

Computational Microscopy

bridging the gap between simple models and complex reality

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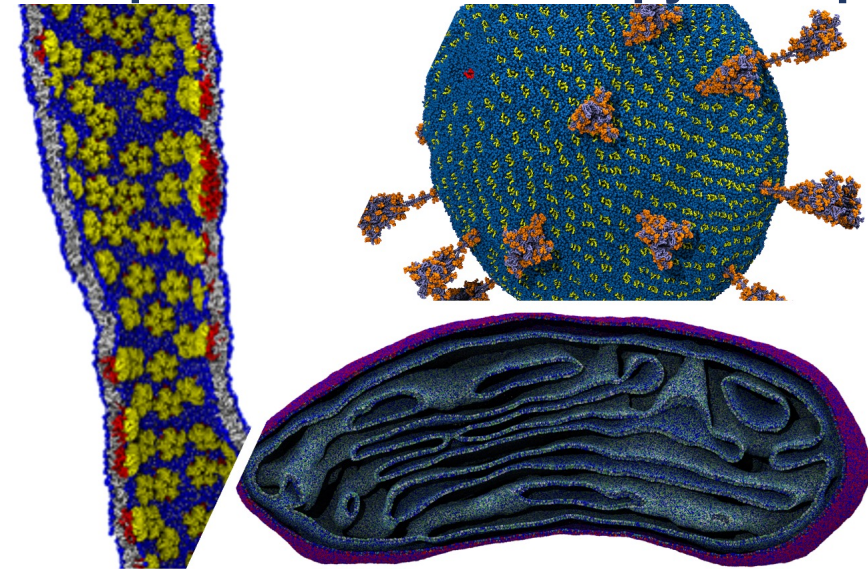
Isabell Lindahl



Brian Ratnasinghe



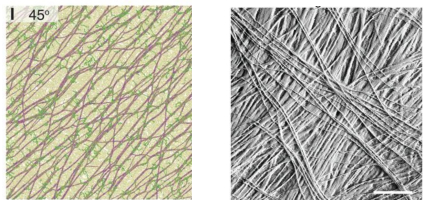
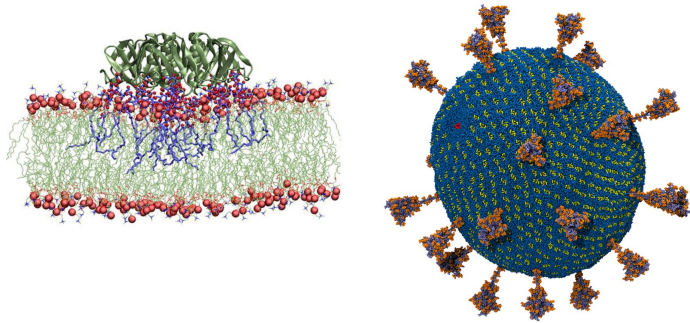
Computational Microscopy Group



Research topics

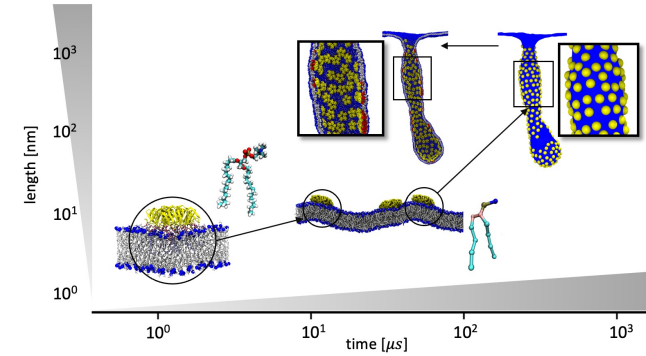
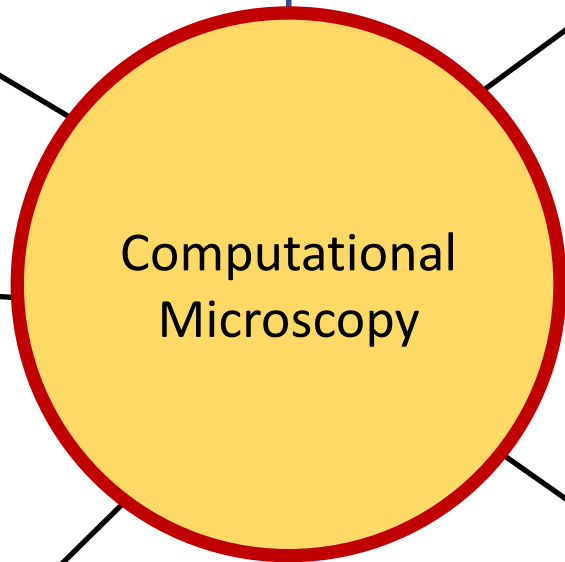
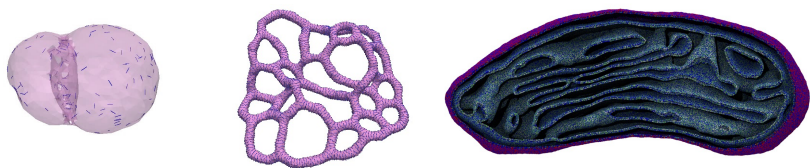
Development

