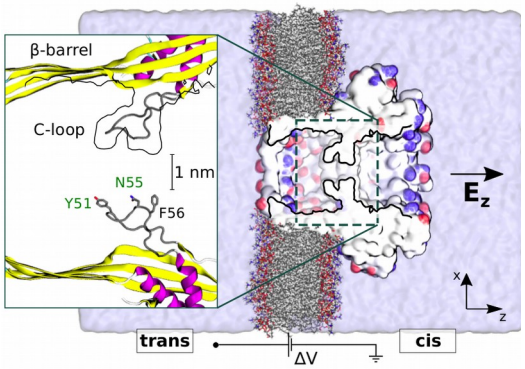
Master degree thesis: Nanopore protein sensing

Proteins perform a huge number of functions in living organisms, thus all the new techniques allowing their precise, fast and accurate characterization at single-molecule level would represent a burst in proteomics with important biomedical impact [1]. Nanopore based sensors constitute a promising approach to single molecule protein sensing being able to detect sequences, structural elements and folding states of proteins and polypeptide chains [2].

In the last years, we employed computation methods (mainly all-atom molecular dynamics simulations and coarse-grained models) to analyse the transport phenomena across nanopores [3-4] for application in proteins sensing and sequencing [2].

Presently, we are focusing on two main research topics, namely: i) the employment of electroosmotic flow to control the molecule capture by the pore and ii) the dielectrophoetic capture and trapping of molecules in solid state and biological nanopores.



The CsgG nanopore, currently used as template for designing the pore embedded in commercial devices for DNA sequencing. The image refers to the simulation set-up we employed to characterize the ion and water flow through the pore under an applied voltage [4]

References

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[2] Chinappi, M., & Cecconi, F.. Protein sequencing via nanopore based devices: a nanofluidics perspective. Journal of Physics: Condensed Matter. (2018)

[3] Bétermier, F., Cressiot, B., Di Muccio, G., Jarroux, N., Bacri, L., Morozzo della Rocca, B., ... & Tarascon, J. M. (2020). Single-sulfur atom discrimination of polysulfides with a protein nanopore for improved batteries. Communications Materials, (2020)

[4] Di Muccio, G., Morozzo della Rocca, B., & Chinappi, M. (2021). Geometrically Induced Selectivity and Unidirectional Electroosmosis in Uncharged Nanopores. ACS Nano (2022)