Sequence-determined membrane-activity of amphiphilic polymers

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Abstract

Using the bond-fluctuation model with explicit solvent we study self-assembled lipid bilayer membranes interacting with random copolymers under variation of the fraction, H, of hydrophobic monomers between H=0 (hydrophilic homopolymer) and H=1 (hydrophobic homopolymer). For intermediate values of H we observe localization of the polymer close to the bilayer-solvent interface as well as bridging accross the lipid bilayer. Here, the polymer conformation is reorganized by placing hydrophobic dominated parts in the bilayer's core and hydrophilic dominated parts in the solvent phase. We characterize this reorganization by using the number of pairs of hydrophobic and hydrophilic monomers, where both are surrounded by the preferred environment. In our model we observe a maximum of this order parameter close to H=0.6 . Close to this maximum we observe a maximum of bilayer permeability with respect to solvent. Our results based on a larger "population" of random copolymers with H=0.6 suggests that heterogeneity of the sequence on a scale smaller than the lipid size determines their membrane activity (see Fig. 1(a)). Larger amphiphilic blocks, on the other hand, tend to reorganize in accordance to the lipid ordering as can be seen in multi-block-copolymers (see Fig. 1(b)) and might therefore reduce bilayer perturbation.

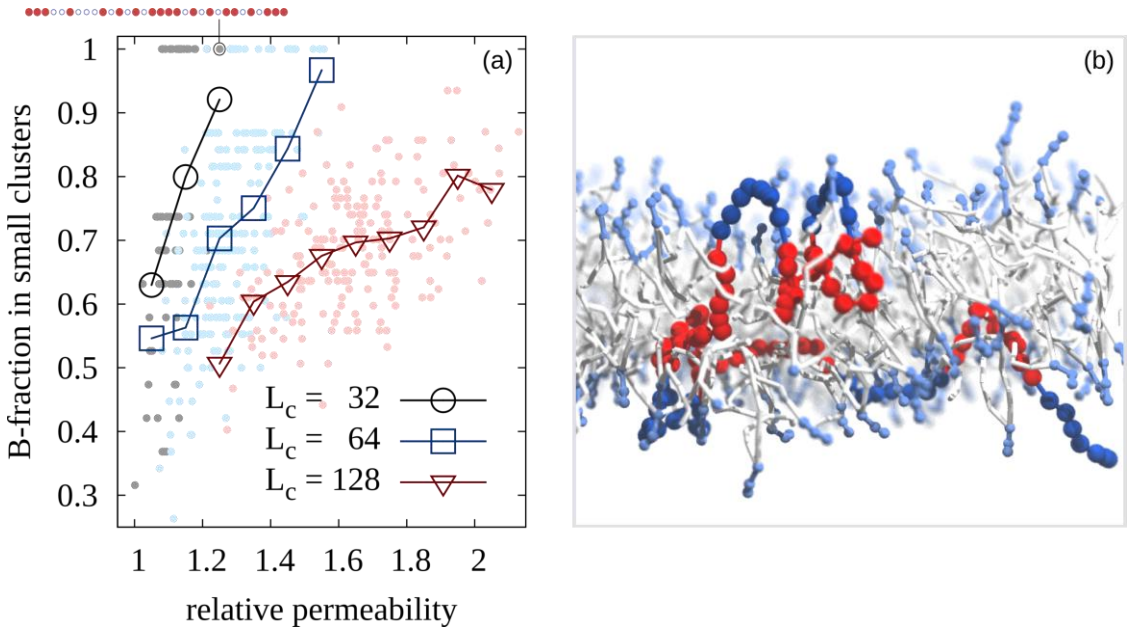

Fig. 1. **(a)** Influence of the sequence distribution of the random copolymer on the polymer-induced solvent permeability of a model membrane relative to an unperturbed membrane. Full circles show the fraction of hydrophobic monomers in small clusters (<5 monomers) of individual random sequences (sampled over $5x10^7$MCS). One of the sequences is illustrated at the top. Open symbols show "population" averages as function of permeability for various chain lengths, L_C. **(b)** Simulation snapshot of a multi-block-copolymer with H=0.6 and hydrophobic parts with a length of 10 monomers (red). Lipid tail length is 5 monomers.