# Computational Modelling of Nanosensor Responses to Odor Molecules

Supervised by

Prof. Gianaurelio Cuniberti

Dr. Rafael Gutierrez

Dr. Arezoo Dianat

Kick-Off Meeting

Narges Ghasemi

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# Smart Electronic Olfaction for Body Odor Diagnostics (**SMELLODI**)

# Functions of the human olfaction system;

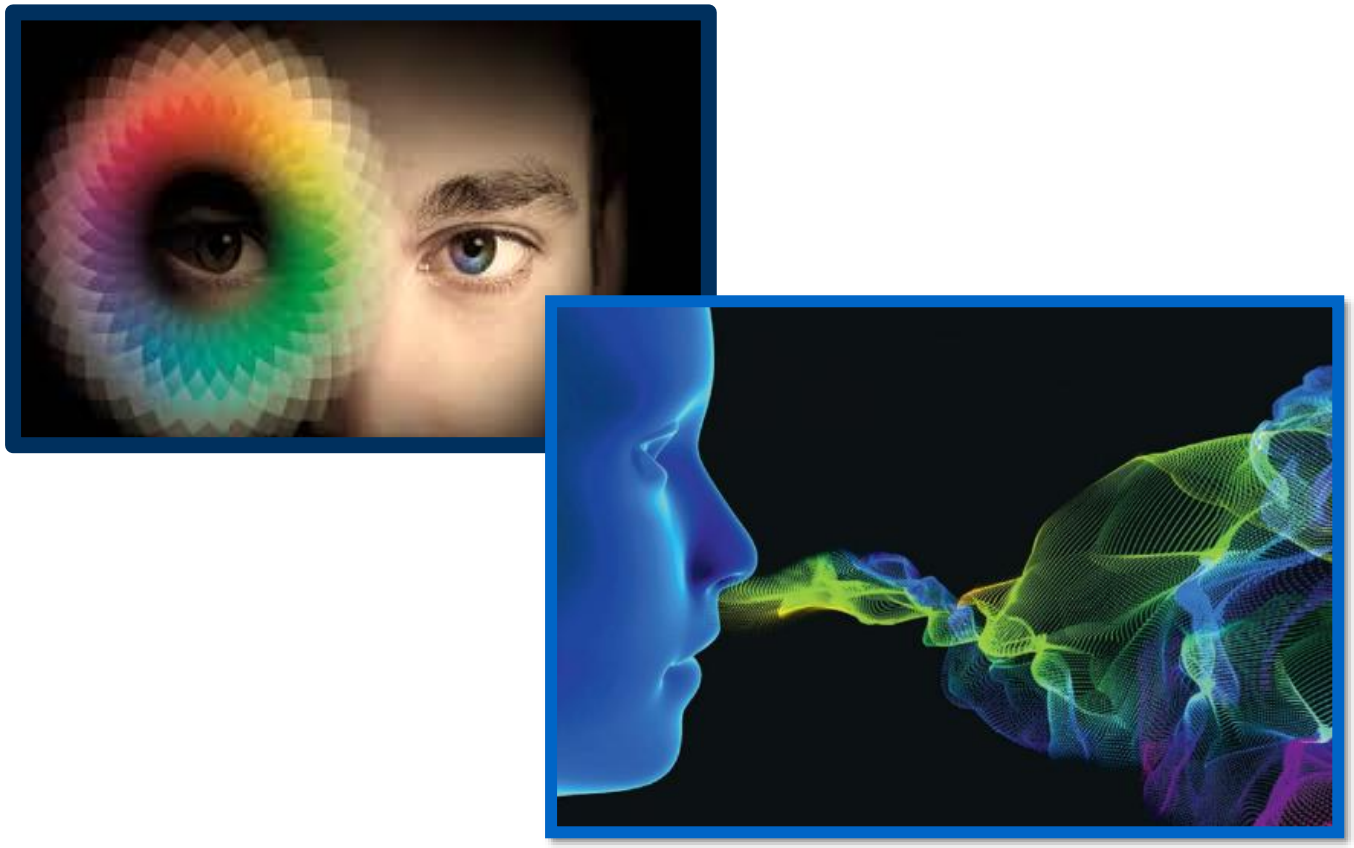
- Social communication
- Avoidance of environmental hazards
- Ingestive behavior
- Disease detection

## Nanoengineering Approaches Toward Artificial Nose

# Serious Challenge

- The biological olfactory system is highly discriminative and sensitive compared to the other sensory systems.

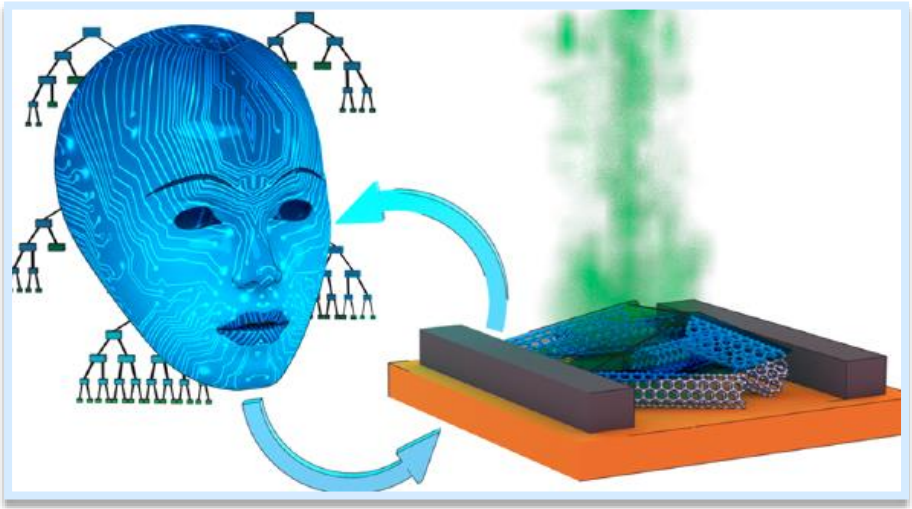
- A single odor source typically emits a combination of many unique odorant molecules that vary in composition



