

## M2 Internship: Viral self-assembly and defect dynamics

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Abstract: A virus is a molecular object mainly composed of a genome and a protective proteic shell. Various morphologies of these thin shells, ranging from ideal icosahedron to conical shape, are observed across viral families. Thin shell elasticity allows to rationalize the observations of most shapes based on the value of the spontaneous curvature of the shell. We recently showed that the self-assembly pathway is dictated by the need of relaxing the mechanical stress that is inherent to the growth of a curved substrate. For high spontaneous curvature, the growing structure must incorporate defects, mainly disclinations or pentamers. The position of these defects will determine the overall shape of the virus and therefore its curvature.

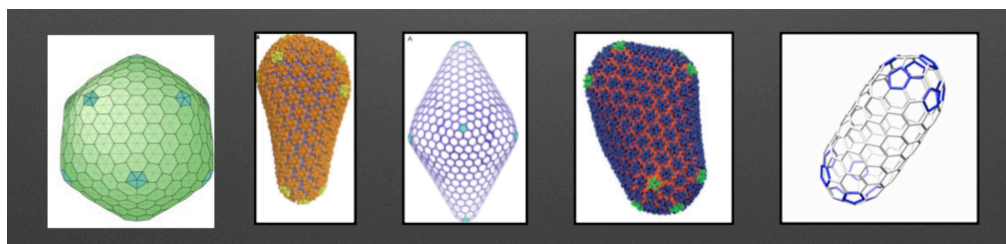
By performing nanoindentation with AFM on different virus, it is possible to change the shape of the shell. The question to be addressed theoretically within this internship is to model the elastic response of such experiments, focusing in particular on the role played by the defects, and their position and dynamics. The model to be designed and analyzed should take into account the dynamics of the defects and their interaction as the shape of the supporting shell is changed. We will use numerical methods in order to minimize the energy of the deformed shell, and we will use also scaling approach in order to rationalize the numerical observations.

Several extensions to this work can lead to a consistent Ph-D program: various questions related to the nucleation of the defects during self-assembly, their out-of-equilibrium properties ; the nucleation of defects in the protein with some external scaffold , etc...

Some references on viral capsid shape, and thin shell elasticity

[1] Wagner J., Zandi R., *The robust assembly of small symmetric nanoshells*, **Biophys. J.** 109, 956 (2015).

[2] Buenemann M., Lenz P. *Elastic properties and mechanical stability of chiral and filled viral capsid*, **Phys. Rev. E** 78, 051924 (2008).



**Figure :** Various viral morphologies corresponding to different distribution of pentameric defects.

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