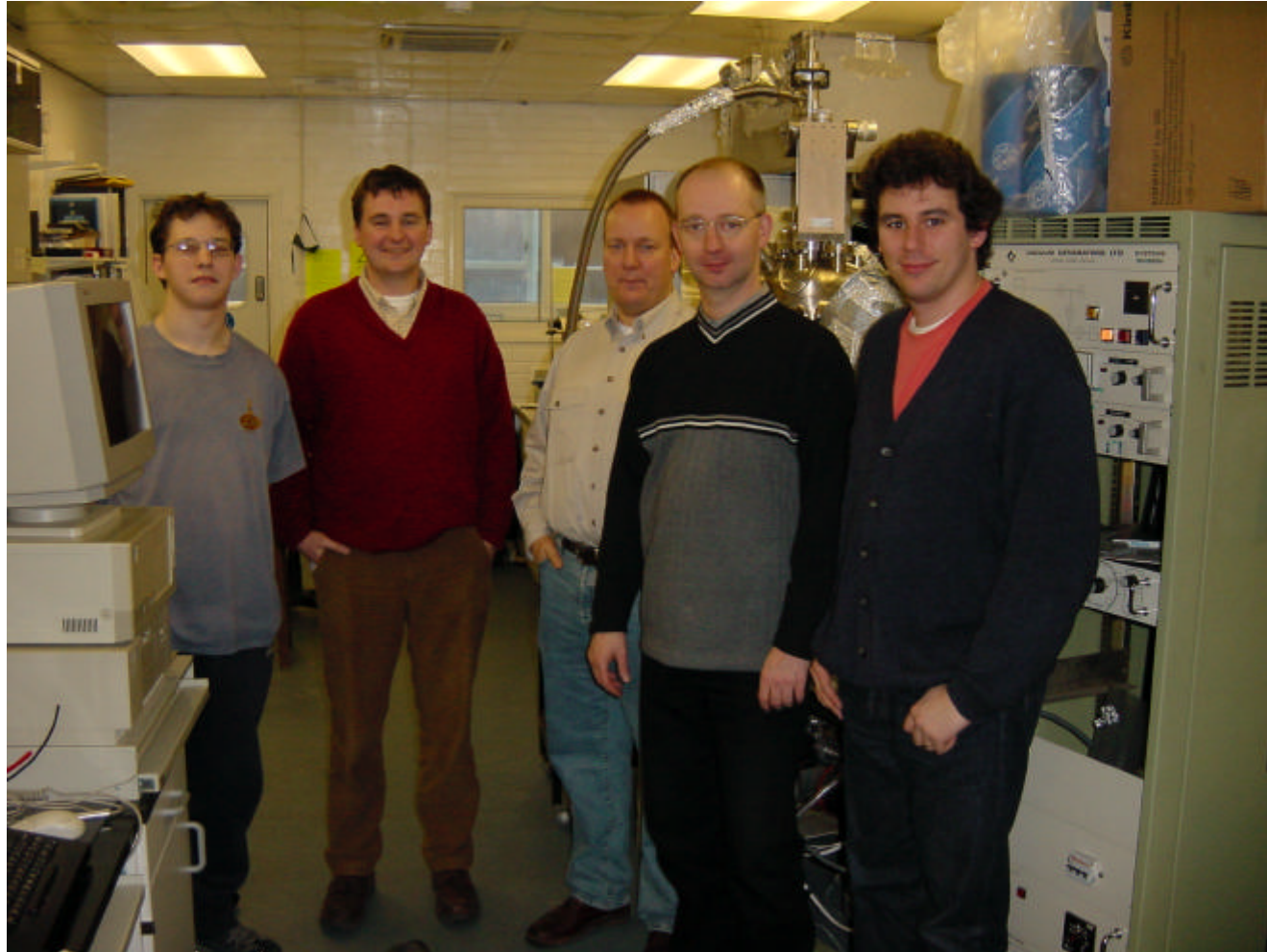
We hope that particularly the young researchers will make extensive use of the links established to DIODE partners during the meeting.

The *Newsletter* will deal with the following items:

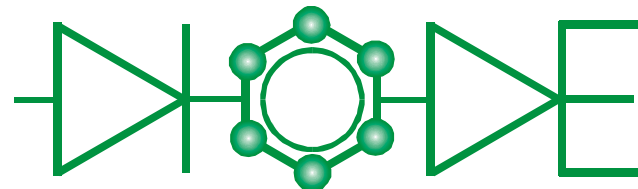
- **Young researchers**
- **Research**
- **Networking**
- **Training**
- **Meetings**
- **AOB**



