FROM COMPUTATIONAL DESIGN TO MOLECULAR ELECTRONICS ON NANOPATTERNED SURFACES

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The 16th edition of the National Seminar of Nanoscience and Nanotechnology
Bucharest, Library of the Romanian Academy, June 6th 2017
Outline

✓ Starting the nano-device construction:
  ✓ construct the surface,
  ✓ construct the active layer,
  ✓ evaluate their properties

✓ Assessing the device electronic properties:
  ✓ DFT calculations

✓ Real case: hybrid organic – inorganic diode based on ZnO/FePc junction

SPM-MBE facility at NIRDIMT Cluj

http://grid.itim-cj.ro/
https://erris.gov.ro/INGRID---GRID-System-1
EXPERIMENT: HOW TO BUILD A MOLECULAR LAYER ON A SURFACE?

- surface preparation
- molecule deposition
- characterization via STM images
Examples: Fabrication of nanostructured, ultra-flat thin films as promising substrates for molecular electronics\textsuperscript{1,2}

Sub-monolayer molecular deposition: FePc on Au(111) case study

2D-STM image for 200 nm thickness of FePc/Au(111)

2D-STM image for sub-monolayer FePc/Au(111)

2D-STM image of Au(111) surface with atomic defects

Roughness RMS=0.32 nm
THEORY: HOW TO DESIGN THE PROPERTIES OF MOLECULAR DEVICES

- periodic structure calculations (slab model)
- computational technique: DFT
  - charge transfer
  - density of states
  - molecule-substrate interaction geometry
Examples: molecules on surfaces

\(\sigma\)-bonded molecule (alpha glycerophosphocholine) in interaction with Au surface; positive and negative electric charge effect\(^1\).

Molecular self-assembly on metallic surface (cysteine on gold)\(^2\)

Calculation of unimolecular device properties (rutenium-di-terpyridine sandwiched between two gold electrodes)\(^3\)

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\(^3\) C. Morari, L. Buimaga-Iarinca et al, Nature Scientific Reports 6, 31856 (2016)
Practical approach for FePc on Au(111) case study

Main idea: the molecular structure and parameters have to be stable in the adsorption state when structural deformation occurs on the surface (i.e. lab-made/cheap surfaces)

Computational details:
Molecule (FePc) – 57 atoms; Au(111) surface – 7x7x3 atoms; lattice parameter 4.08 Ang.
The molecule and first Au layer set free to relax their position
Relaxed until a gradient < 0.03 eV/Ang;
Spin-polarized calculations
We used the SIESTA code in VdW setup, with the BH* functionals.

Charge transfer between FePc and Au substrate

CONCLUSION

Charge transfer between molecule and surface differ for each case (left images)

BUT
is small - little or no difference for the Fe atom (right images)

So
It may be possible to build devices using ‘lab-made’ surfaces

Δρ=0.001 Å/B³
Δρ=0.01 Å/B³

Model 1

Model 2

Model 3

Red – FePC accept charge from the surface; Blue – FePC loose charge to the surface
EXPERIMENTAL IMPLEMENTATION: HYBRID ZnO/FePc NANO-DIODE

Transparent and flexible electronics
Organic-inorganic hybrid diode
In the near-future:

Thin-film MOLECULAR TRANSISTOR on transparent and flexible substrate
CONCLUSIONS

We construct the surface by MBE $\rightarrow$ design and assess the device properties by DFT $\rightarrow$ construct the molecular device components $\rightarrow$ assemble the device $\rightarrow$ perform complete measurements and characterizations.

From design to proof-of-concept: calculations, fabrication and characterization – we integrate all the steps to produce nanometric-scale organo-metallic flexible devices.
Financial support is gratefully acknowledged from UEFISCDI, CAPACITIES – Module I – Large investment projects for 2PM/I/07.10.2008, UEFISCDI, for PN-II-ID-PCCE-2011-2-0027, ANCSI, Core Programme for Project PN16-30 02 01.