Kim et al., Frontiers in Chemistry, Volume 9, 2021

## Chemoresistive sensors

- Metal-oxide-semiconductors (MOS)
- Conductive polymers
- Nanomaterials like graphene, carbon nanotubes



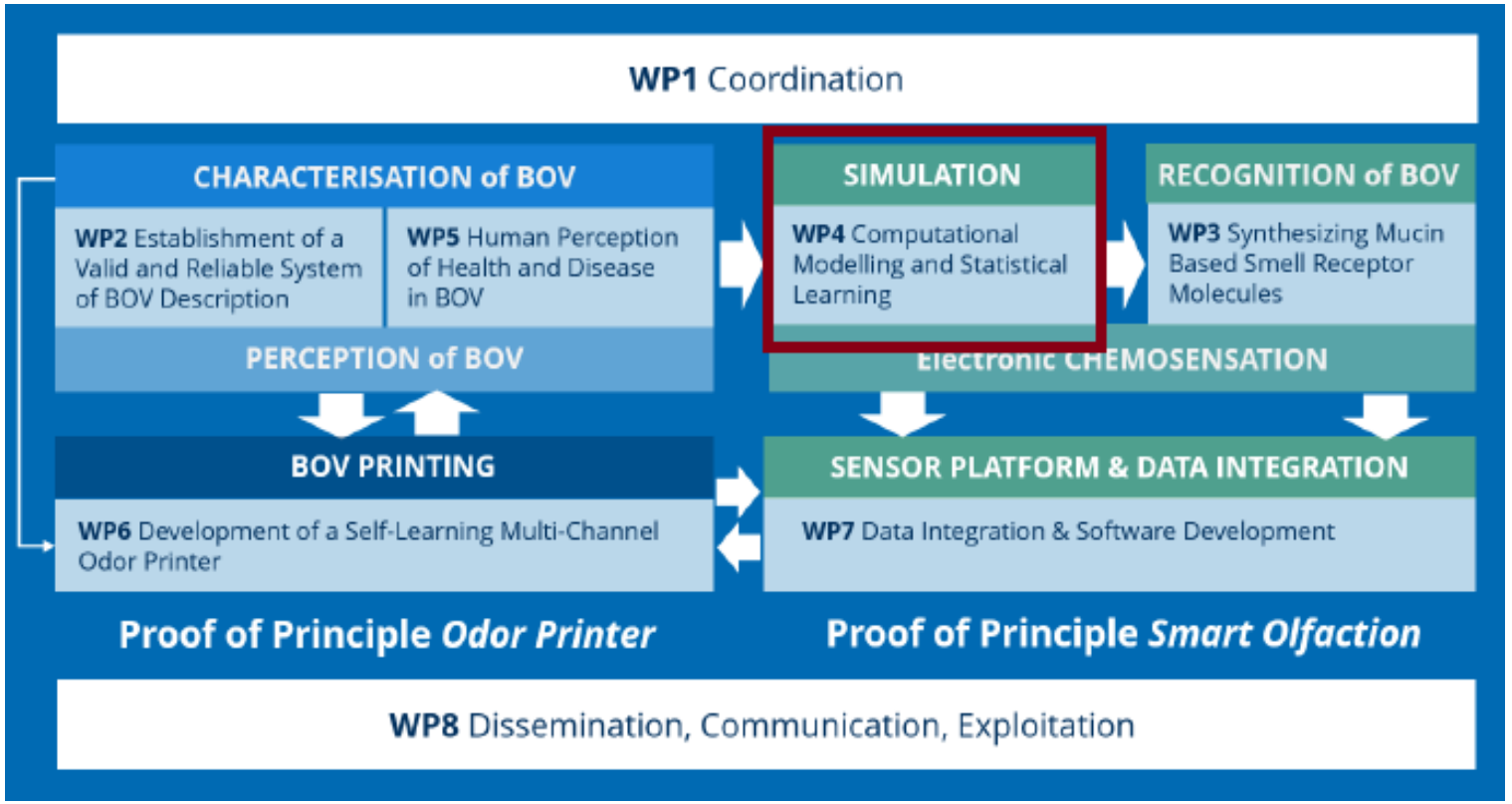
Schroeder et al. ACS Sens. 2019, 4, 2101−2108,

**Advantages**:

- ➢ Excellent carrier mobility
- ➢ High mechanical strength
- ➢ Low fabrication cost
- ➢ Being adaptive through the functionalization of the sensing material envisioned in SMELLODI

## Three components of SMELLODI;

- the development of an eNose platform
- Study of healthy and pathological body odor perception by individuals
- The controlled synthesis of odors




Work packages included in SMELLODI

# Motivation

- In order to improve or tune the sensitivity and selectivity of graphene surface, the functionalization of graphene nanoribbons with artificial receptors should be investigated.