# Visit to UWA



IHP Research Training Network

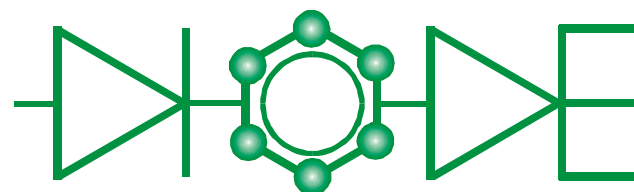


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# Visit to UAM



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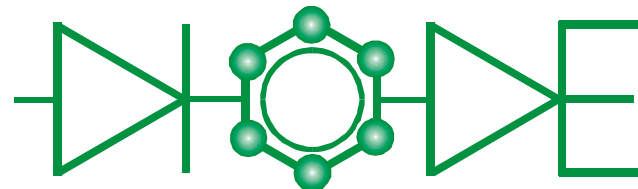


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# Administrative



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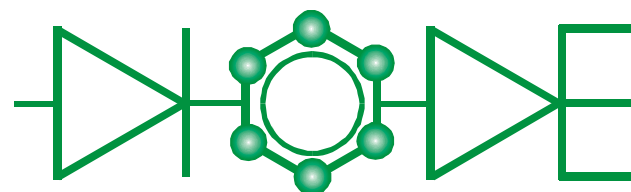
*DRTZ*  
*TUC*

# YR Employment Statistics

Partner	Young researchers financed by contract so far (person-months)			Contract deliverable of young researchers to be financed by the contract (person-months)		
	Pre-doc	Post-doc	Total	Pre-doc	Post-doc	Total
TUC	51	0	51	36	24	60
UAM	19	24	43	24	24	48
TUB	8	0	8	24	24	48
TCD	32	0	32	48	12	60
Rome	22	1	23	32	6	38
UWA	34	3	37	36	36	72
UGHP	17	2	19	42	6	48
<b>Total</b>	<b>183</b>	<b>30</b>	<b>213</b>	<b>242</b>	<b>132</b>	<b>374</b>



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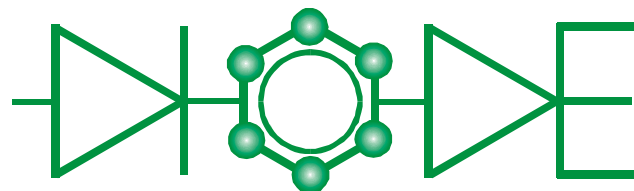
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*TUC*

# DIODE Budget Use

Participant	Cost Categories (spent to date)				Estimated Eligible Costs (foreseen in the contract)			
	Personnel	Networkin g	Overheads	Total	Personnel	Networkin g	Overheads	Total
TUC	72.800	32.200	21.000	126.000	156.584	18.416	35.000	210.000
UAM	76.600	29.200	21.160	126.960	127.000	41.000	32.000	200.000
TUB	33.400	6.000	7.880	47.280	152.807	14.193	33.000	200.000
TCD	46.500	15.600	12.420	74.520	123.586	43.100	33.314	200.000
Rome	31.500	28.500	12.000	72.000	106.500	27.500	26.000	160.000
UWA	128.400	21.400	29.960	179.760	195.000	39.000	46.000	280.000
UGHP	28.800	9.100	7.580	45.480	104.200	20.800	25.000	150.000



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# Young Researcher

TUC: **Georgeta Salvan**  
**Gianina Gavrilă**  
**Mihaela Gorgoi**  
**Miruna Noaghi**

UAM: Rafal Oszwaldowski  
**Nicoleta Nicoara**  
(Florian Landstädter)

TUB: (Radoslav Parashkov)  
Georgi Ginev

TCD: Gregory Cabailh  
Justin Wells

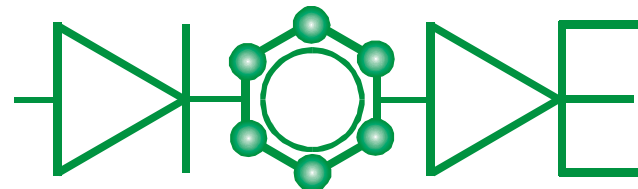
Rome: **Marieta Gheorghe**  
**Tiffany Ziller**

UWA: Joachim Steiner  
(Ivan Cerillo)  
Abel Brieva  
Javier Mendez

UGHP: (Fabio Della Sala)  
(Jaroslav Vacek)  
**Bernadette Szücs**



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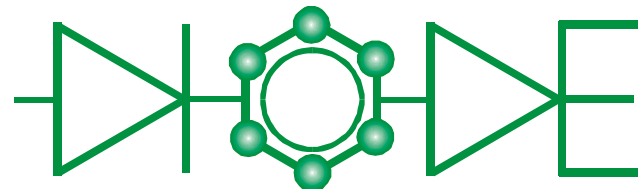
# Finally:

The DIODE network has helped enormously

- to attract additional (national) funding,
- to raise the awareness for the activities of the DIODE members,
- to build stronger links between the members.



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