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# Bacteria trapping on porous silicon: development of copper-free click-chemistry active surfaces

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Sepsis is a blood bacterial infection that can lead to death in few hours in the most severe cases. Sepsis diagnosis requires blood culture for several days because of the low blood concentration of bacteria (1 CFU/mL) before mass spectrometry (MS) analysis.

Our objective is to develop chemically functionalised porous silicon (pSi) surfaces to trap selectively bacteria from blood and identify them by infrared desorption-ionisation on silicon (DIOS)-MS in few minutes.

Bacteria will be specifically trapped on the pSi surface thanks to immobilisation of a nanobody (Nb) via copper-free click reaction with dibenzocyclooctyne (DBCO-PEG-silane molecules) modified surfaces.

## Porosification

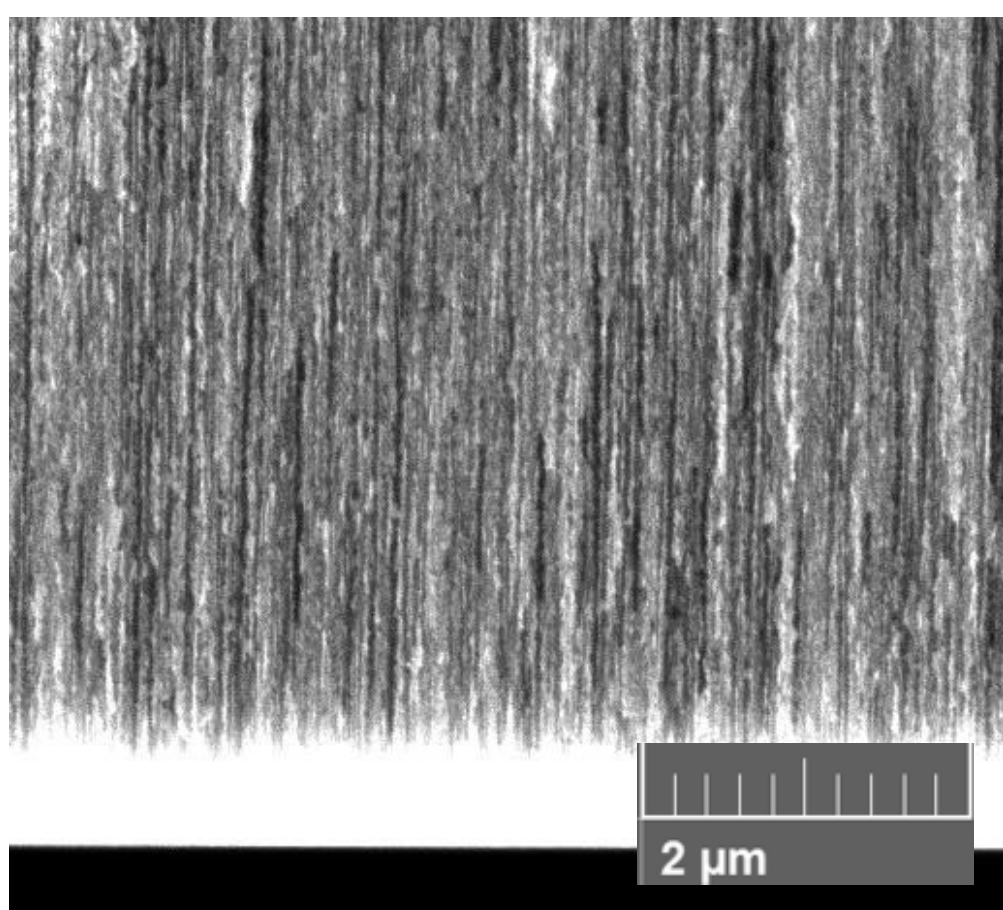
### Electrochemical etching

Silicon wafer parameters

Resistivity	0.001-0.005 Ω.cm
Diameter	2"
Thickness	300 μm
Type	P, Boron doped
Orientation	100

