

## **Node 5:**

### **Dept. Electr. Eng. University of Rome Tor Vergata**

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DIODE Young Researchers:

Marieta Gheorghe, Ph.D. student  
Tiffany Ziller, Post Doc

Other researchers related to DIODE project:

Alessandro Bolognesi, PhD  
Alessandro Pecchia, Post Doc

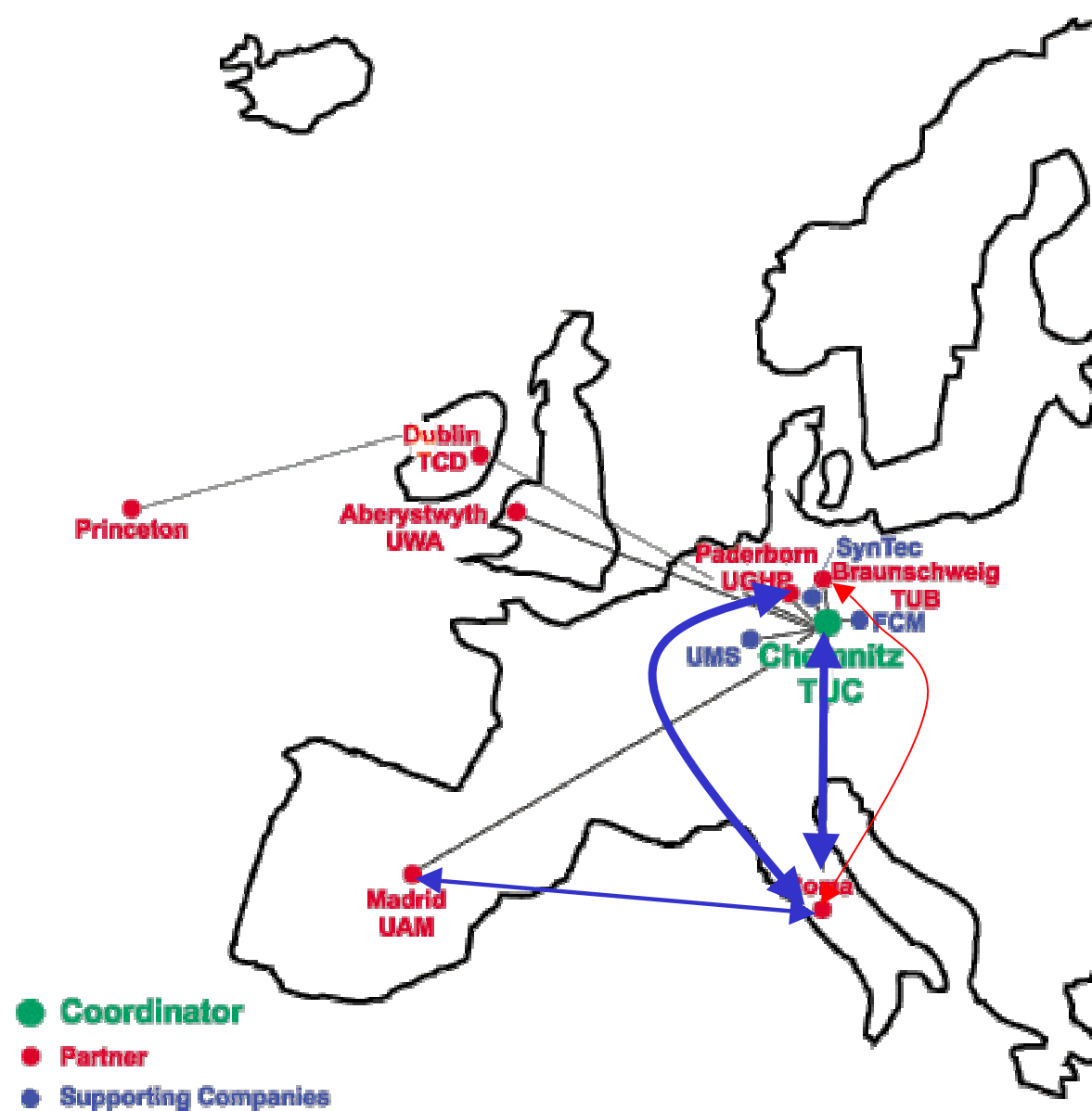
# What we do for young researcher ?

