TECHNISCHE UNIVERSITÄT DRESDEN

smellodi

European Innovation Council

Funded by the European Union

complex nano materials

SMELLODI.
Smart Electronic Olfaction for Body Odor Diagnostics.
Computational research.

CMD30 – Fismat 2023

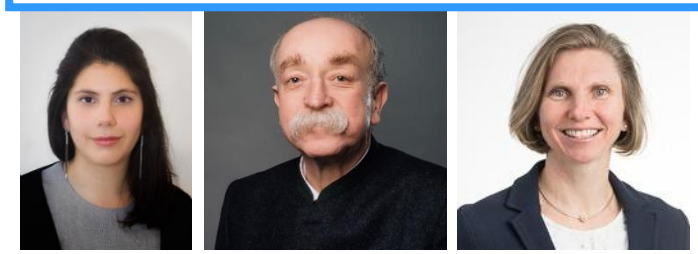
5th September, Milan

Chair Materials Science and Nanotechnology

Institute for Materials Science, TU Dresden

Dr Nina Tverdokhleb

e-mail: nina.tverdokhlib@tu-dresden.de



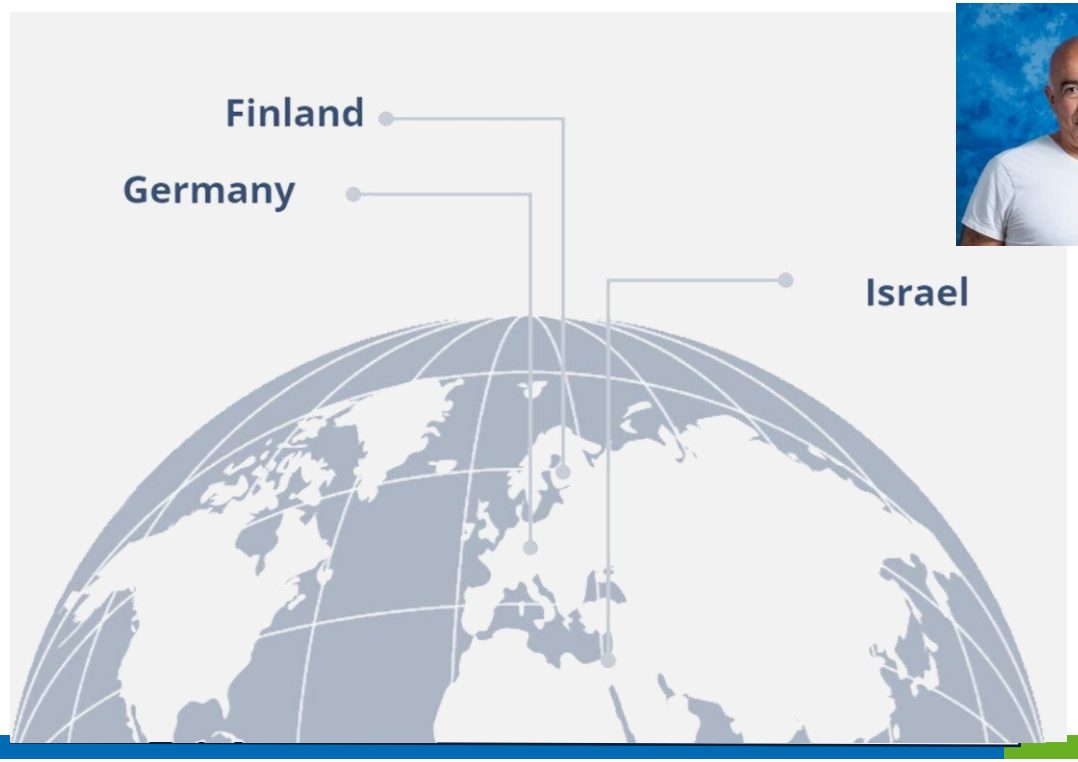












Finland
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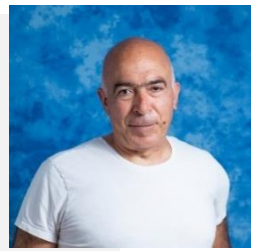
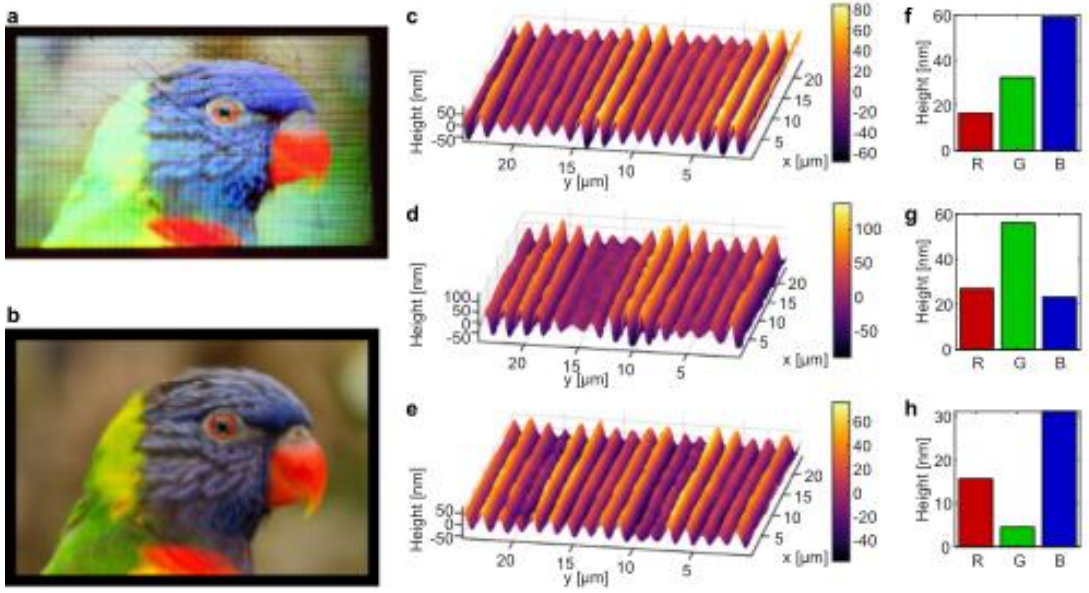






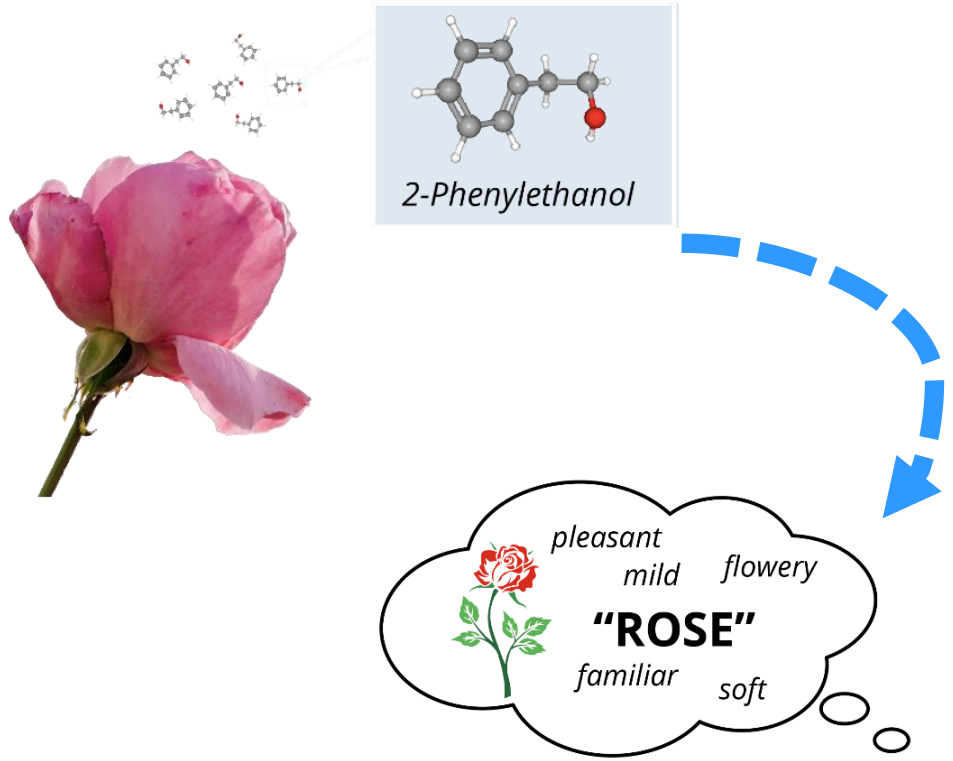
Starting Point: *Digital Senses*

Visual system



Structural colours

Olfactory system



A. Priimagi & co.
Sci. Rep. **10**, 19642 (2020)

Motivation:

Computational Modelling and Statistical Learning

BACKGROUND

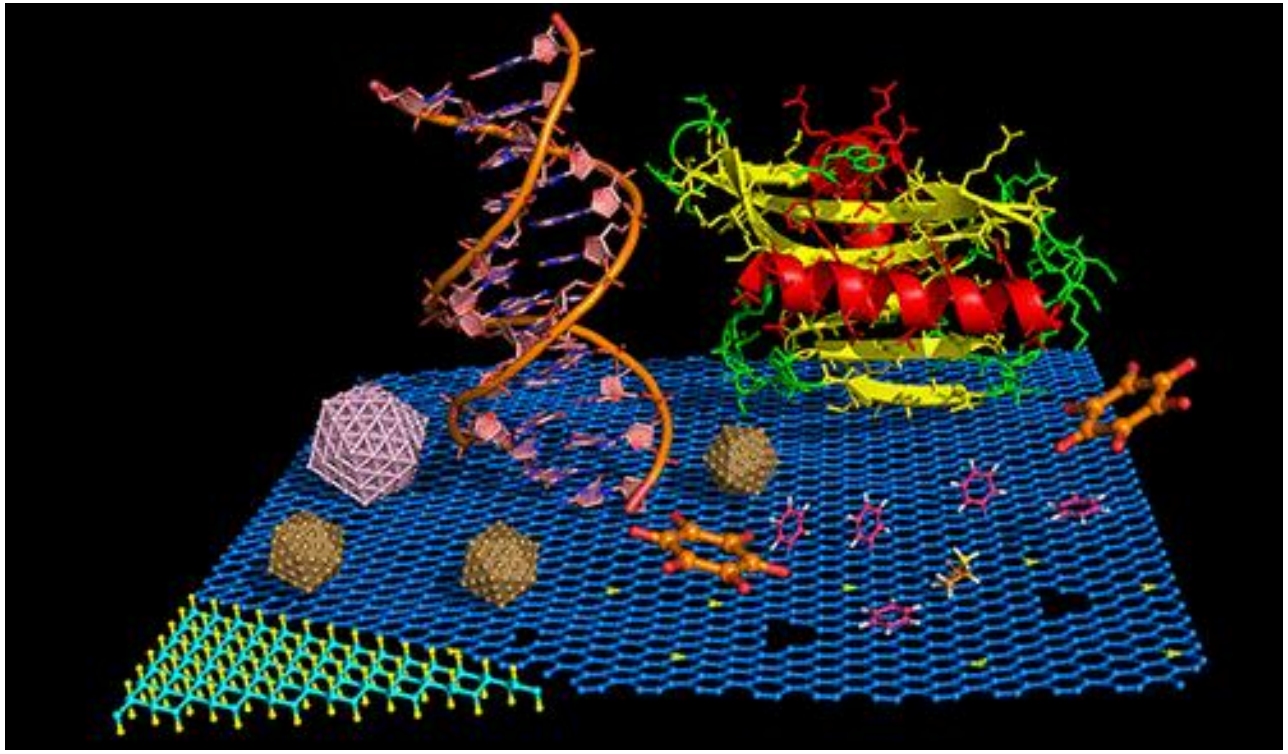
We aim at correlating **microscopic** molecular **features** to **sensor response** *via* atomistic and mesoscale simulations

OBJECTIVES

a) Atomistic descriptors for relevant odor molecules
b) Structural stability and receptor-substrate binding energies
c) Atomistic characterization of analyte - receptor binding
d) Mesoscale modeling of sensor response within an effective FET model
e) Predicting sensor signals from molecular descriptors and binding features using artificial neural networks

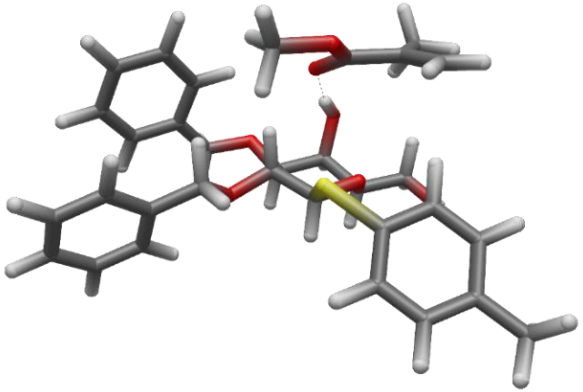
Substrate Functionalization

Non-covalent functionalization of graphene through π - interactions allows for the attachment of functional groups to graphene without interfering with the electronic structure of the material.



Chem. Rev. 2012, 112, 11, 6156−6214
Publication Date:September 25, 2012
https://doi.org/10.1021/cr3000412