Process parameters

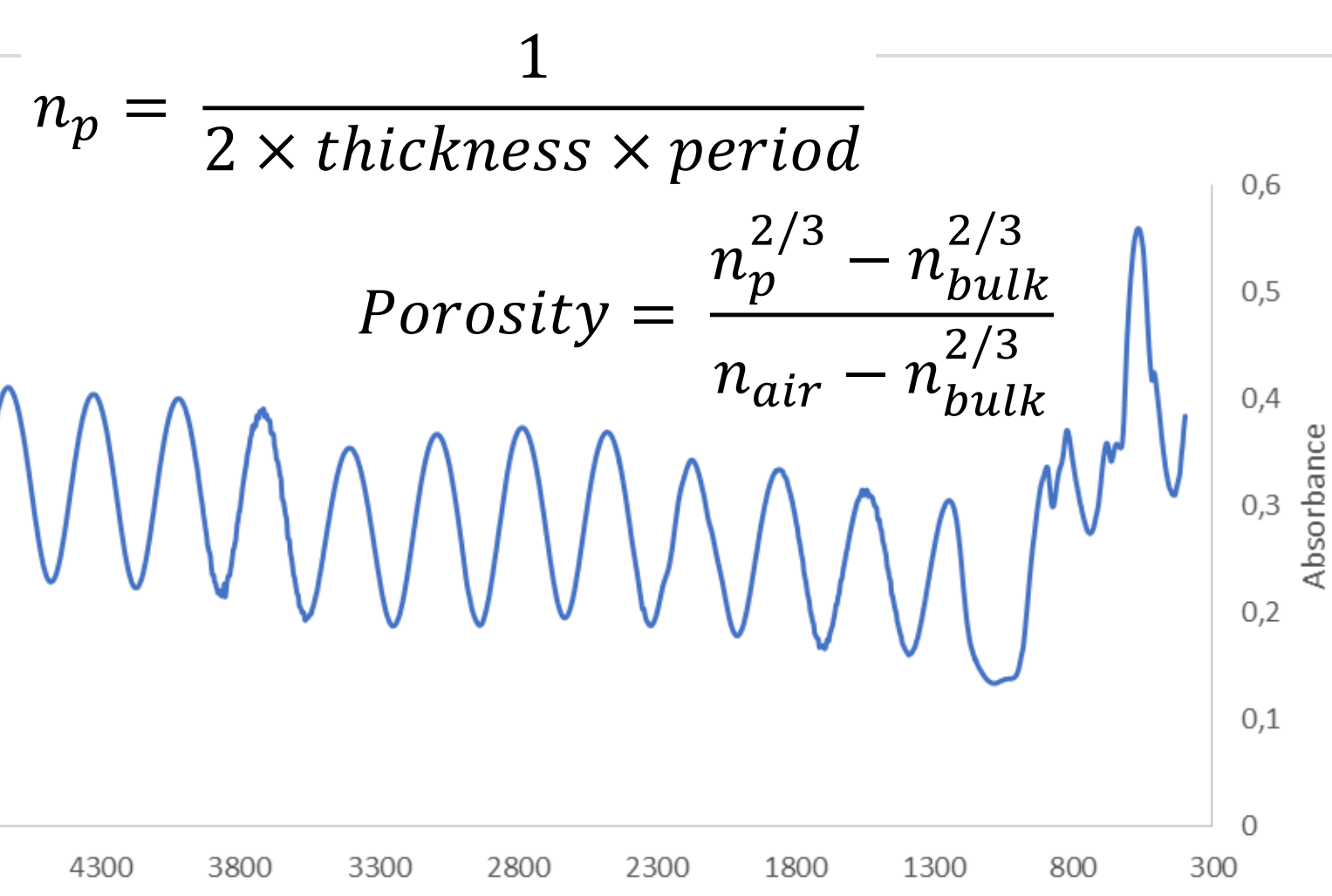
Current Density	200-2000 mA
Etching time	5-30 min
HF concentration	12,5%-37,5%



