Clathrin aggregation by rotational brownian dynamics

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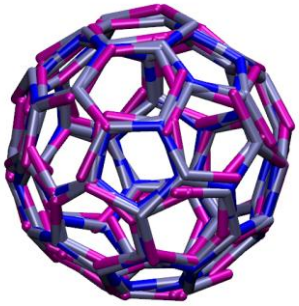
The processes of endo- and exocytosis are associated with the transport of nutrients, hormones and proteins in to and out of living cells. When these molecules enter a cell, they are collected and encapsulated in vesicles for further transport to a destination within the cell. Likewise, the products of organelles are encapsulated before being transported to the edge of the cell. The central protein in the formation process of these vesicles is clathrin. Clathrins are proteins that have three long legs that enable them self-assemble into vesicles and transport cargos within the living cell.

We investigate the formation and structure of clathrin cages by means of computer simulations. To achieve this, we have developed a highly coarse-grained patchy particle model by representing a clathrin protein as a rigid triskelion with interaction sites on the legs. To simulate their dynamics, we have developed a novel Brownian Dynamics algorithm to describe the realistic motion of the protein. Our Brownian Dynamics Algorithm overcomes complications traditionally associated with rotational dynamics of anisotropic particles.

We will show results of the self-assembly of clathrin[1] into cages on a time-scale that is comparable to experimental data. In addition, the simulated cages are structurally similar to those observed by in vitro experiments and the simulations predict the clathrin interaction strength [2].



Clathrin cage obtained from Brownian Dynamics Simulations

[1] I.M. Ilie, W.K. den Otter and W.J. Briels, in preparation (2014)
[2] W.K. den Ottern and W.J. Briels, Traffic, 12 (2011)