Computational methods



XTB

Semiempirical Extended Tight-Binding Program Package v6.6.0
D4-ATM dispersion

DFTB

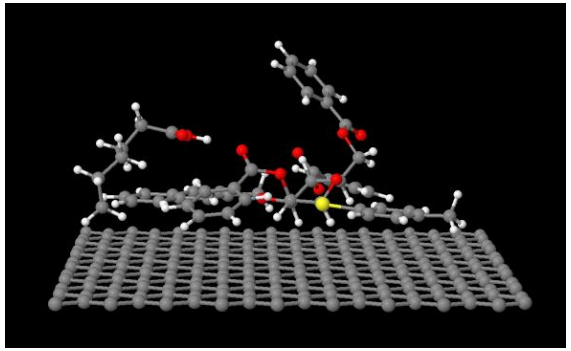
3ob parameters
D3 dispersion

VASP

PBE XC-functional
D3 dispersion

Work function

$$W = -e\Phi - E_F$$



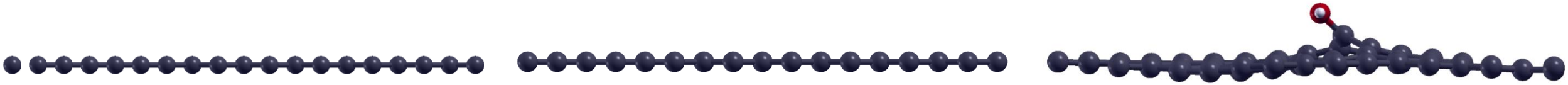
NAMD
Scalable Molecular Dynamics

Structures of graphene, N-gra and OH-gra

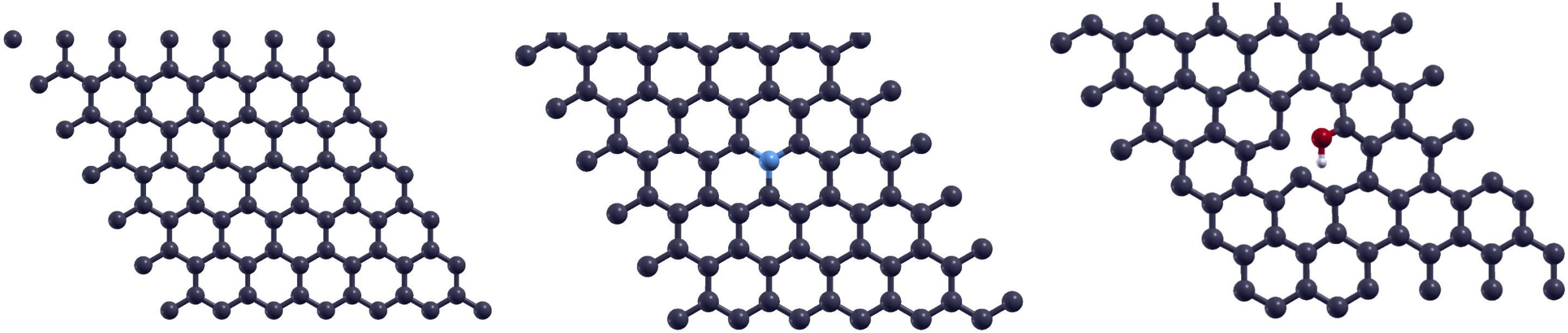
(a) Graphene (gra)