pSi : 20 nm diameter, 12 μm depth, 70% porosity

pSi characteristics

Pores depth	3 - 30 μm
Pore size	10 - 100 nm
Porosity	35 - 80 %

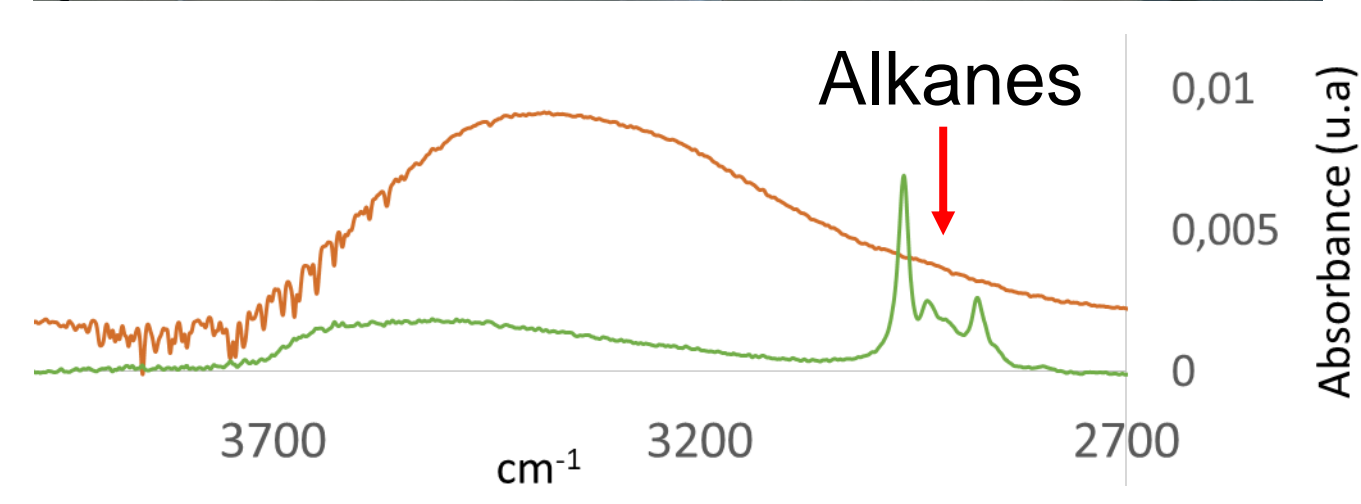
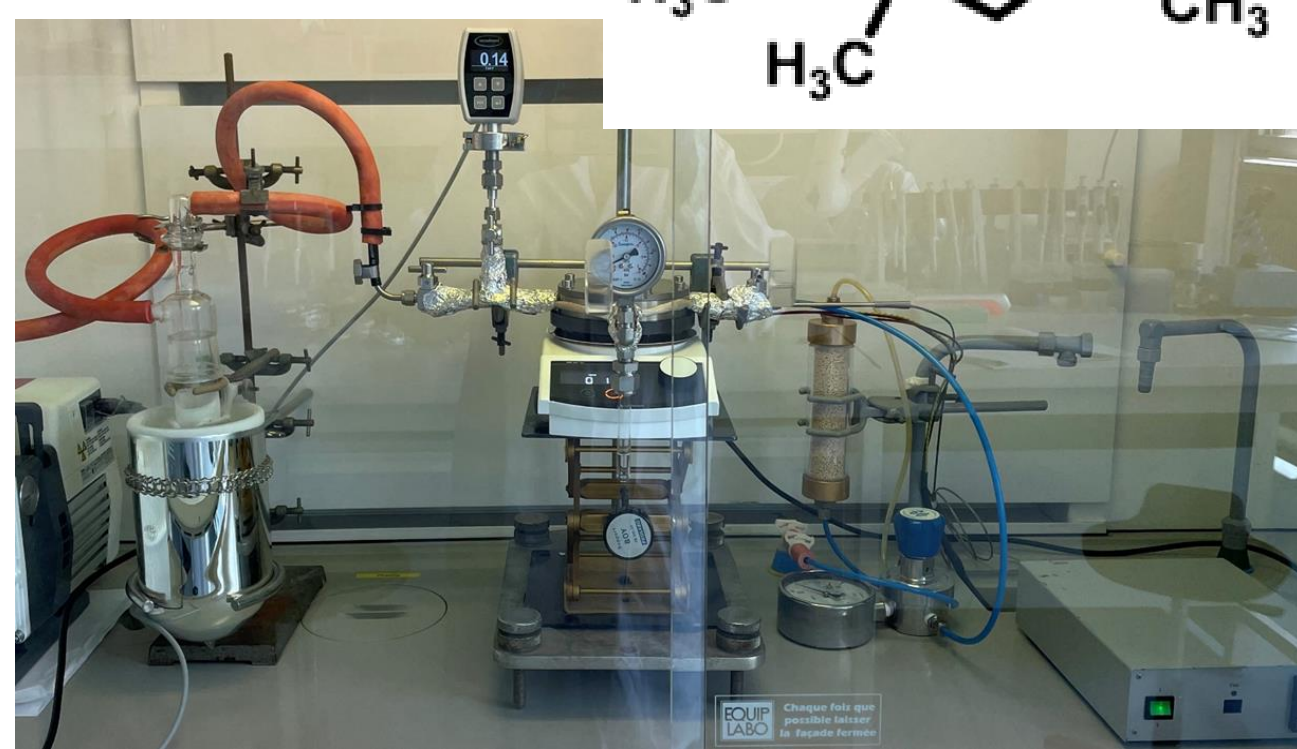
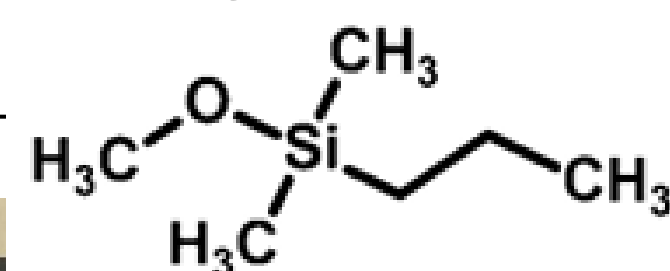