# Research Plan

- A consistent set of molecular descriptors will be defined for the odor molecules.
- The focus will be on mucin-derived glycans and glycopeptides receptors
- Structural optimization will be performed to address stable conformations and binding energies of receptors on CNTs and the graphene surface
- Based on the stable structures, an atomistic calculation of transport characteristics of analyte-receptor interactions will be carried out.

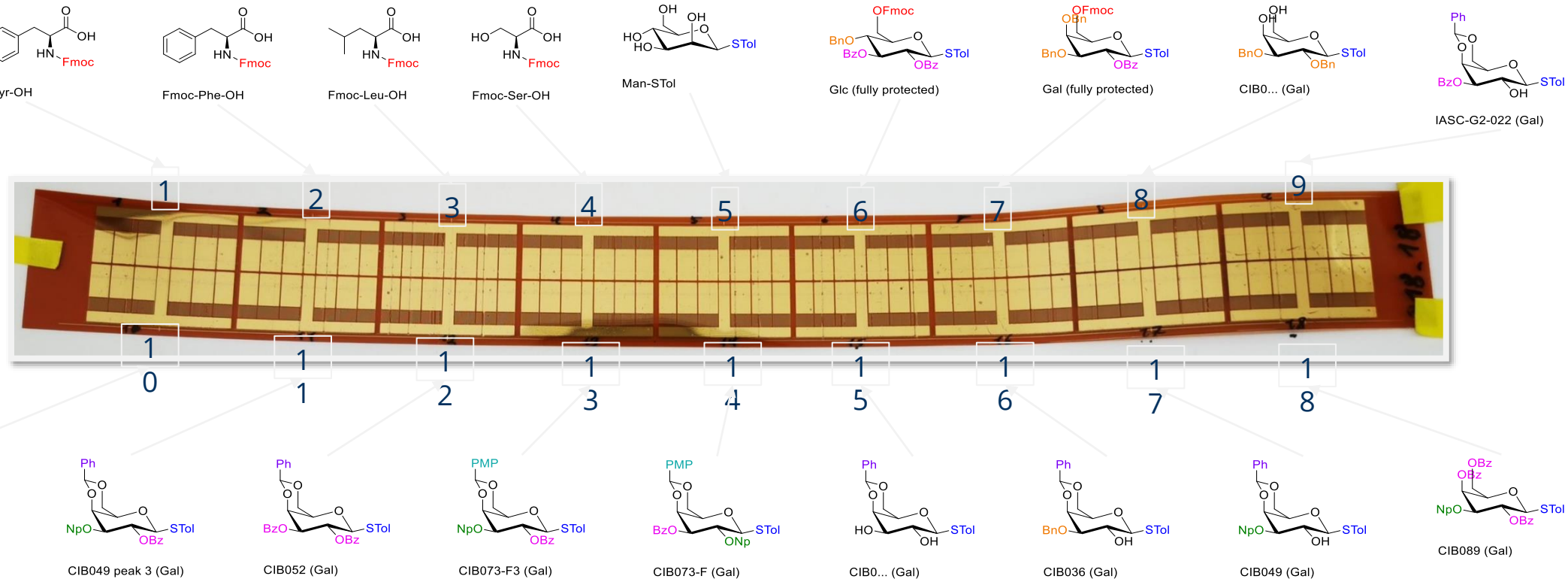
**Simulation setup:**

- Functionalization of Graphene nanoribbon by Mucin-derived artificial receptors.
- Adding odor molecules to functionalized nanoribbon.

**Computational method:**

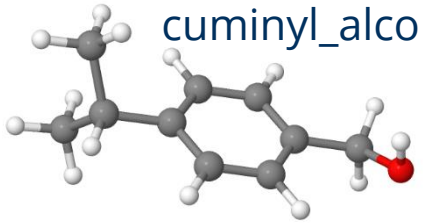

- Method: **DFTB**
- Geometry optimization with *Dispersion corrections*
- Electron transport calculations with *SCC correction*