virial and toxic particles

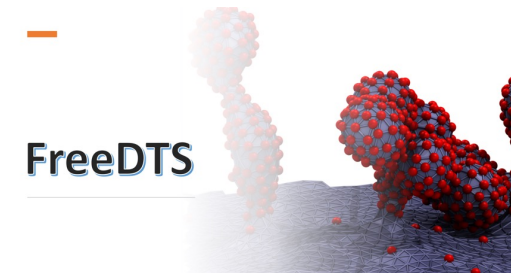


Green materials

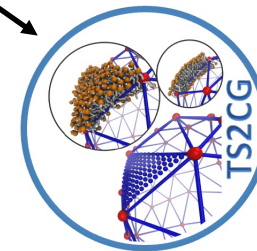
emergence of intracellular forms



multiscale simulations scheme

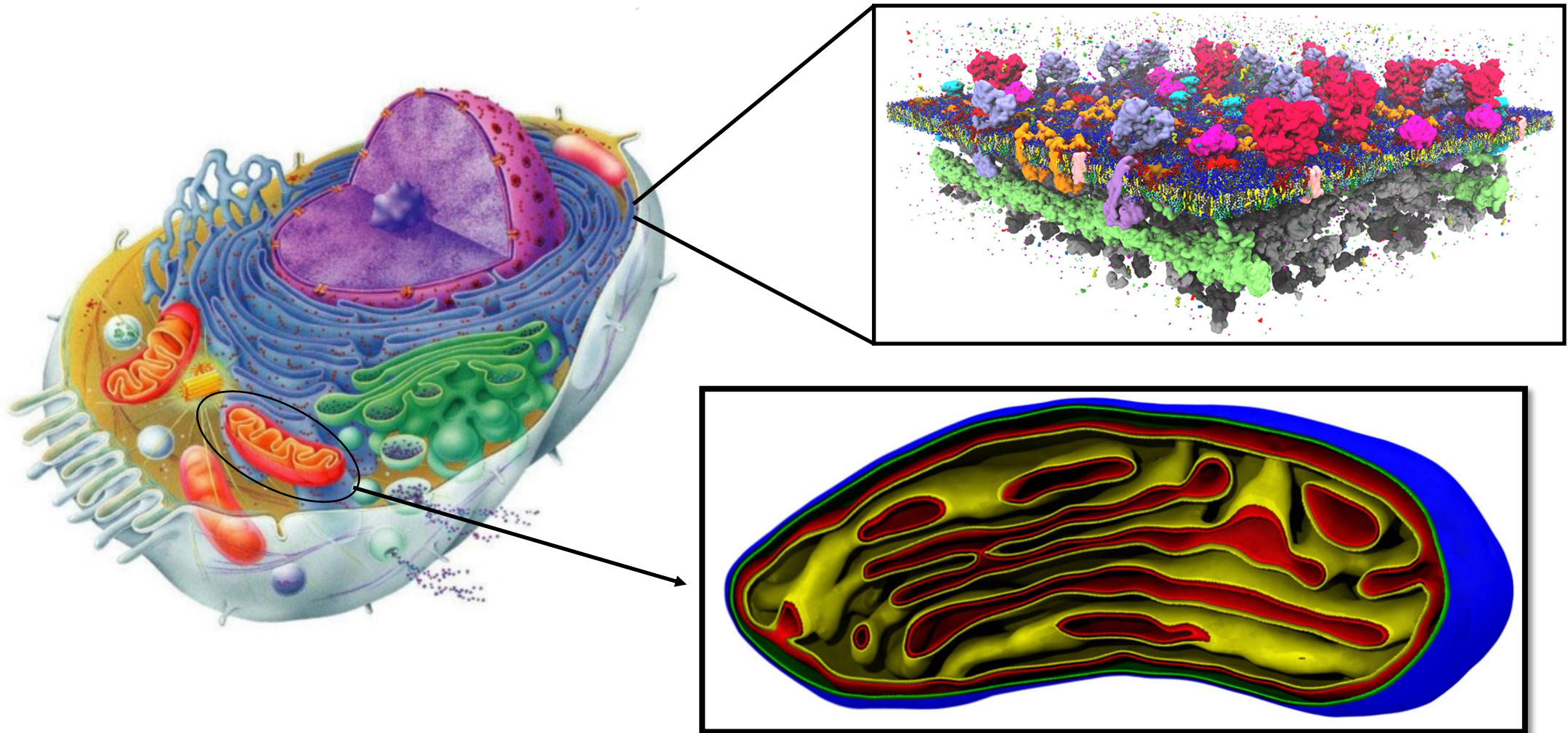


mesoscale simulation software

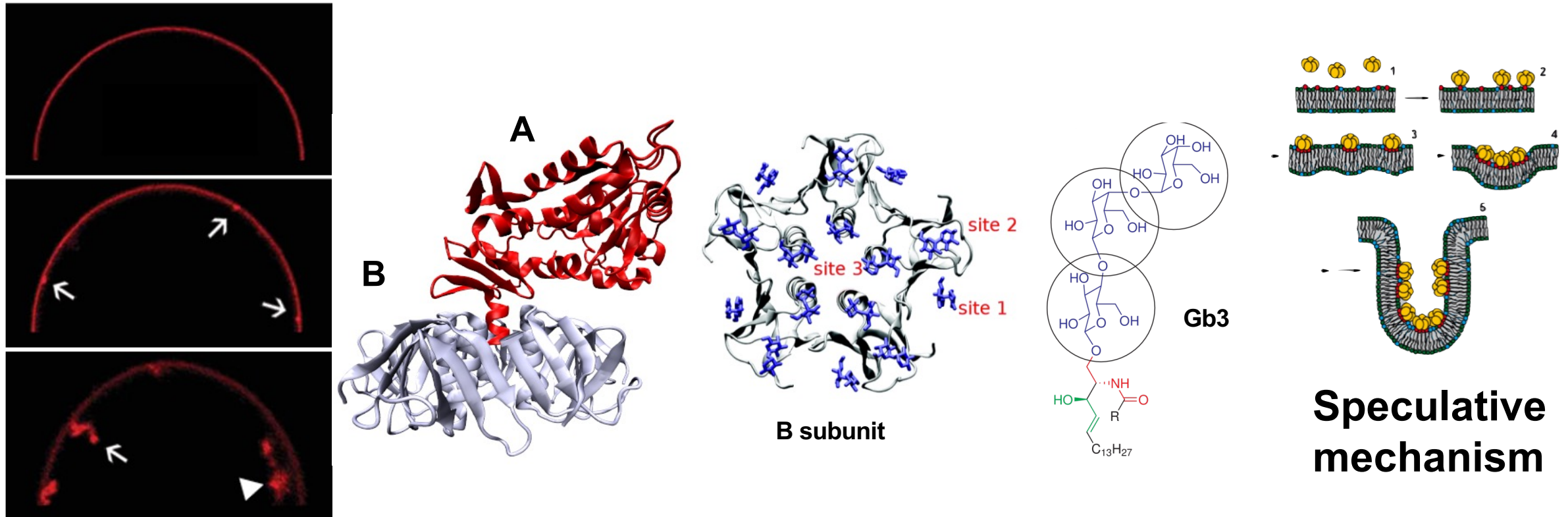