## Surface functionalisation

### Gas Phase

Propyldimethylmetoxysilane (CH<sub>3</sub>-short)

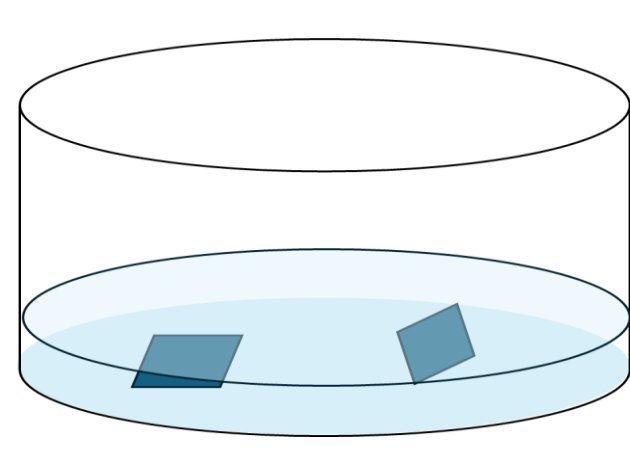
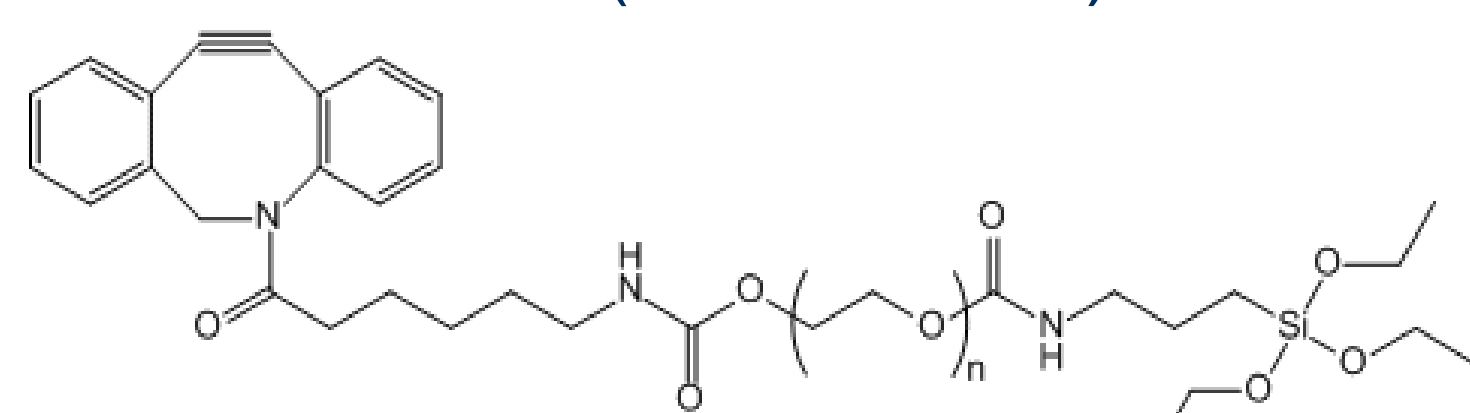
20 Torr of silane at room temp., then 4h (16h) curing at 180°C (120°C)



