Abstract Submitted for the MAR13 Meeting of The American Physical Society

Diblock organization of individual nucleoporin amino acid sequence determines overall structure and function of the nuclear pore complex DAVID ANDO, University of California, Merced, YONG WOON KIM, Korea Advanced Institute for Science and Technology, ROYA ZANDI, University of California, Riverside, ED LAU, Lawrence Livermore National Laboratory, MICHAEL COLVIN, University of California, Merced, MICHAEL REXACH, University of California, Santa Cruz, AJAY GOPINATHAN, University of California, Merced — The transport of cargo across the nuclear membrane is highly selective and accomplished by a poorly understood mechanism involving hundreds of nucleoporins within the nuclear pore complex (NPC). Currently, there is no clear picture of the overall structure formed by this collection of proteins within the pore, primarily due to their disordered nature. We perform coarse grained simulations of both individual nucleoporins and grafted rings of nups mimicking the *in vivo* geometry and supplement this with polymer brush modeling. Our results indicate that different regions or "blocks" of an individual NPC protein can have distinctly different forms of disorder and properties and that this appears to be a conserved feature. Furthermore, this block structure at the individual protein level is critical to the formation of a unique higher-order polymer brush architecture. Our results indicate that there exist transitions between distinct brush morphologies (open and closed states of the gate), which can be triggered by the presence of cargo with specific surface properties. The resulting transport mechanism, that we propose, is fundamentally different from existing models and points to a novel form of gated transport in operation within the NPC.

> David Ando University of California, Merced

Date submitted: 11 Dec 2012

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