structure builder for next generation MD simulations

Biomembranes



Initial stage of Shiga toxin internalization



W. Romer et al, *Nature* (2007); H. Ling et al, *Biochemistry*, (1998).

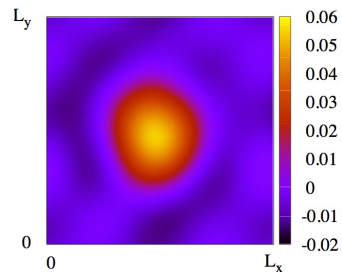
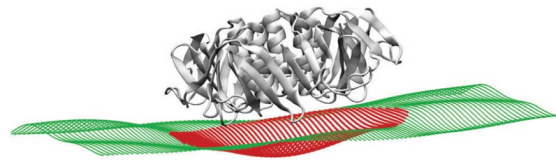
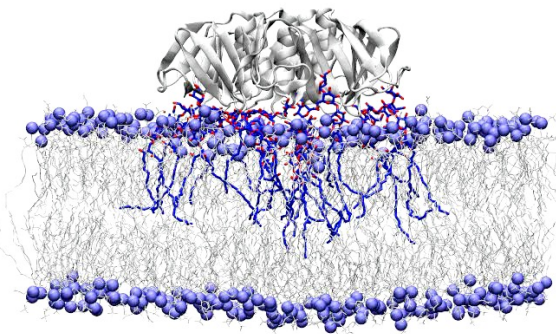
Formation of tubular invaginations