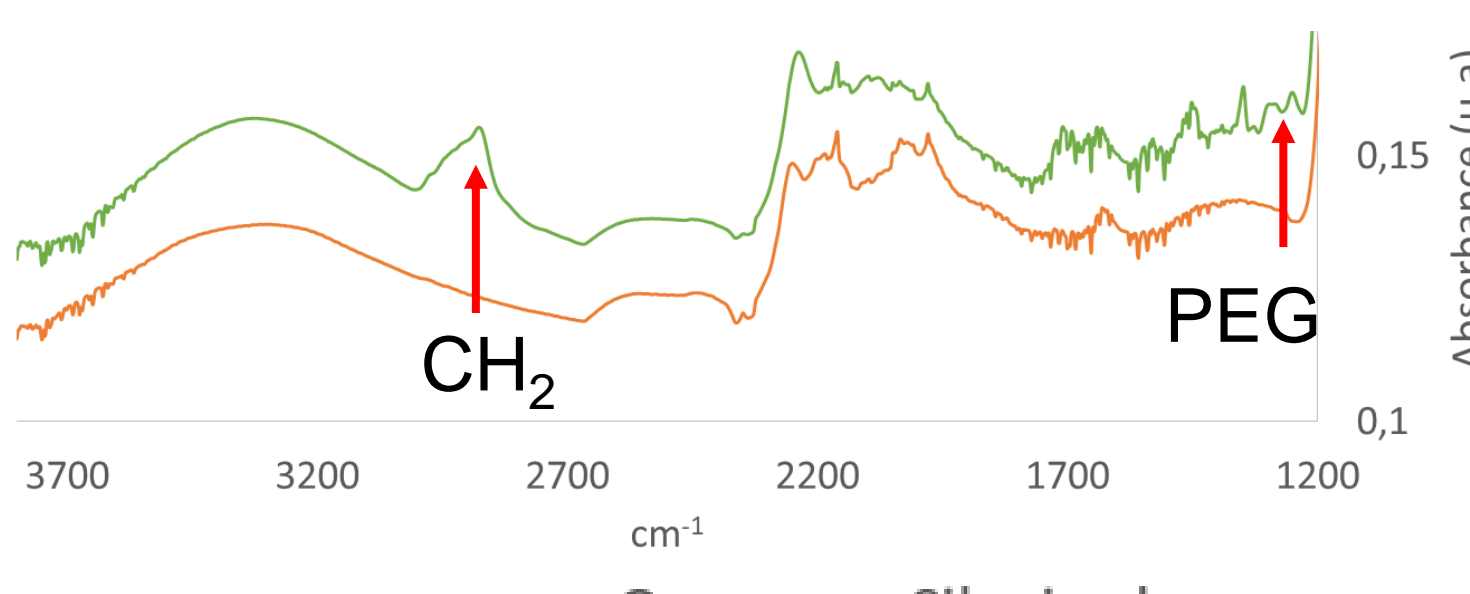
FTIR-ATR : pSi before / after CH<sub>3</sub>-short modification