# Mucin-derived artificial receptors, suggested by S. Yitzchaik

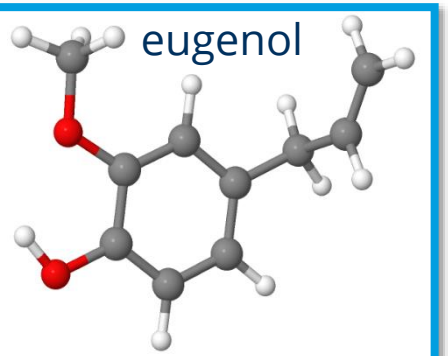


# Selected odor molecules

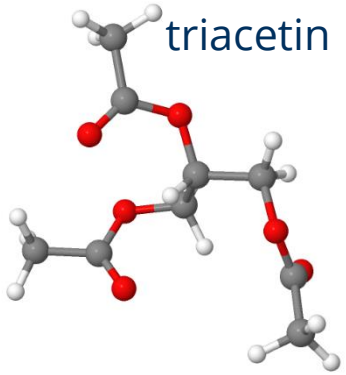
cuminyl_alcohol



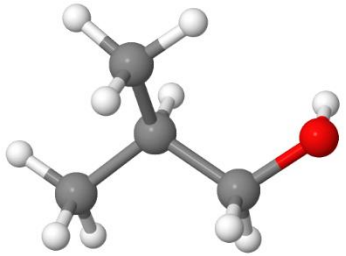
eugenol



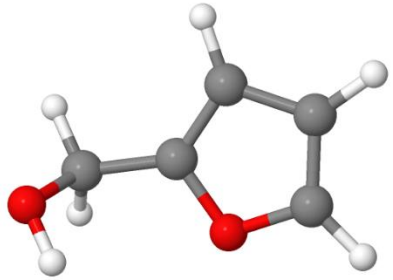
triacetin



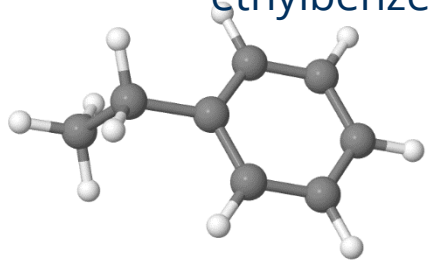
2methylpropanol



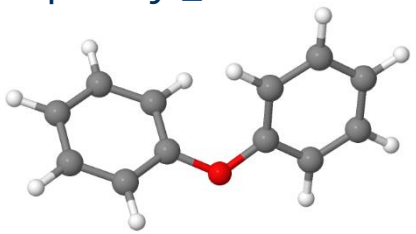
furfuryl_alcohol



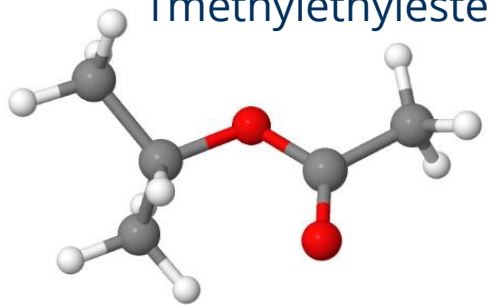
ethylbenzene