(b) N-gra

(c) OH-gra

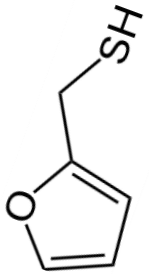


- Front view -



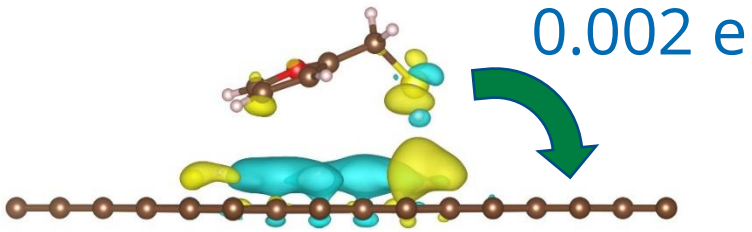
- Top view -

Charge density difference distribution (CDDD) for systems graphene-odorant

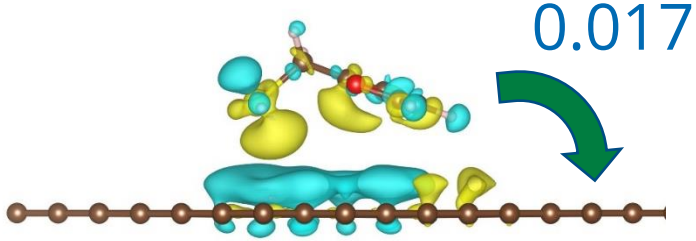


Losing
Gaining

(a) Coffee+gra



(b) coffee+N-gra

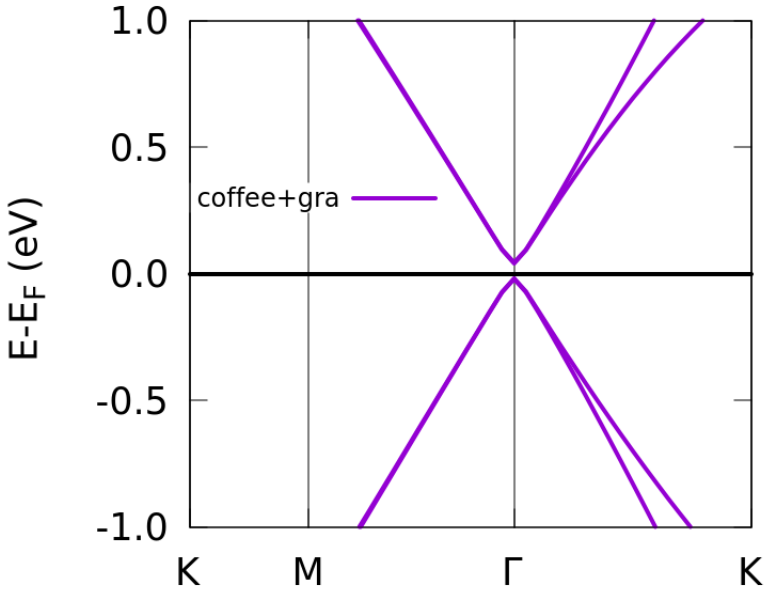


(c) coffee+OH-gra

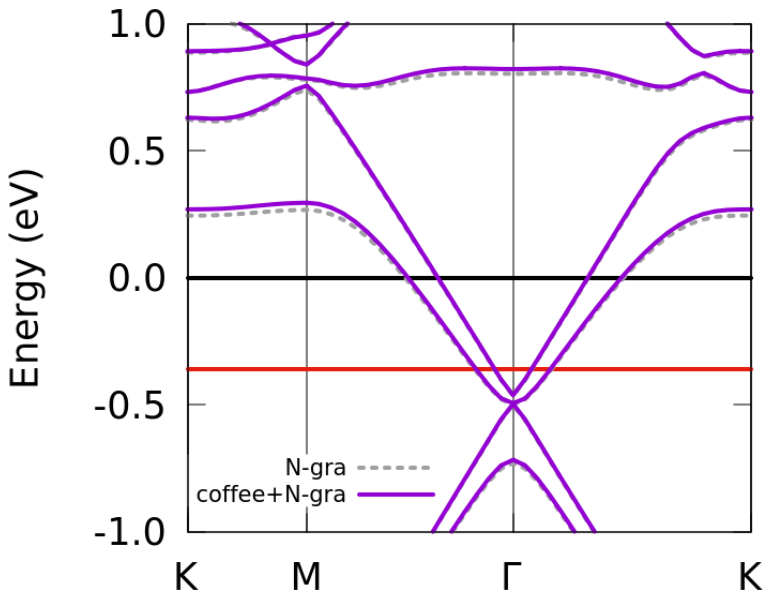
[2] Computational Materials Science, 36(3):354–360, 2006.