### Liquid Phase

Dibenzocyclooctyne-PEG(2000Da)-silane (DBCO-PEG)



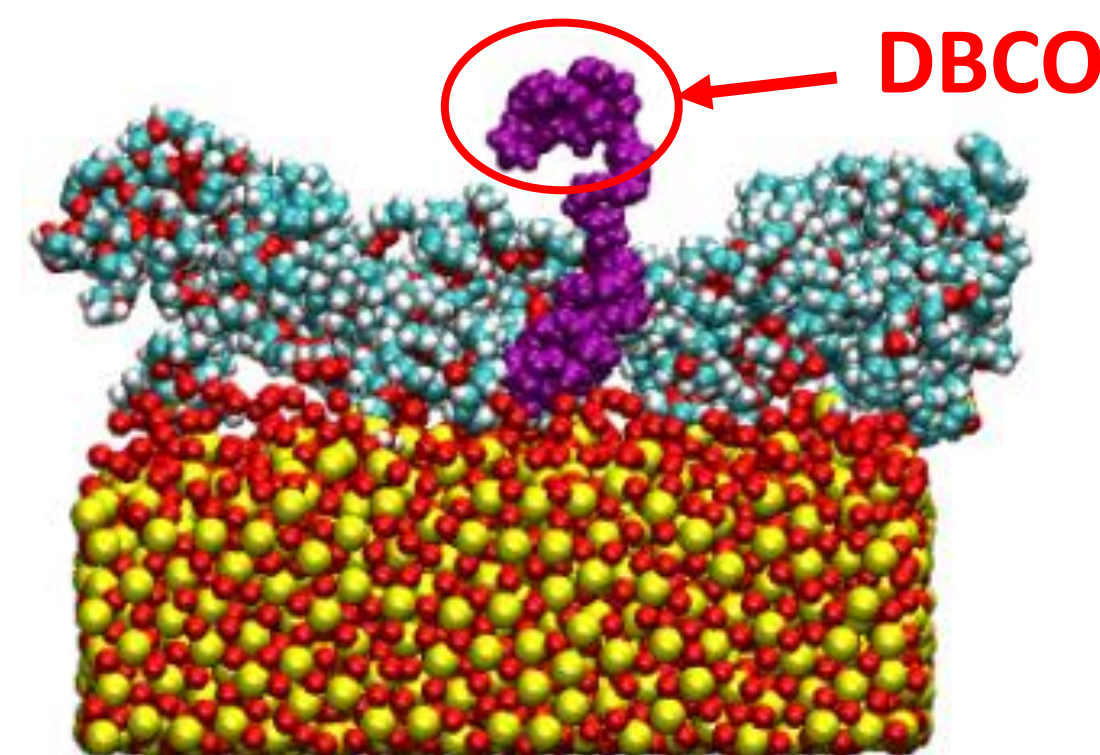
anhydrous ethanol with 0.14% of acetic acid + DBCO-PEG (10<sup>-3</sup> mol/L) for 16h. Curing (50°C, 30 min)



