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Contribution ID: **4325** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

(G*) Simulation of the effects of charge on the kinetics of a triblock copolymer hopping across a membrane

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We examine the kinetic process of an anionic A-block from an ABA triblock copolymer hopping between the solvophillic, cationic A-domains of an ABA triblock copolymer membrane. One motivation is to use this toy model to provide insight into the nature of a rapid, charge-mediated reconstitution mechanism observed for anionic membrane proteins reconstituted into cationic ABA triblock copolymer membranes. We use dynamic self-consistent field theory (dSCFT) to efficiently simulate this interacting, many-chain system, and we introduce screened electrostatics by coupling the Poisson-Boltzmann equation into the dSCFT equations. We equilibrate membranes by imposing the condition of isotropic stress and find that, under this condition, the area per A block is an increasing function of the charge on the A block. dSCFT enables us to track the position of each polymer bead, and to observe rapid hopping events as the anionic A-block traverses the solvophobic membrane mid-block. By measuring many such events, we create a probability distribution for the time interval between hops. We will present results for the behaviour of this distribution as we change the charge per A-block, and the charge asymmetry between A blocks. Our results could suggest whether it is direct charge interactions, or indirect effects like softening of the membrane, that are mainly responsible for modifications to the free-energy barrier to A-blocks hopping across the membrane.

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Keyword-2

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Keyword-3

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