all-atom

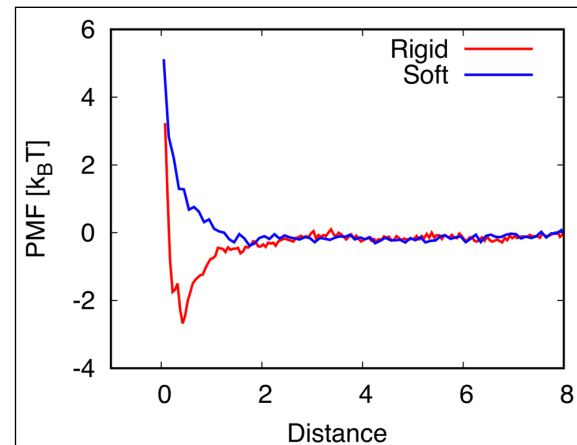
Coarse-grained

mesoscale

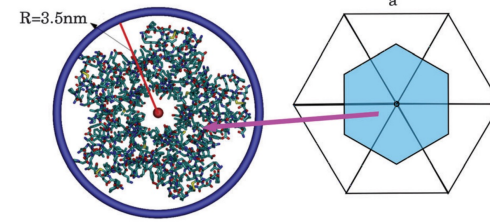
no CG info



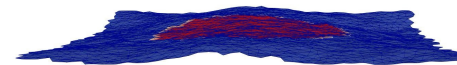
$$\langle 2H_0 \rangle = \langle C_0 \rangle = 0.07 \text{ nm}^2$$