FTIR-ATR : pSi before / after DBCO-PEG<sub>34</sub>-silane modification

## Molecular Dynamics Simulation

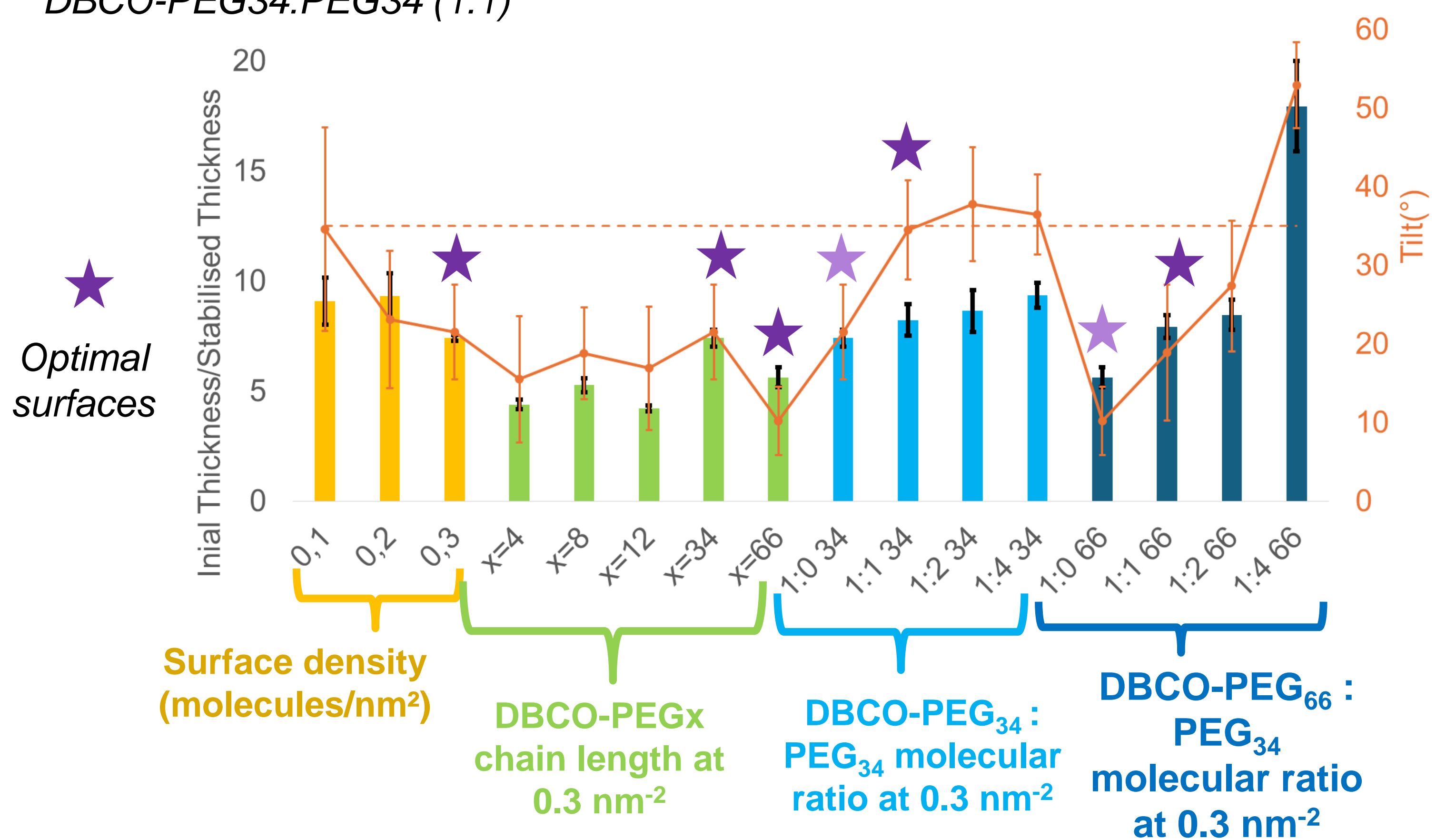
### Molecular Dynamics (MD) Simulation (Gromacs 2023.2)



