

Abstract Submitted
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Physical modeling of the conformation of the unfolded proteins of the Nuclear Pore Complex ANTON ZILMAN, Department of Physics, University of Toronto, MICHAEL OPFERMAN, Department of Physics and Astronomy, Pittsburgh university, ROB COALSON, Department of Chemistry, Pittsburgh University, DAVID JASNOW, Department of Physics and Astronomy, Pittsburgh university — Nuclear Pore Complex (NPC) is a biological “nano-machine” that controls the macromolecular transport between the cell nucleus and the cytoplasm. NPC functions without direct input of metabolic energy and without transitions of the gate from a “closed” to an “open” state during transport. The key and unique aspect of transport is the interaction of the transported molecules with the unfolded, natively unstructured proteins that cover the lumen of the NPC. Recently, the NPC inspired creation of artificial bio-mimetic for nano-technology applications. Although several models have been proposed, it is still not clear how the passage of the transport factors is coupled to the conformational dynamics of the unfolded proteins within the NPC. Morphology changes in assemblies of the unfolded proteins induced by the transport factors have been investigated experimentally in vitro. I will present a coarse-grained theoretical and simulation framework that mimics the interactions of unfolded proteins with nano-sized transport factors. The simple physical model predicts morphology changes that explain the recent puzzling experimental results and suggests possible new modes of transport through the NPC. It also provides insights into the physics of the behavior of unfolded proteins.

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