$$U = -1.5 + \cos 5\vartheta$$

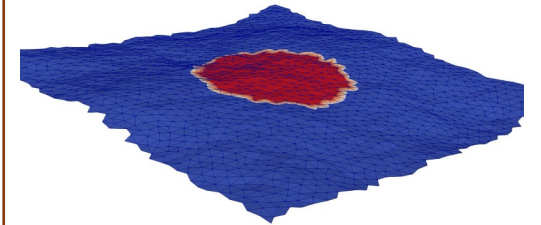


$$a = 6.7 \text{ nm}$$

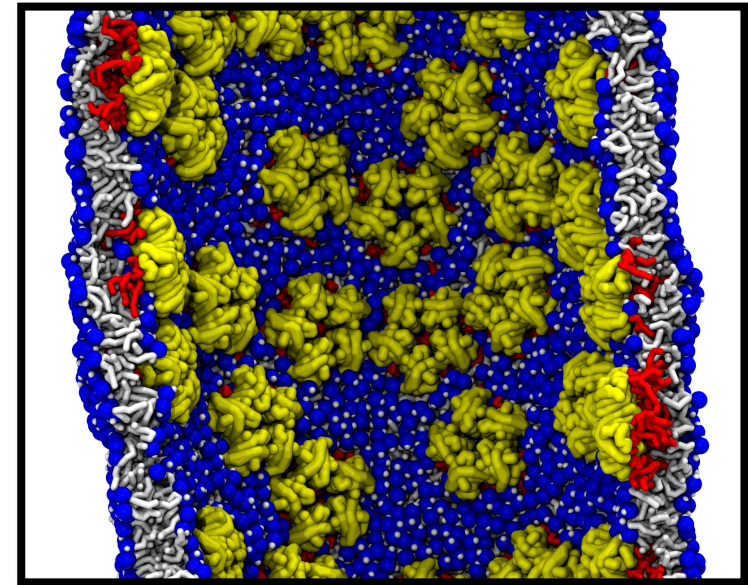
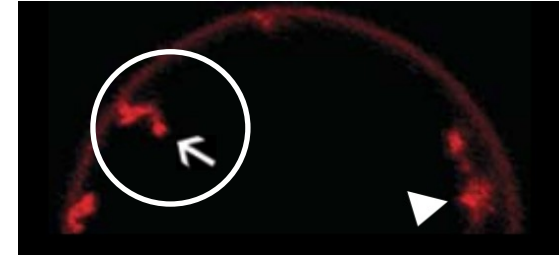
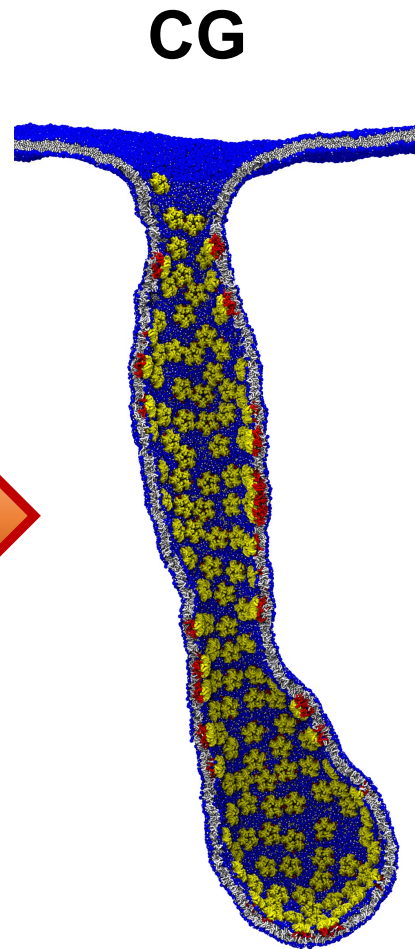
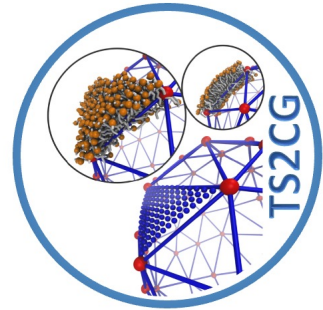
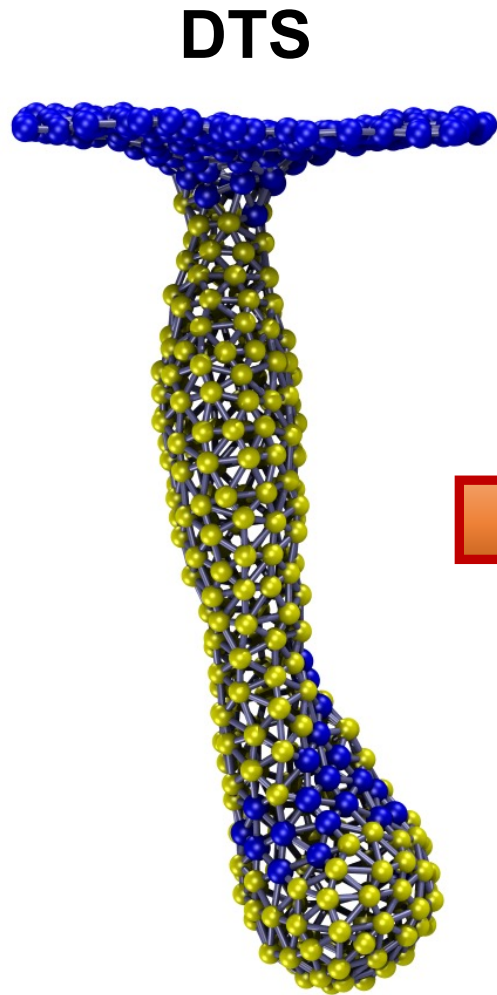


