Translocation of amphiphilic polymers through lipid bilayer membranes - balanced hydrophobicity versus polarization

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Abstract

We discuss adsorption and passive translocation of amphiphilic polymers such as random copolymers[1] through self-assembled lipid bilayer membranes. By using the bond fluctuation model with explicit solvent[2,3] we consider copolymers of hydrophilic and hydrophobic sites with random sequence as well as alternating sequence of short blocks (see Fig. 1) under variation of the fraction, H, of hydrophobic units and chain length. Our results indicate a point of balanced hydrophobicity, $H_L = 0.6$, where a slight excess of hydrophobic monomers compensates an additional insertion barrier due to the self-organized packing of the bilayer. Translocation events of shorter polymers through the membrane can be observed close to the balanced condition $H = H_L$. For longer chains, translocations are suppressed due to the polarization of the amphiphilic molecules with respect to the lipid-solvent interface. Close to the point of balanced hydrophobicity, the polymer induces dynamic and static perturbations in the bilayer and increases permeability with respect to solvent. We give a more general outlook on how to design membrane active polymers with a desired emphasis on either translocation or permeabilization on the onset of balanced hydrophobicity.

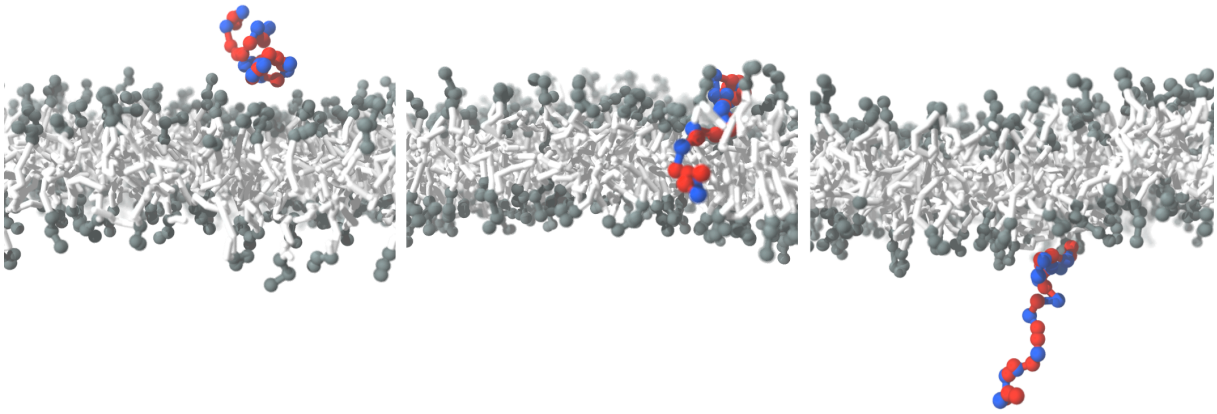

Fig. 1: Simulation snapshots during the translocation of an alternating copolymer of short hydrophilic and hydrophobic blocks with $H = H_L$ and a total length of 32 repeat units.

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