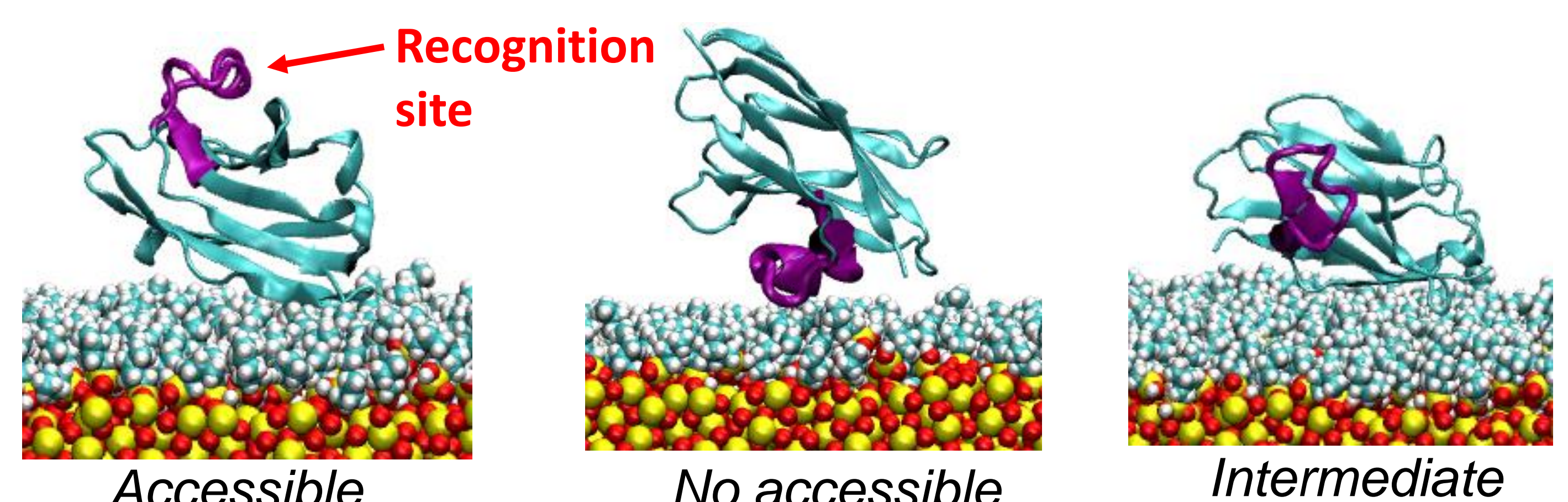
30 ns simulation, average of triplicate

Optimisation of the accessibility of the DBCO groups by tuning surface modification

SiO<sub>2</sub> surface modified by a mix DBCO-PEG<sub>34</sub>:PEG<sub>34</sub> (1:1)



### Adsorption of a nanobody(Nb) (3 orientations, 7 surfaces)



	Bare SiO <sub>2</sub>	CH <sub>3</sub> -short	PEG <sub>34</sub>	DBCO <sub>34</sub>	DBCO <sub>34</sub> :* PEG <sub>34</sub>	DBCO <sub>66</sub>	DBCO <sub>66</sub> :* PEG <sub>34</sub>
Most probable orientation	No Access.	Access.	No Access.	No Access.	Inter.	Inter.	Inter.
Relative E(kJ/mol)	1060	1389	760	394	287	0	604

\* 1:1 molecular ratio

None of the surface gives any deformation of the Nb (RMSF<3Å)

CH<sub>3</sub>-short : gives an orientation compatible with bacteria trapping but is the less stable

DBCO<sub>66</sub> : recognition site on the side but the highest stability

## Conclusion and Perspectives

Experimentally, we managed to make some reproducible protocols for each silane in two different ways. Furthermore, we successfully made some pSi with large pores (100 nm) even if we have to optimise the protocol to increase porosity. For the simulation, the deformation and the orientation of Nb were studied following physisorption. According to the simulation, CH<sub>3</sub>-short gives the orientation where the recognition site is accessible while the DBCO<sub>66</sub> gives the most stabilised system. We will investigate antifouling properties of the different surfaces by determining the structure of the interfacial water layer (water molecule diffusion coefficient, coordination number...), and graft a Nb with a covalent bond to look at the deformation of the recognition site. Then, these simulation works will be used to explain experimental results. The different pSi modified surfaces, presented above, will be elaborated (with at least pore diameter of 100 nm but 1 μm would be preferred if possible). Nb will be grafted by click-chemistry on the DBCO groups. Then, bacteria trapping efficiency will be evaluated by fluorescence spectroscopy, and compared to the results obtained with adsorbed Nb.

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