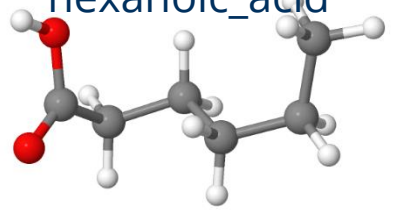
diphenyl_ether



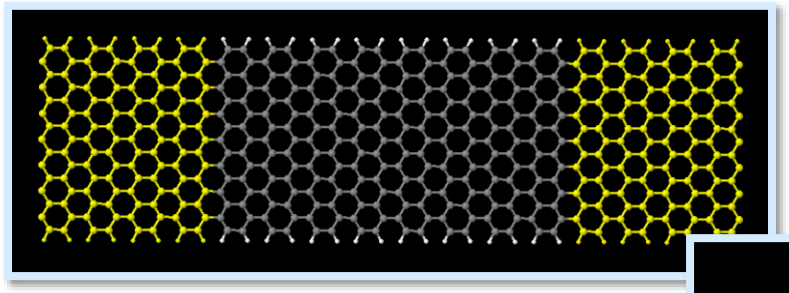
1methylethylester

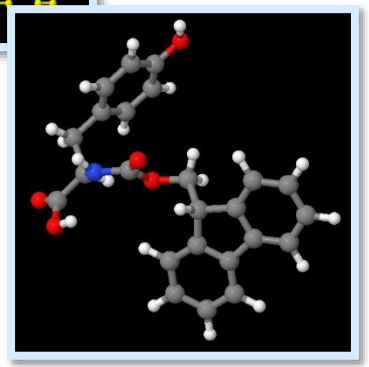


hexanoic_acid

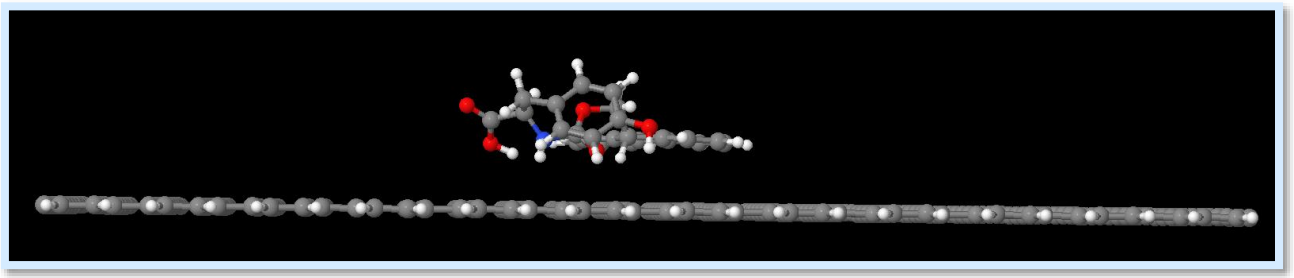


# Functionalization of Graphene nanoribbon by artificial receptors

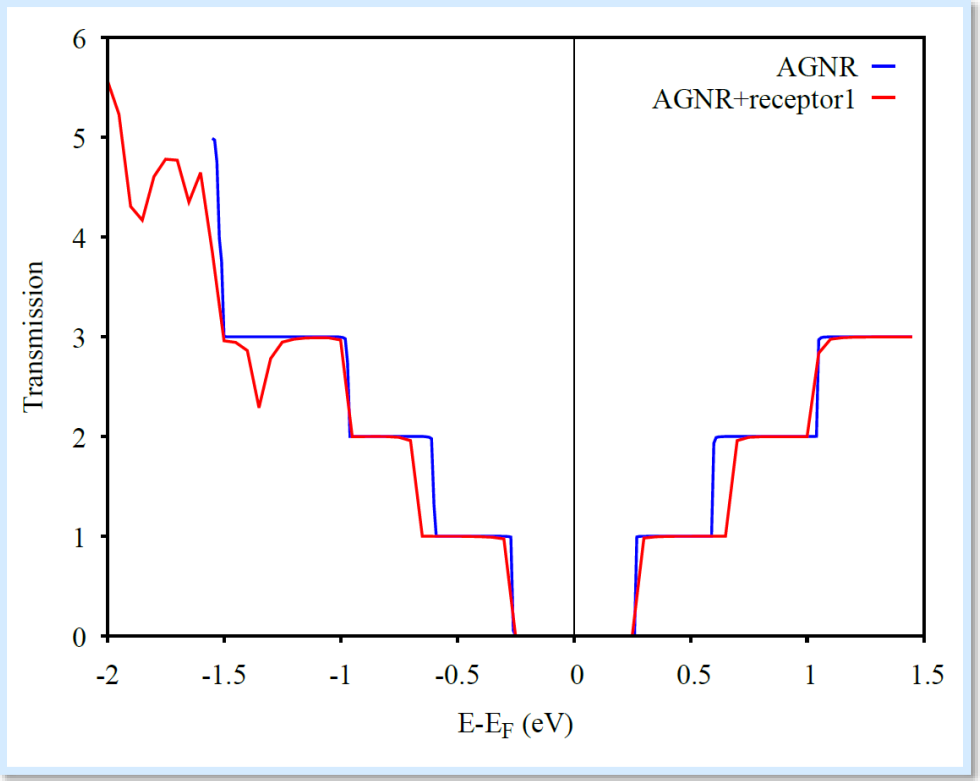


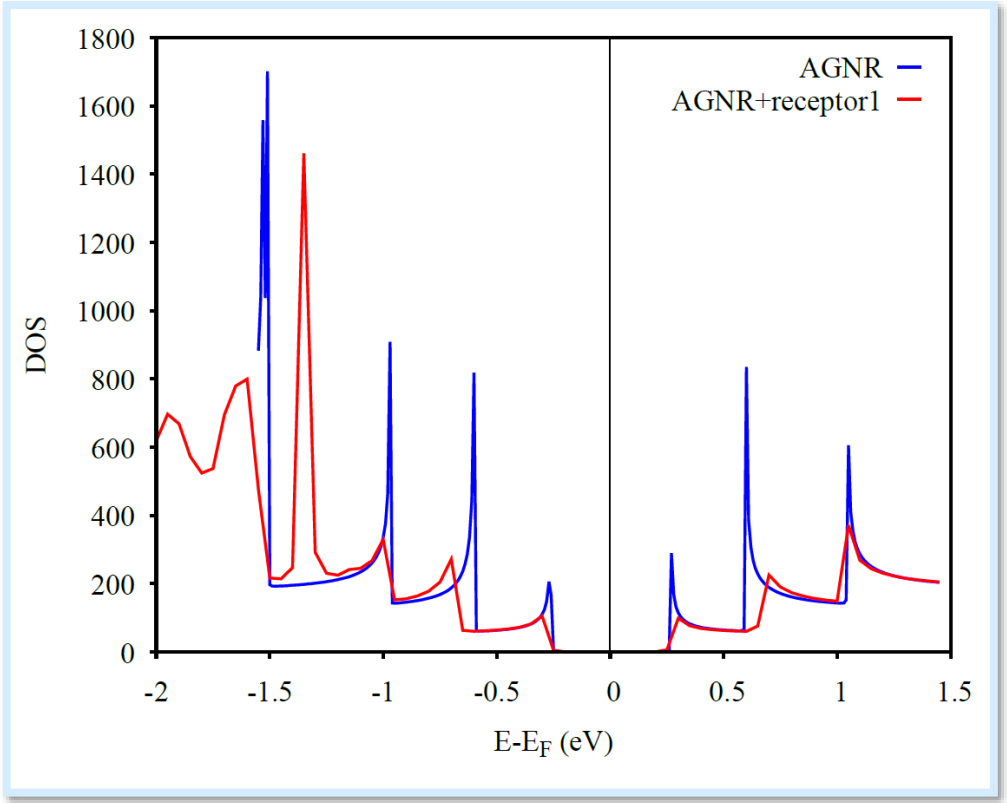


**Fmoc-Tyr-OH**



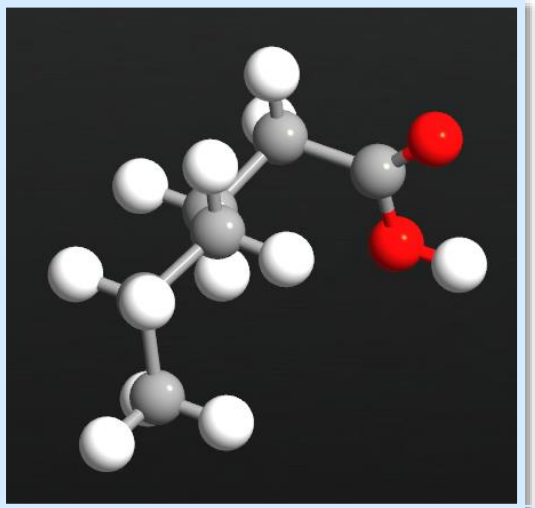
# SCC Transmission and DOS in AGNR with and without the receptor



