1.2. Virus: Detección de interacciones hidrofóbicas e hidrofílicas de polisacáridos
Viruses: Sensing hydrophobic and hydrophilic interactions of polysaccharides (Glycans)

(Tutor: Horacio V. Guzman, horacio.guzman@uam.es**)**

Viruses are an extremely simple form of life that consists of a genome inside a capsid, made of a combination of proteins, lipids, and glycans (i.e., polysaccharides). Although glycans have been considered for several viruses as secondary virus components, thorough studies [1,2] of the SARS-CoV-2 glycosylated surface have demonstrated the key role they can play when identifying possible antibody binding-sites. The glycans have also explained an innovative camouflage mechanism of the SARS-CoV-2 spike proteins, which hinders the rapid detection of the human immune system by steric repulsion. Recent findings have modeled the shape of glycans in the spike protein to map steric accessibility to find realistic epitopes for structure-based vaccine design [1]. This work has considered several properties of the spike proteins, like the rigidity, sequence conservation, among others. However, the adsorption of such polysaccharides to the solid liquid interface in relevant environmental conditions has not been tackled yet. In particular, we want to determine if certain adsorption preferences of glycans onto hydrophobic or hydrophilic surfaces may modify their structure and, hence, allow the adsorption of hydrophobic and hydrophilic residues onto the substrate activating the protein-surface interaction. This is a highly relevant material-design question, as substrates trapping viruses can be an efficient strategy to prevent virus propagation. And on the other hand, relevant for the antibody-design, which corresponds to the disease treatments.

In this project, the student will help develop a computational algorithm for calculating the adsorption energies capable of exploring the different glycans short-range interactions. Such endeavors would enable us to evaluate the preferential adsorption surfaces, and determine configurations where the steric interactions are minimal. The surface molecular dynamics mode is available at the host group [3], as well as the modeling of Glycans, which may also include international collaborations with Germany and Slovenia. The theoretical methods used in this project involve the calculation of binding energies and the structural analysis of adsorption. Those calculations will be performed at High-Performance-Computing facilities. Prior experience in programming (C, C++ or Python) would be helpful.

[1] M. Sikora et al. PLoS Comput Biol 17(4), 2021: e1008790. https://doi.org/10.1371/journal.pcbi.1008790
[2] B. Turnova, M. Sikora, et al. Science 370 (2020)
[3] https://tinyurl.com/goCompModeling

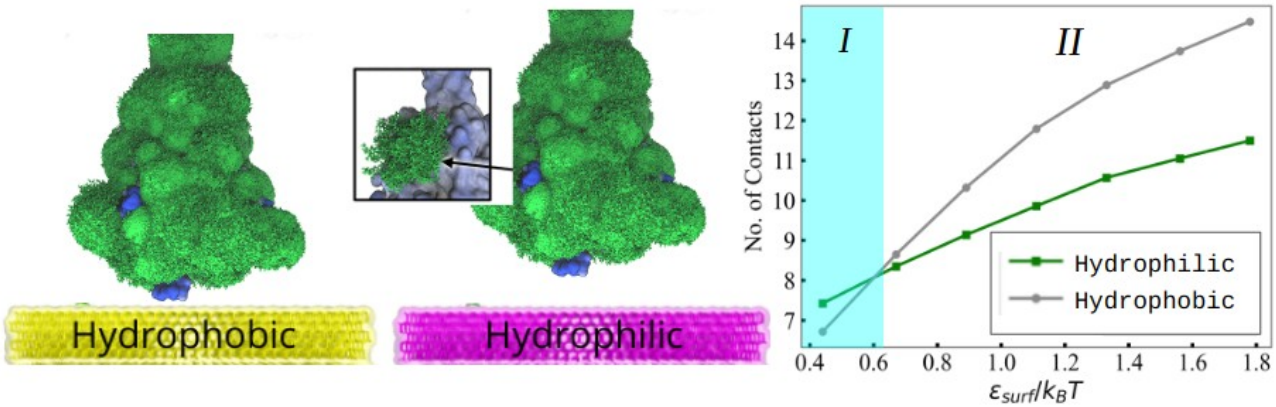

Figure 1: Computational model of two spike proteins, surrounded by Glycans, adsorbing onto hydrophobic and hydrophilic surfaces. The adsorption phenomenology is rich in behavior showing different regimes, which depend on the attractive strength of the surface, tuned by their contact angles.