P.05 Modelling of the Nuclear Pore Complex

D Osmanovic

University College London, UK

The Nuclear Pore Complex (NPC) forms a selective gate for all transport between the nucleus and the cytoplasm in the living cell. Its selectivity for larger macromolecules relies on changes in a permability barrier that is formed by unstructured proteins, induced by interactions of these proteins with so-called importins and exportins. The exact mechanism by which this works is unknown. We have modelled the NPC as a polymer-coated cylindrical pore via classical Density Functional Theory (DFT) and Monte Carlo (MC) approaches, to show that - for physiologically relevant parameters - the pore can act as a bi-stable switch, in which small changes in polymer-polymer interaction causes the system to switch between a closed, centrally condensed state and an open state in which the polymers condense at the pore wall. We have then extended this work to look at the effects of different macromolecules upon the conformation of the polymers in the pore. We will present direct comparisons of our results to experiments done on the NPC.

[1] Bistable collective behavior of polymers tethered in a nanopore, D Osmanovic et al. Phys. Rev. E Stat. Nonlin. Soft Matter Phys., 85 (2012), p. 061917

[2] Physical Modelling of the Nuclear Pore Complex, D Osmanovic et al. (Review Article) Soft Matter , 2013, 9, 10442

[3] Model Inspired by Nuclear Pore Complex Suggests Possible Roles for Nuclear Transport Receptors in Determining Its Structure, D Osmanovic et al. Biophys. J. 105, 2013, 2781