1.2. Virus: Interacciones electrostáticas y adsorción en sustratos corrugados
Viruses: electrostatic interactions and adsorption onto corrugated substrates

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Viruses are an extremely simple form of life that consists of a piece of nucleic acid inside an capsid, made purely of proteins, or, as in the common flu and COVID-19 viruses, of a combination of proteins and lipids The infection mechanism of viruses involves the attachment of the capsid onto biological substrates, that are naturally corrugated at the nanometer scales. In the case of virus with purely protein capsids, the adsorption process brings into play rich electrostatic interactions and possibly structural changes of the capsid. It has been recently shown that these electrostatic interactions between the capsid proteins and the substrate are highly localized [1,2]. In this project, we want to explore the interplay between the charge distribution, the symmetry of the capsid, and the nanometer-scale properties of the substrate in the adsorption process. In particular, we want to determine if certain adsorption geometries may modify the structure of the virus capsid and, hence, influence the disassembly process and inhibit the virus activity. This is a highly relevant materials-design and also biological question, as substrates trapping viruses can be an efficient strategy to prevent virus propagation or infection.

In this project, the student will help develop a computational algorithm for calculating the binding energies capable of exploring the different icosahedral symmetries of the virus capsid (based on their T-number). Such endeavor would enable us to evaluate the preferential adsorption symmetry with a high-resolution method considering not only the amino acid but also the atomistic level of the virus capsid. While the corrugated substrate will be coarse-grained from available molecular dynamics simulations of 6 different membranes and 1 modeled self-assembled bilayer. We will then evaluate different polarizable substrates and quantify their adsorption energies. The theoretical methods used in this project involve the calculation of electrostatic interactions (Poisson-Boltzmann equation) and our in-house developed coarse-grained approximation to the van der Waals forces for different capsid symmetries. Moreover, basics of coarse-graining molecular dynamics. Prior experience in programming (C, C++ or Python) would be helpful.

[1] C. D. Cooper, I. Addison-Smith, H. V. Guzman, Nanoscale (2022). https://doi.org/10.1039/D2NR02526D
[2] https://tinyurl.com/goCompModeling

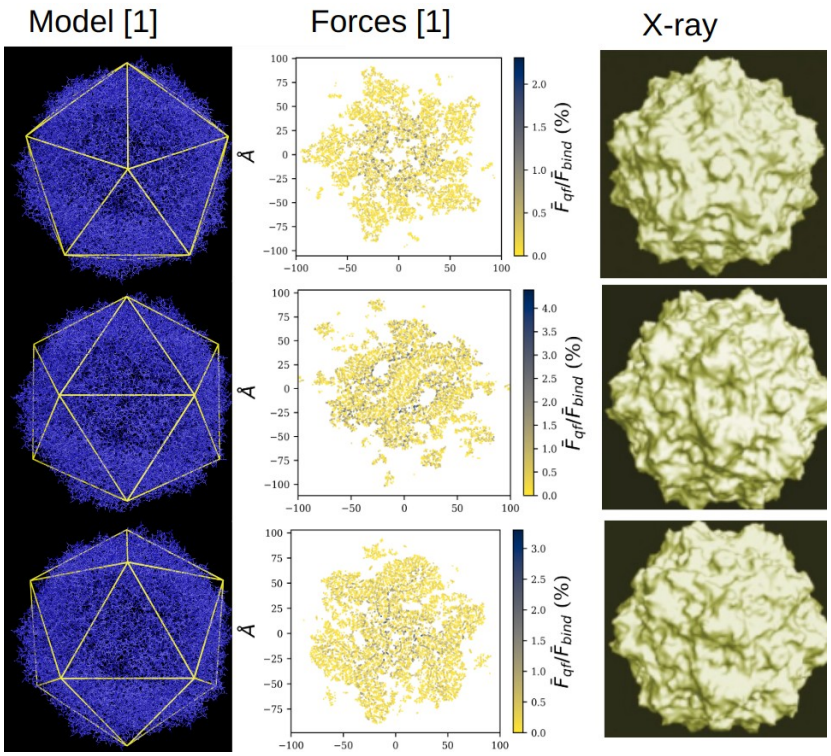

Figure 1: Computational model of an icosahedral virus being adsorbed onto flat substrates. The electrostatic Forces play a key role in identifying the adsorption symmetry.