- Interview
- Accommodation (Relocation Cost)
- Italian language course (University)
  
- The PhD student should also pass an internal (but national) competition
  
- PhD students are enrolled for a three year program
  - First year: Special courses for PhDs (advanced arguments) (150 hours)
  - Second year: Visit to project partners
  - Third year: Final rush
  
- Young researcher are initially trained from “old” people of the group (how to use the cluster, how to compile etc.)
- PhD. Students are then assigned to a PostDoc (the PostDoc supervisor of M. Gheorghe is Dr. Alessandro Pecchia)
  
- After a initial time, also PostDoc of the DIODE project will have their students

Every young researcher have to report each month the scientific activity



# Intranetwork relations



# Two-dimensional Drift-Diffusion Model

We simulate organic devices using an industry standard device simulation tool, namely ISETCAD™, a package able to resolve the standard drift-diffusion equations coupled with Poisson's equation in two and three dimensions:

## Drift-Diffusion equations

$$J_n = -q m_n \tilde{N} y + q D_n \tilde{N} n$$

$$J_p = -q m_p \tilde{N} y - q D_p \tilde{N} p$$

$$\tilde{N} \times (e_0 e_r \tilde{N} Y) = -q (p - n + N_D^+ - N_A^-)$$

$$\frac{\mathfrak{I}n}{\mathfrak{I}t} = \frac{1}{q} \tilde{N} \times J_n + (G - R)$$

$$\frac{\mathfrak{I}p}{\mathfrak{I}t} = -\frac{1}{q} \tilde{N} \times J_p + (G - R)$$

ISETCAD™ is not capable to handle charge transport in organic material, so we have implemented a new model based on the following properties:

- Appropriate density of states
- Field dependent Mobility
- Equivalent Doping
- Traps

Field dependent mobility has been calculated by using a Monte Carlo simulator.