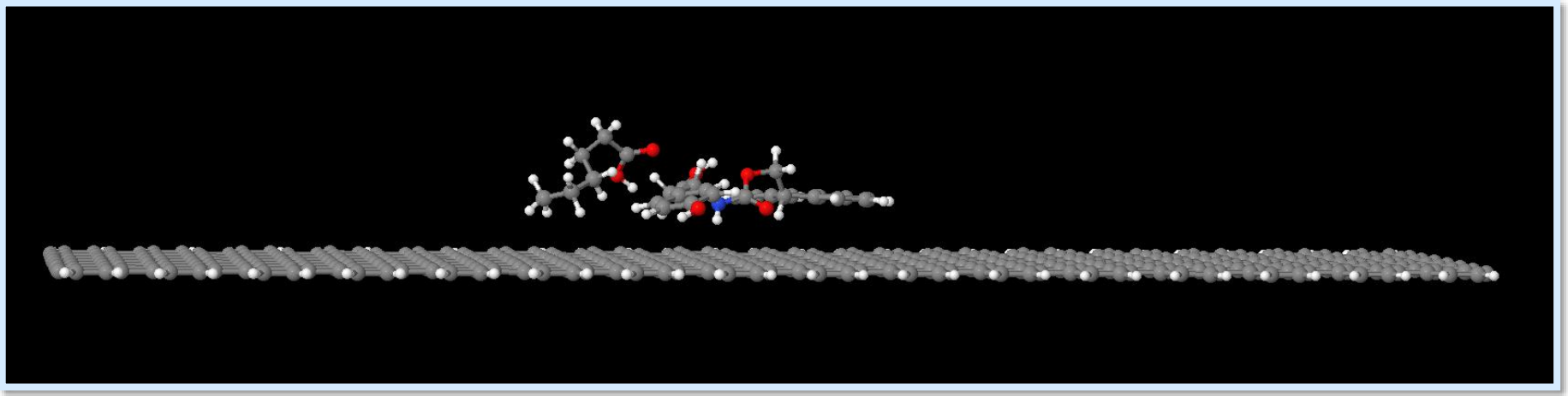




Fermi energy:
AGNR = -4.45 eV
AGNR + receptor1= -4.45 eV

# Interaction between the receptor and the first odor molecule

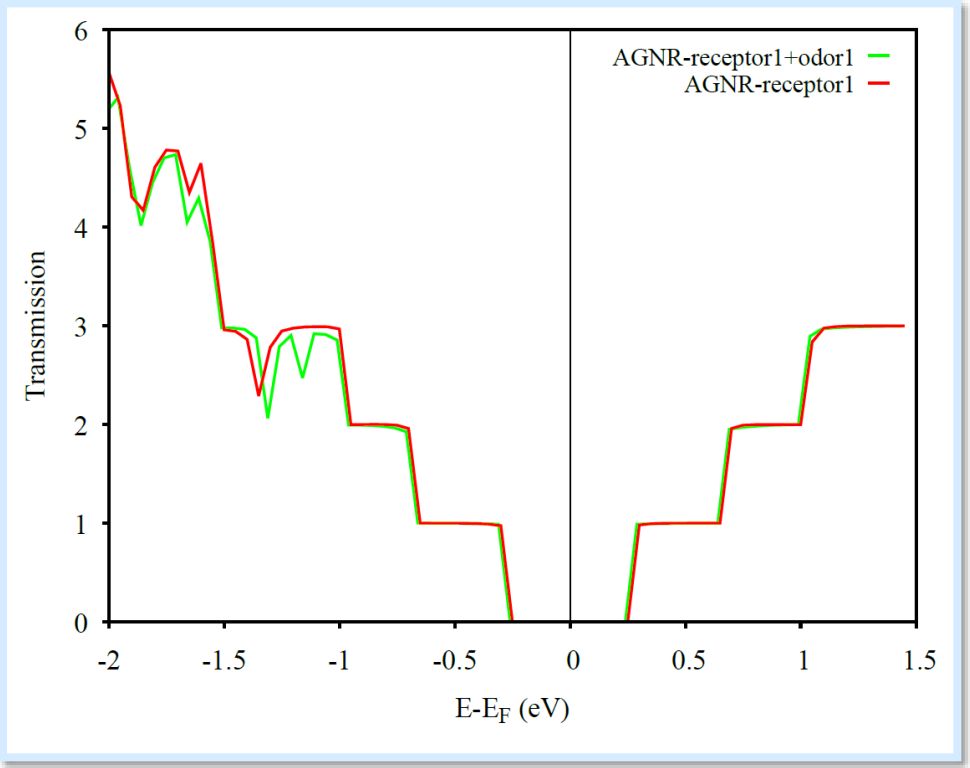