Electronic band structures for coffee adsorption

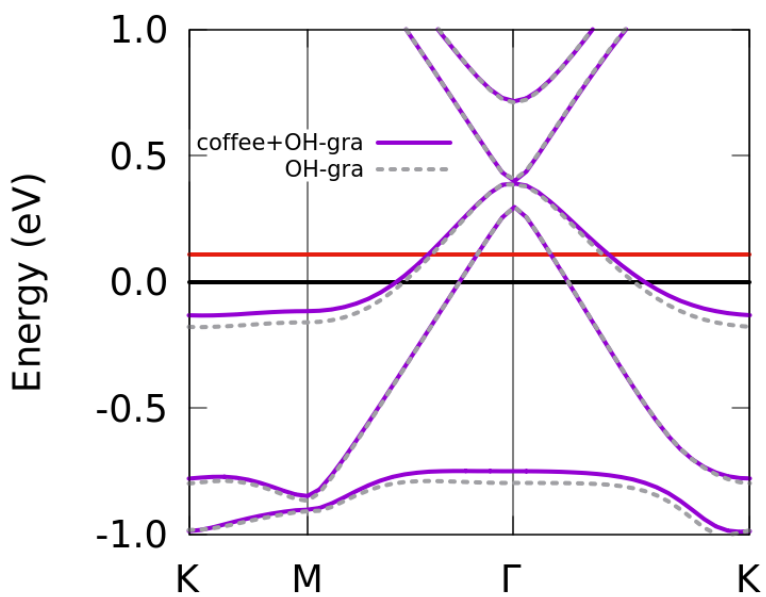
(a) coffee+gra



(b) coffee+N-gra

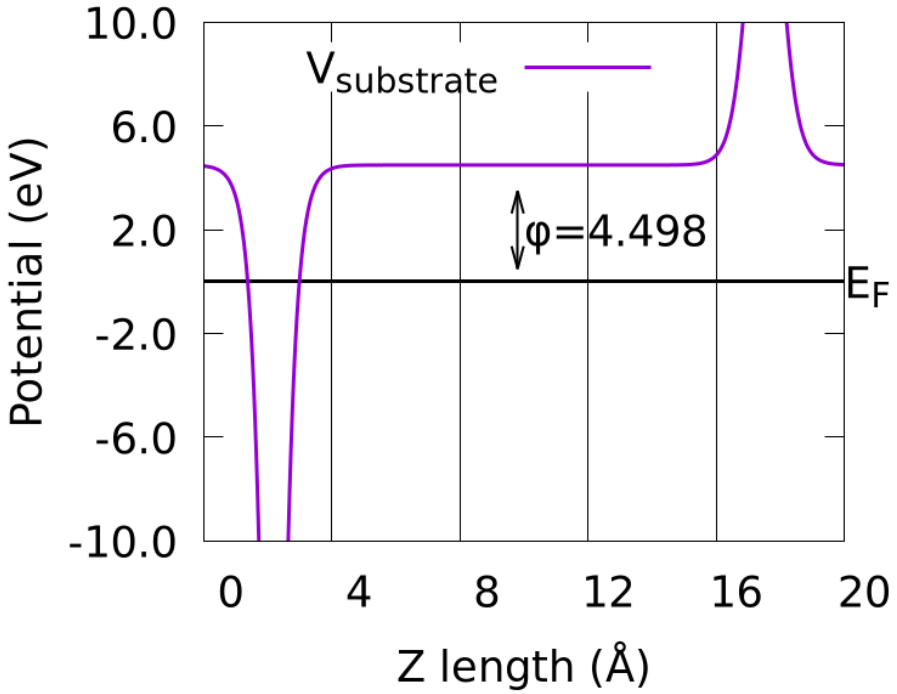


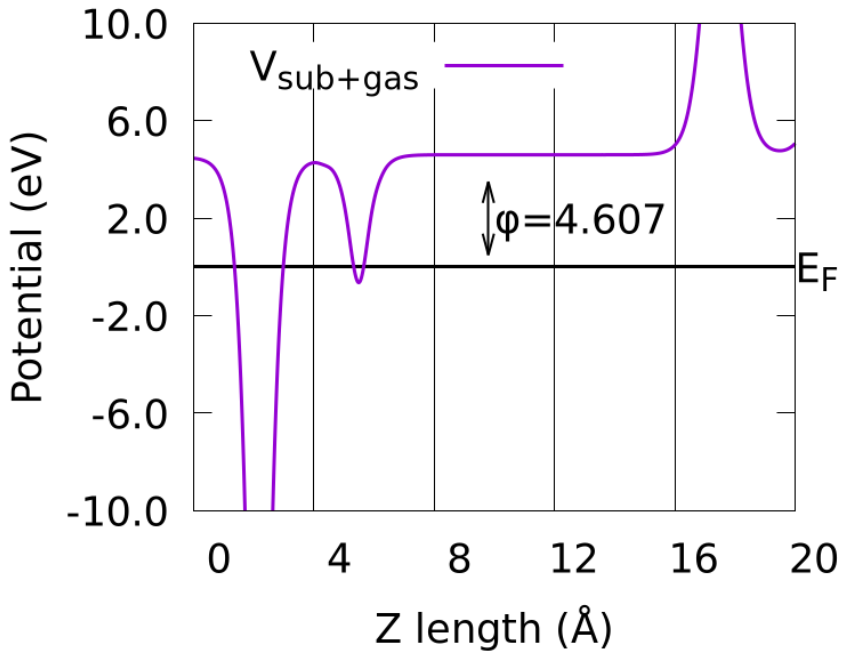