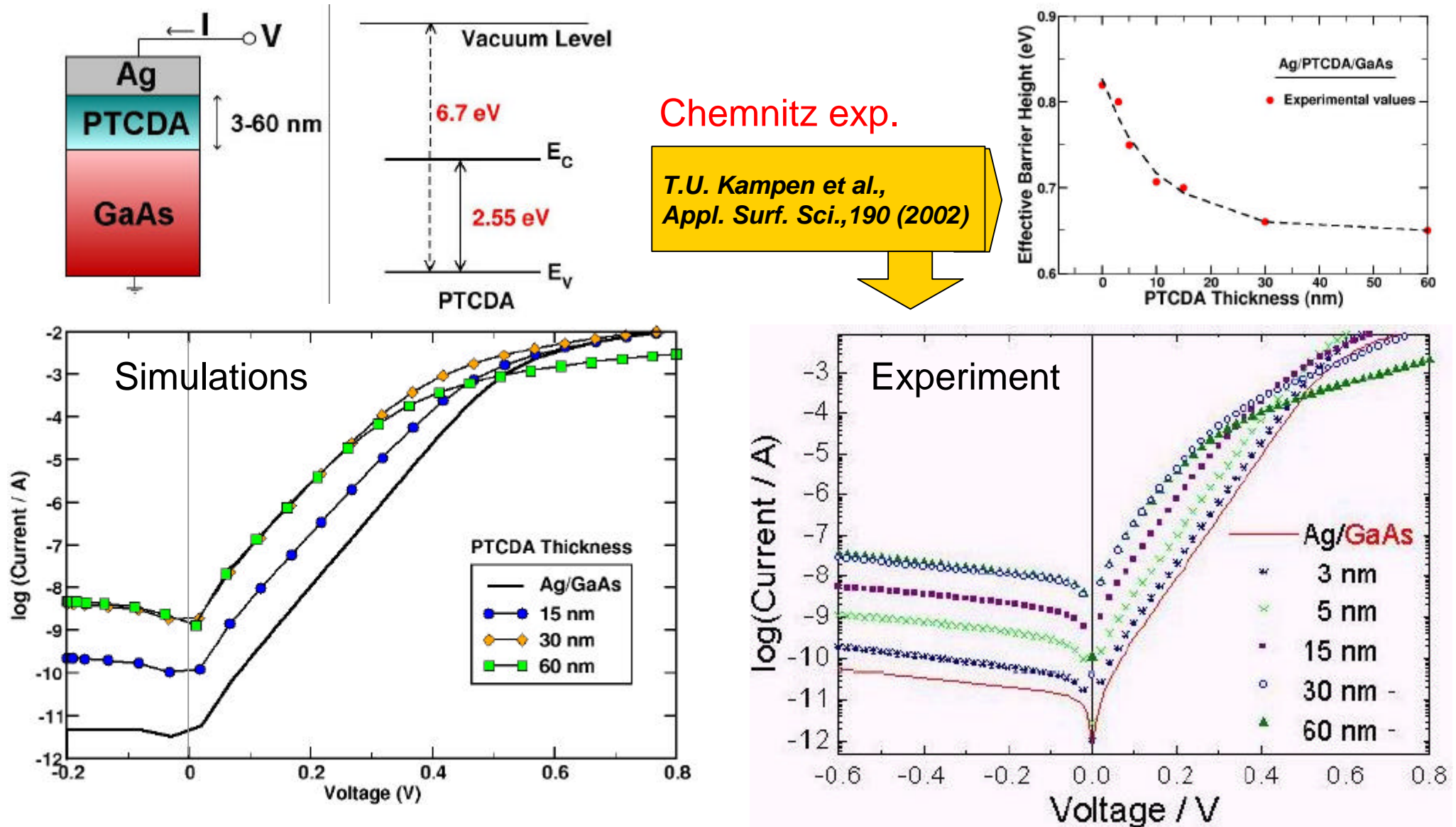




# Organic / Inorganic Devices: Ag/PTCDA/GaAs Schottky barrier

[ Rome – Chemnitz – Braunschweig ]

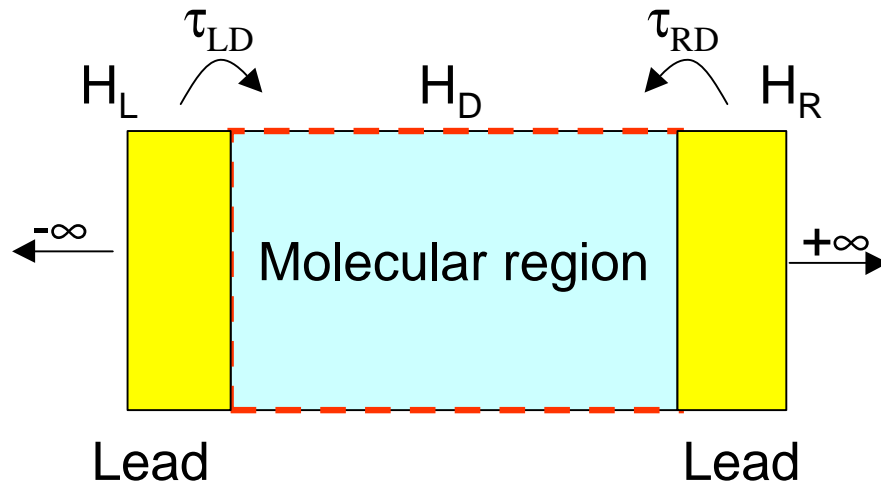
We simulate the behavior of a Ag/GaAs Schottky barrier with a thin layer of PTCDA.



# Tunneling current: Green Function Approach

[ Rome – Paderborn-Madrid]

The Density Functional Tight-Binding developed in **Paderborn** has been extended to calculation of transport properties of organic materials. This has been obtained by using a self-consistent Green-Function approach.



Retarded (r) and advanced (a) Green functions are defined as follow (matrix notation)

$$[(E \pm i\hbar)\mathbf{I} - \mathbf{H}] \mathbf{G}^{r,a} = \mathbf{I}$$

From these definition is possible to calculate:

$$T = \text{tr}(\Gamma_L G_D^r \Gamma_R G_D^a)$$

Transmission coefficient

$$G = \frac{2e^2}{\hbar} T$$

Conductance

$$J(V) = \int_{-\infty}^{+\infty} dE T(E) [f(E - \mathbf{m}_L) - f(E - \mathbf{m}_R)]$$

Current

Extension to Non-Equilibrium Green Function (**Madrid**) is in progress