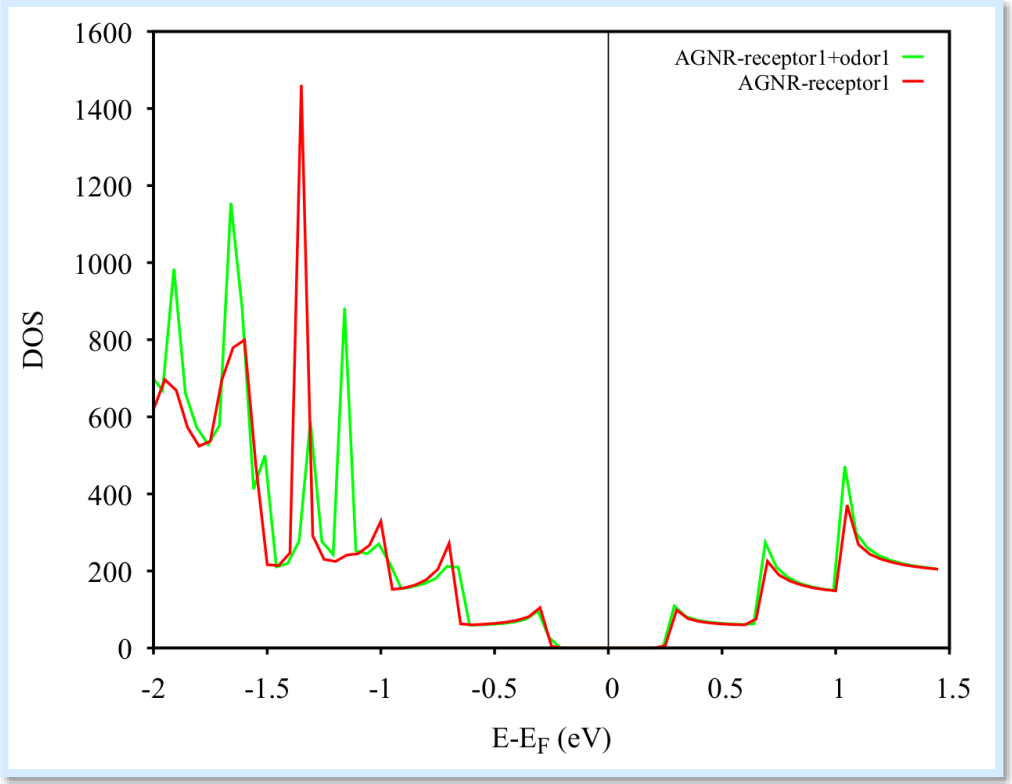
Hexanoic acid: **C6H12O2**



**Binding energy = -1.058 eV**

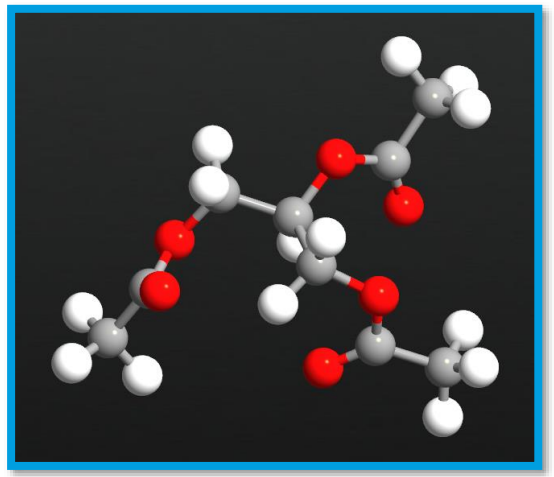
# SCC Transmission and DOS in functionalized AGNR with and without the first odour molecule