(c) coffee+OH-gra



_____ : Fermi level of the complex
_____ : Fermi level of pure surface

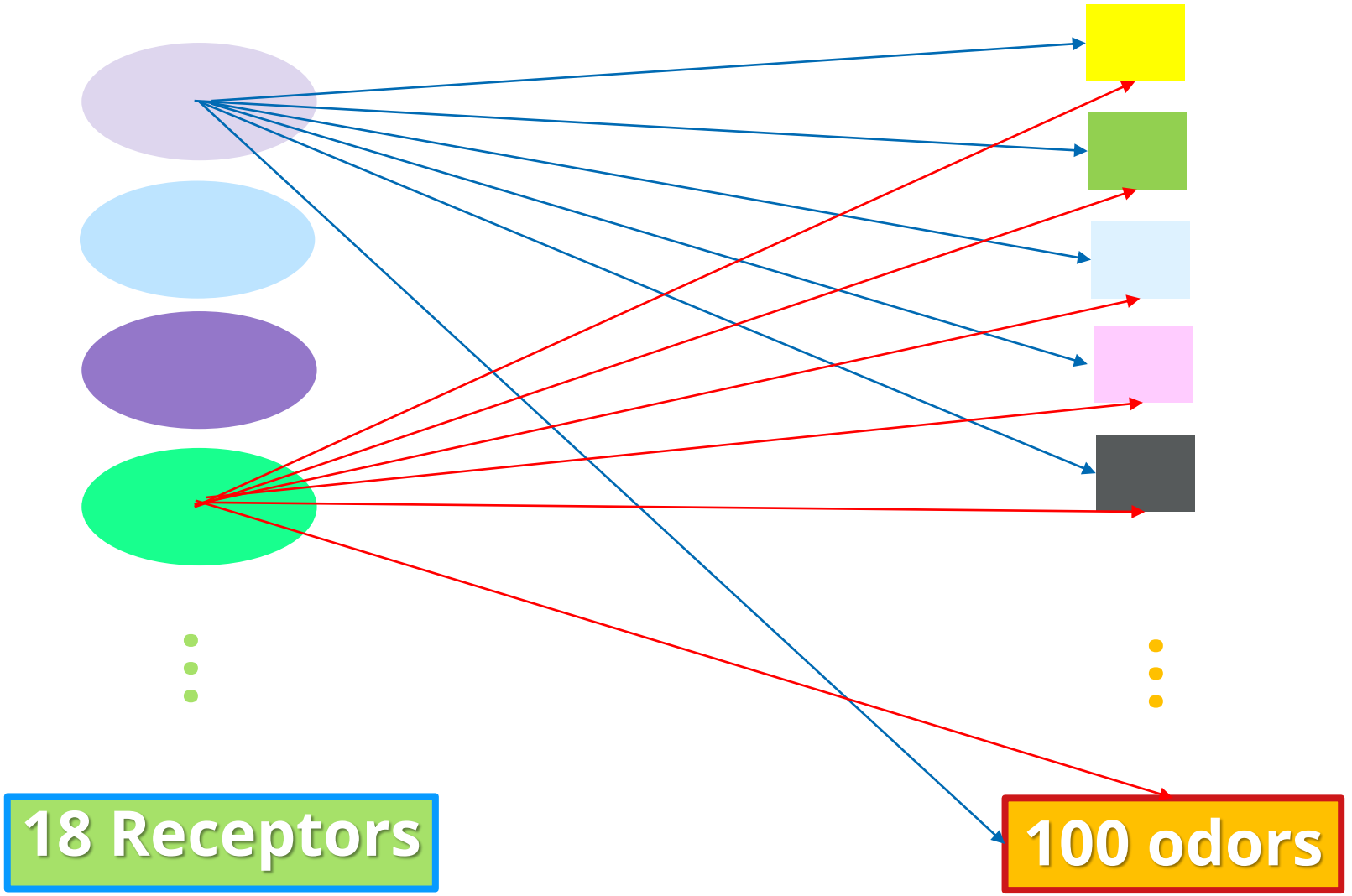
Response: work function φ = E_{vacuum} - E_F