- proteins bound to membrane
- membrane surface

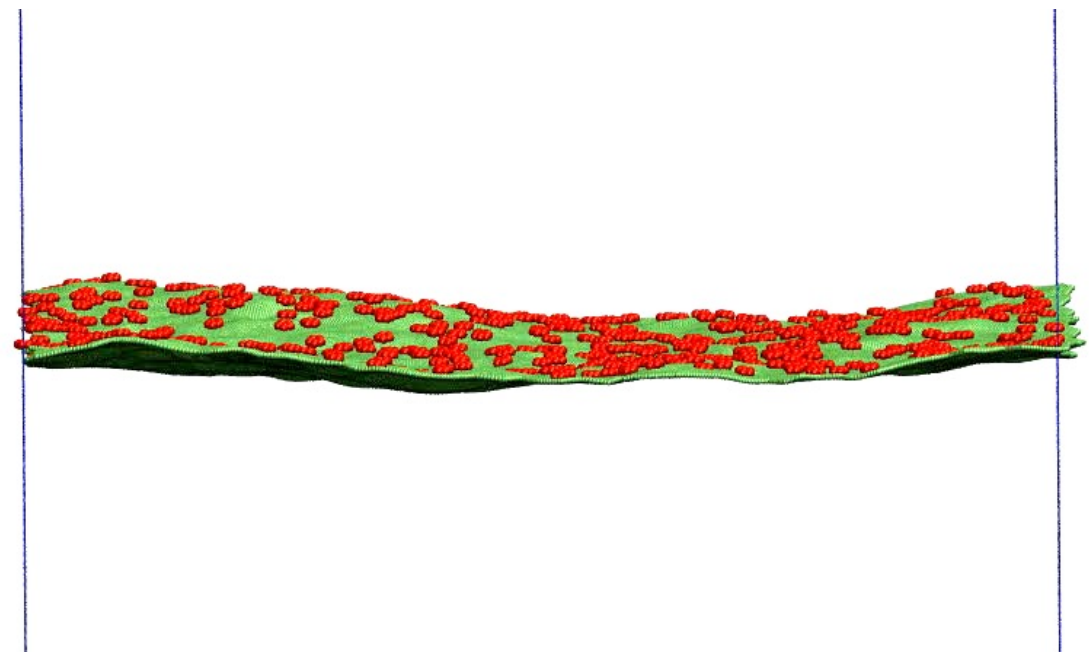
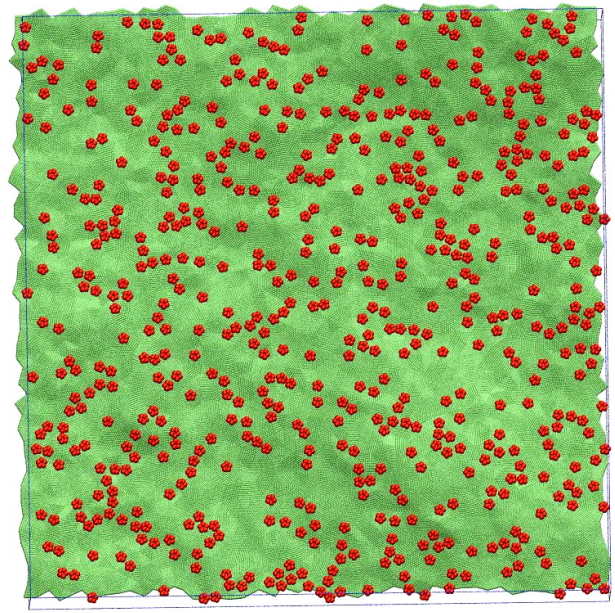
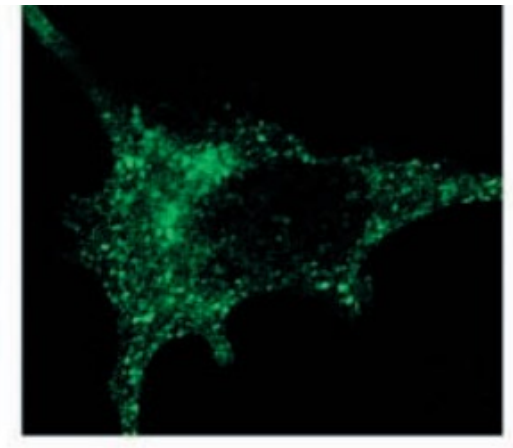
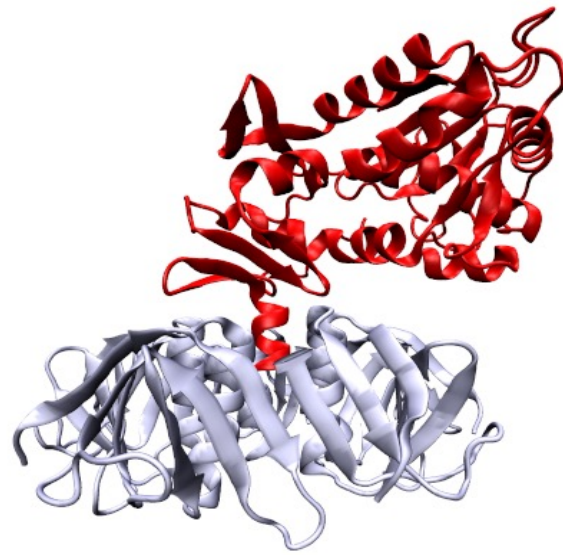
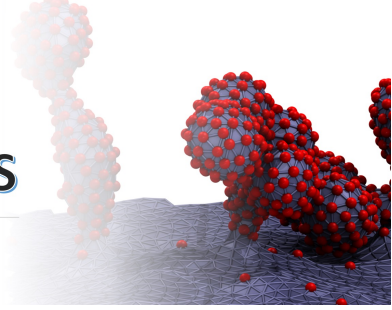
$$U = 0$$



