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Nuclear Pore Complex Protein Sequences Determine Overall Copolymer Brush Structure and Function? DAVID ANDO, University of California, Merced, YONGWOON KIM, KAIST, South Korea, ROYA ZANDI, University of California, Riverside, MICHAEL COLVIN, MICHAEL REXACH, AJAY GOPINATHAN, University of California, Merced — Disordered proteins are an interesting class of unfolded protein biopolymers which are functionally versatile. Their sequences are unconstrained by a sequence-structure relationship, and allow for a wide range of chemical and physical polymer properties. The Nuclear Pore Complex (NPC) contains over one hundred of such proteins (FG nups), which collectively function to regulate the exchange of all materials between the nucleus and cytoplasm. We perform coarse grained simulations of both individual FG nups and grafted rings of nups mimicking the in vivo geometry of the NPC, supplemented with polymer brush modeling. Our results indicate that different regions or "blocks" of an individual FG nup can have distinctly different forms of disorder, and that this property appears to be a conserved feature across eukarya. Furthermore, this block structure at the individual protein level is critical to the formation of a unique higher-order polymer brush architecture. Because the interactions between FG nups may be modulated by certain forms of transport factors, our results indicate that transitions between brush morphologies could play an important role in regulating transport across the NPC, suggesting novel forms of gated transport across membrane pores with wide biomimetic applicability.

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