➔**Δφ = 4.607 – 4.498 = 0.109 eV**

Investigated objects

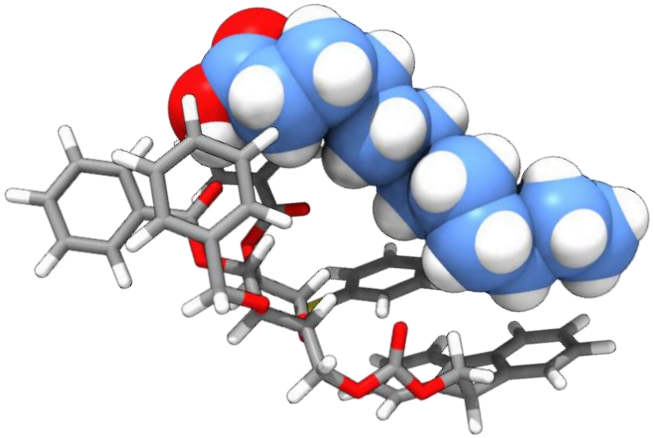


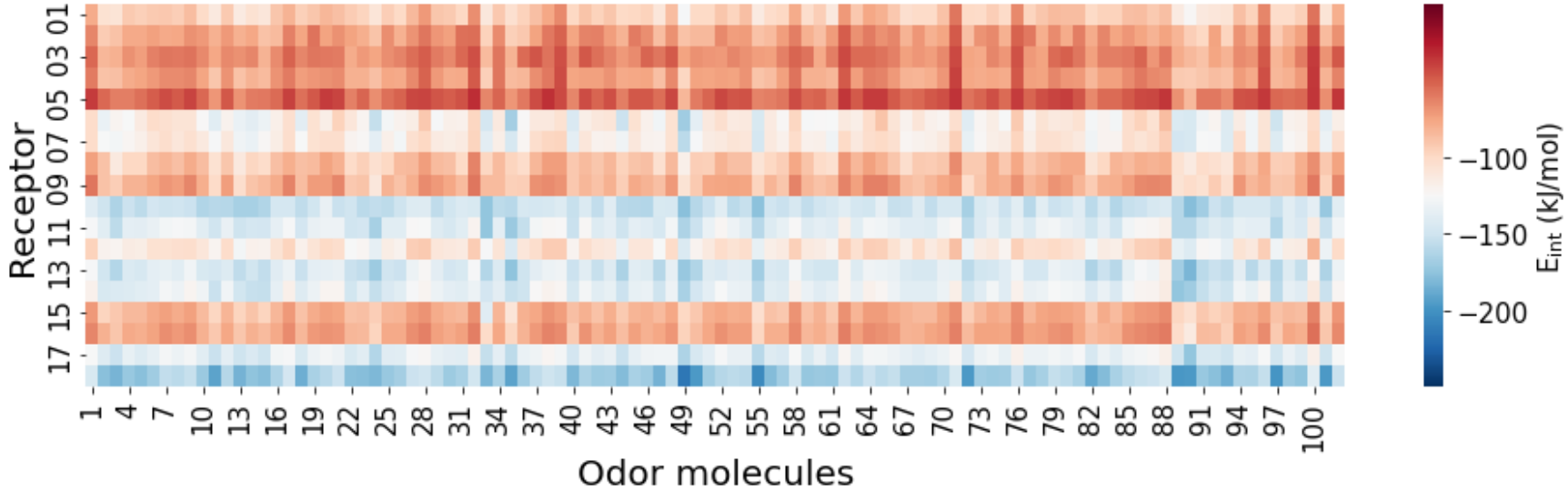
Detector: binding energy

Method – Docking in xTB → find metastable odorant-receptor configurations with the largest (absolute) value of the **interaction energy:**

$$E_{int} = E_{comp} - E_{rec} - E_{odor}$$

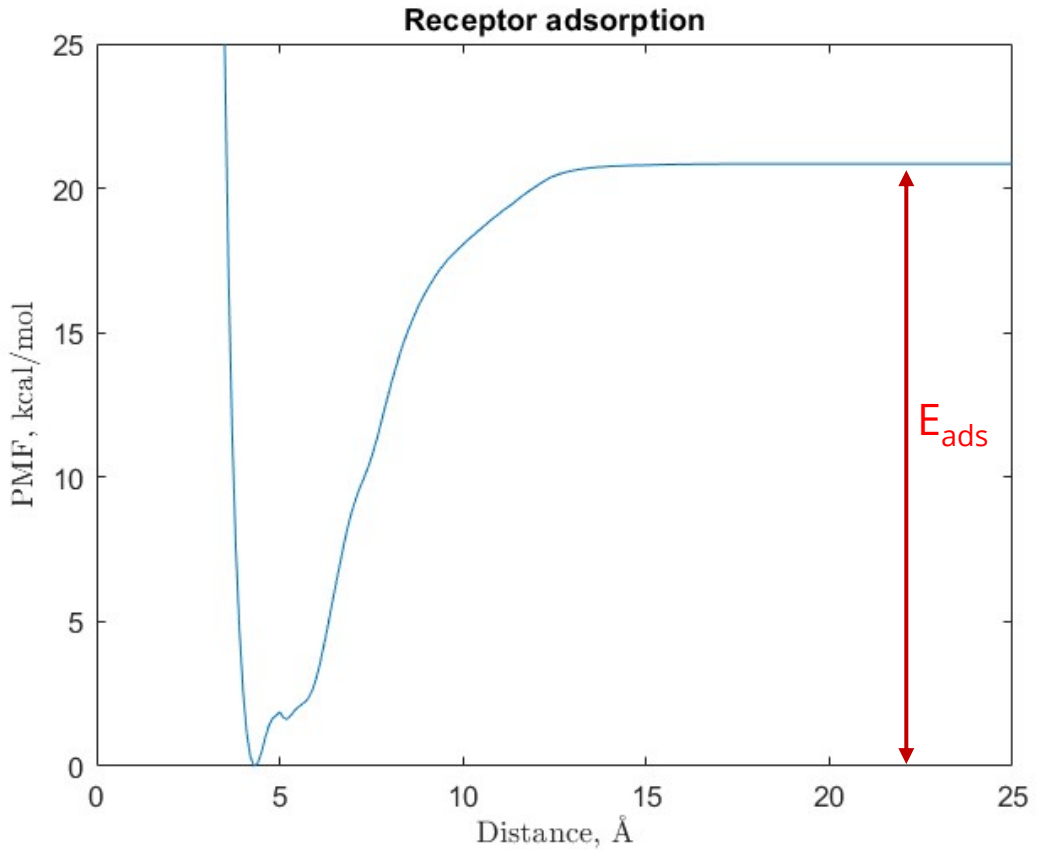
- E_{int} is only an indicator for binding affinity





Potential of mean forces curves of adsorption

Method - Steered molecular dynamic: **Adaptive biasing forces**



~ Recovery time of receptor ?

Conclusions

- Smellodi is working on digitalization of olfaction to detect smells, especially for remote medical diagnostics;
- Charge transfer, band gap, work function, binding energy and recovery time of receptor should be defined as detectors of the sensorics response.

Thank you for your attention!