Molecular architecture of the tube



FreeDTS



Division of artificial cells

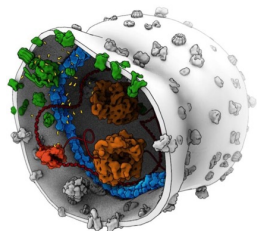


<https://www.syntheticcell.eu/>

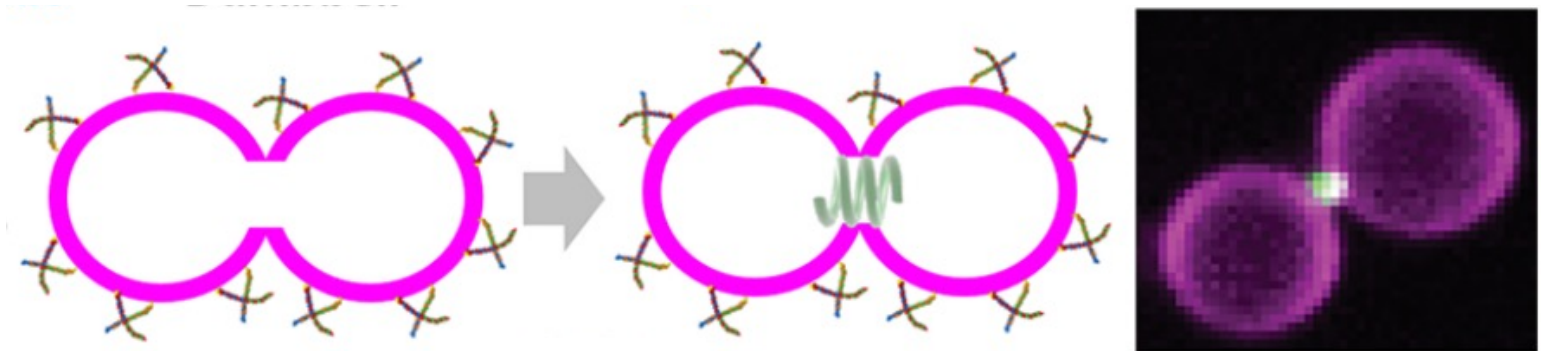
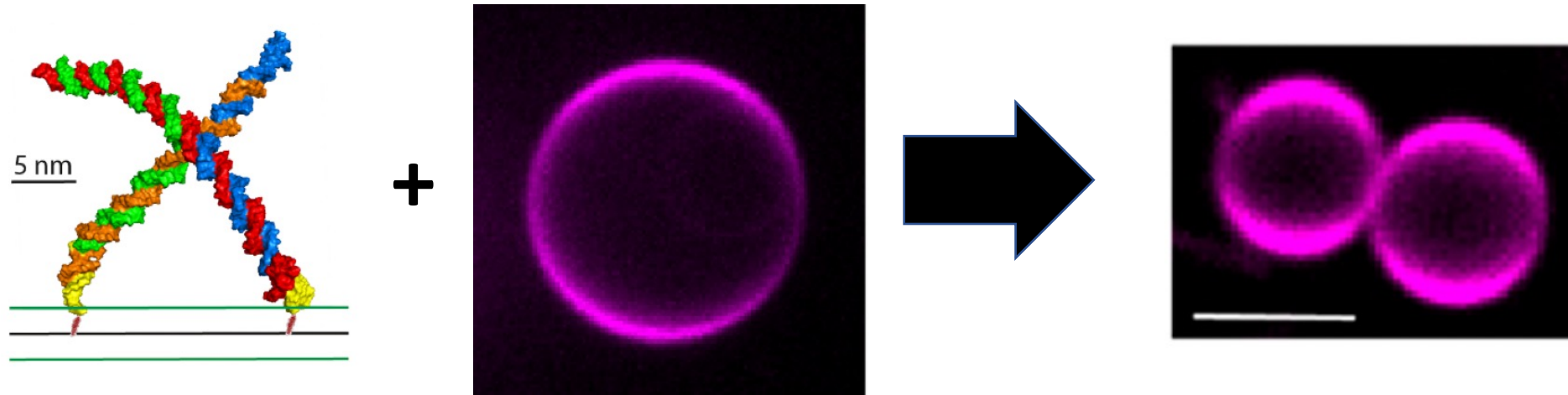