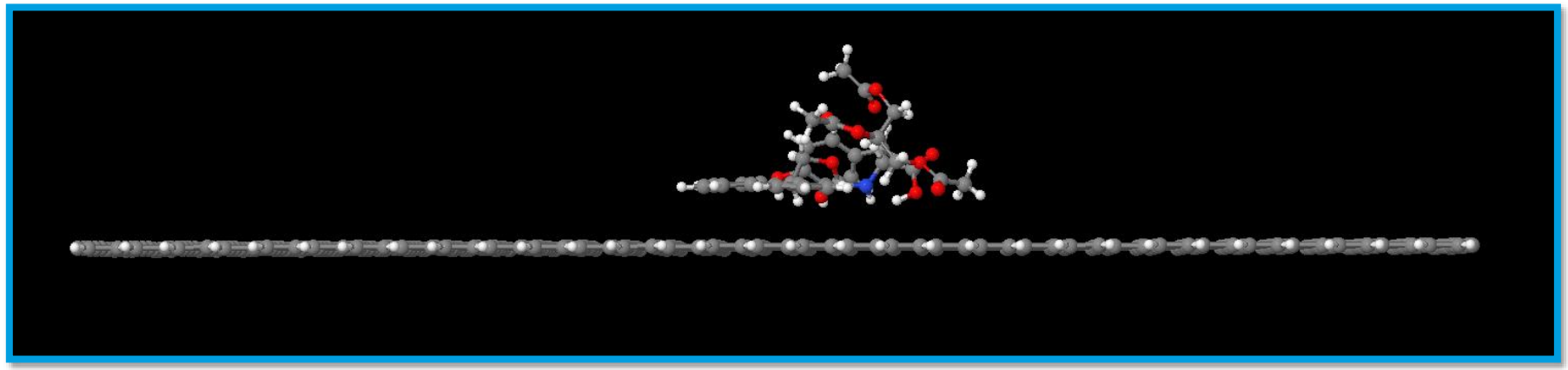




Fermi energy:
Receptor1= -4.45 eV
Receptor1+odor1= -4.44 eV

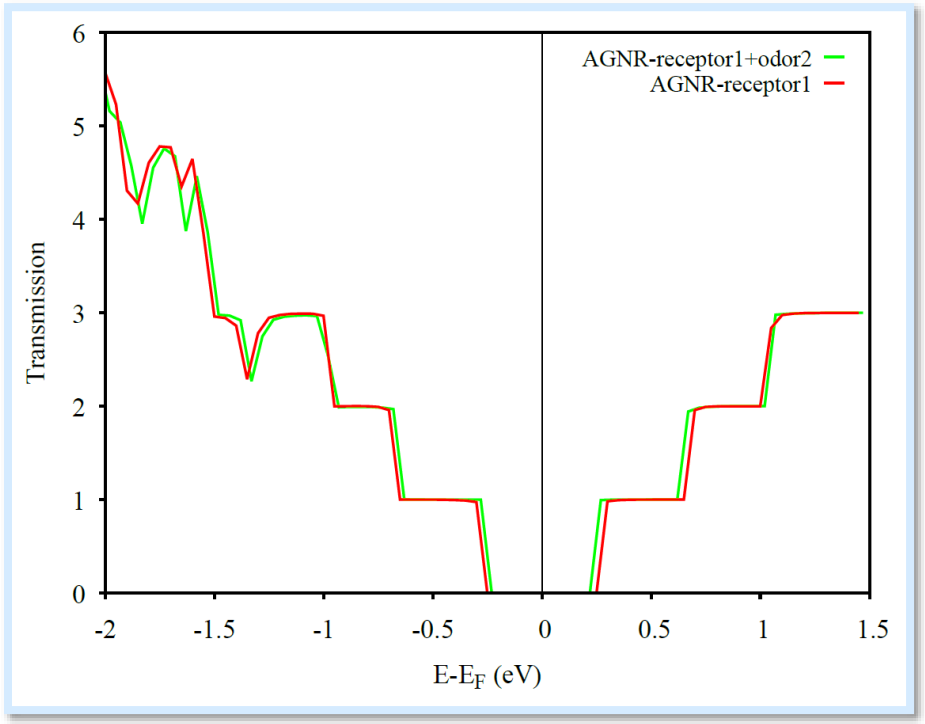
# Interaction between the receptor and the second odor molecule

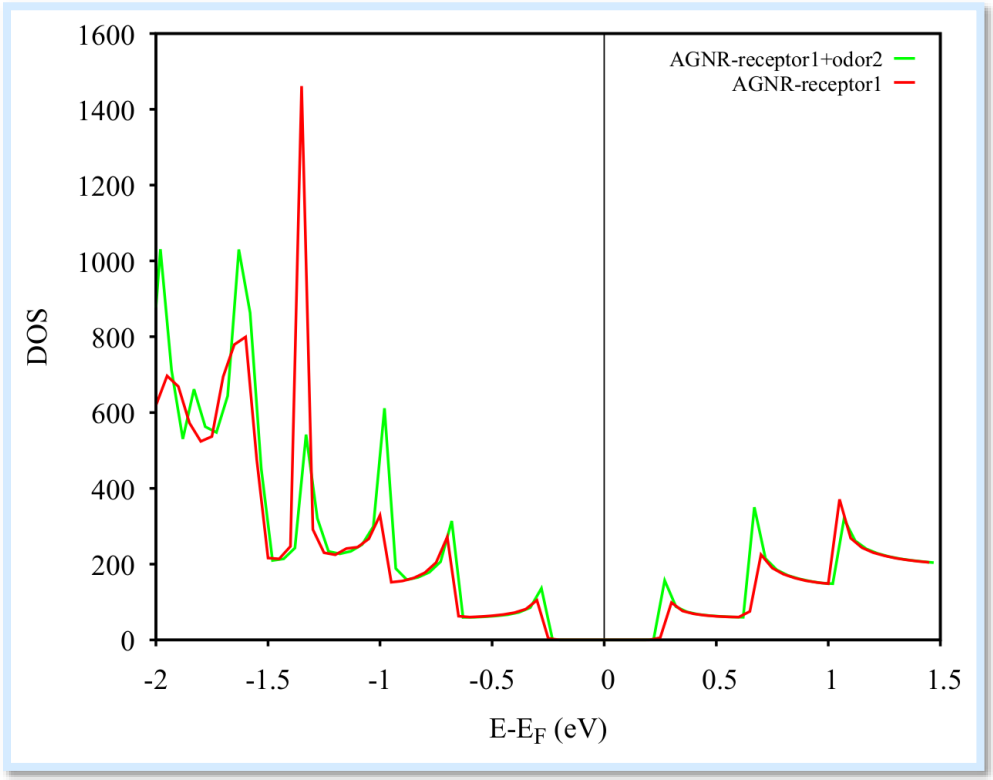


Triacetin: **C9H14O6**



# SCC Transmission and DOS in functionalized AGNR with and without the second odour molecule




Fermi energy:
Receptor1= -4.45 eV
Receptor1+odor1= -4.47 eV

# Conclusion

- The AGNR have been functionalized by one of the artificial receptor(Fmoc-Tyr-OH)
- The interaction between the functionalized AGNR with the odor molecules have been investigated
- The sensitivity in functionalized AGNR seems to be low.

## Suggestion for the next step

- The calculations could be repeated with defective AGNRs.

# Thank you for your attention!