European Synthetic Cell Initiative

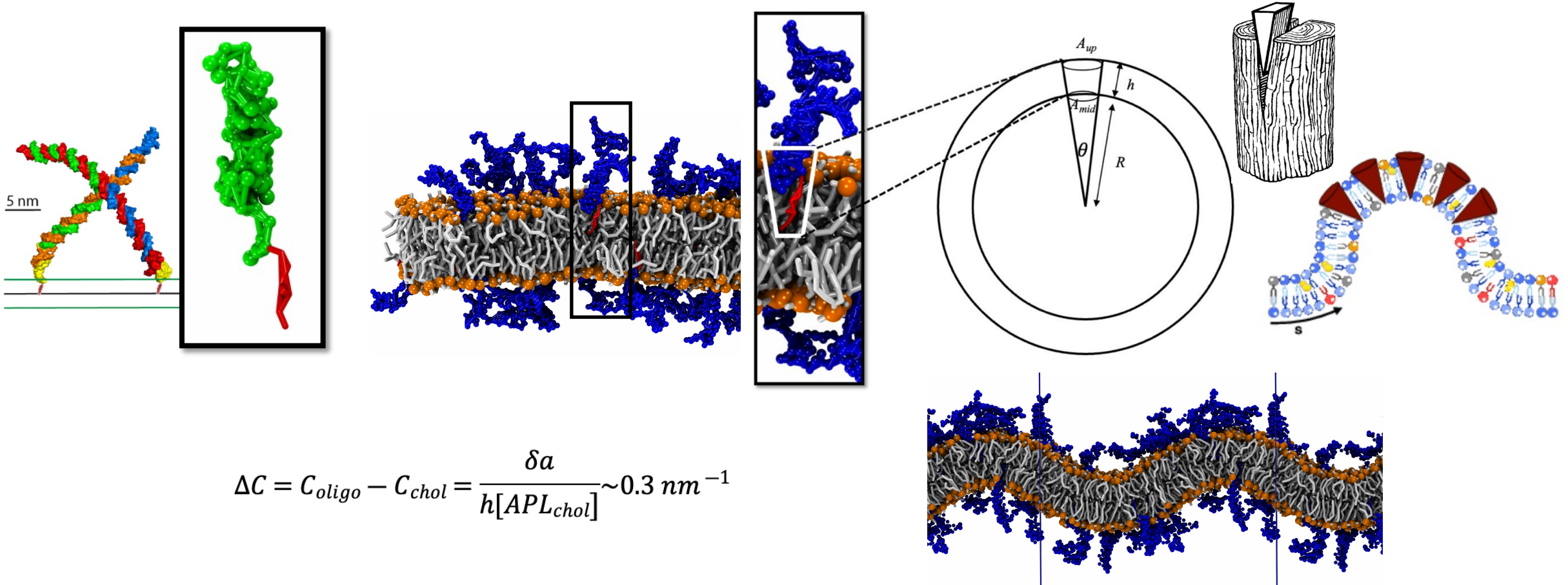
Nature is our next technology



Division of an artificial cell

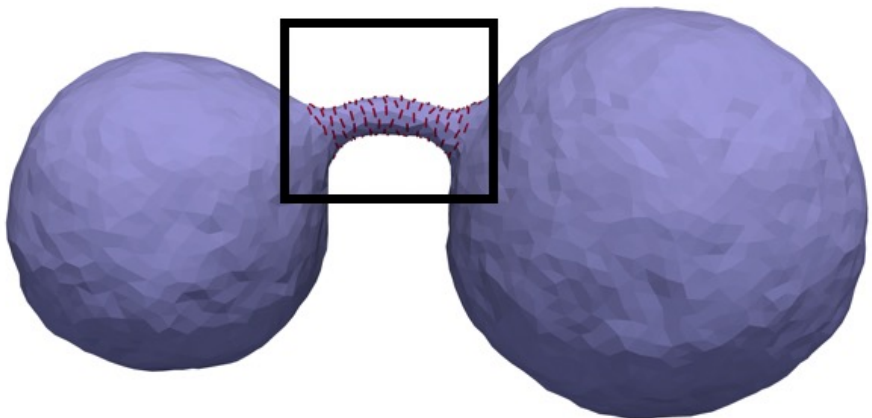
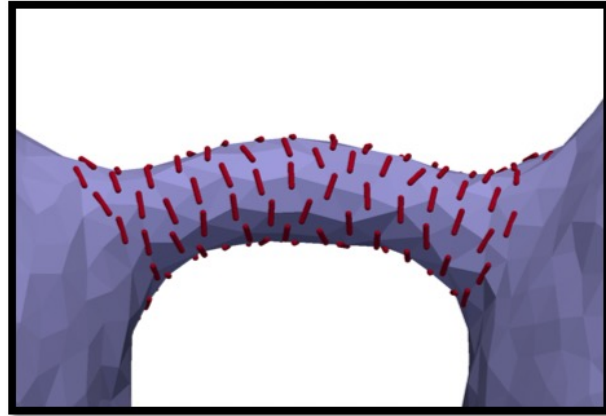


Shaping membranes



Recruitment of enzymatic proteins

negative curvature: binding from inside



positive curvature: binding from inside

