Membrane design with mean-field theory: controlling bilayer domain formation and vesicle size

Martin J. Greenall, *Carlos M. Marques*
Institut Charles Sadron, 23, rue du Loess, 67034 Strasbourg, France – greenall@unistra.fr

Abstract

The design of amphiphilic membranes for applications can be guided and focused by theory and computer simulations. Here, we use mean-field theory to investigate two problems of current practical interest: promoting phase separation in mixed bilayers and fixing the size of vesicles.

First, we build on recently published work[1] to demonstrate how adding oil molecules of a carefully-chosen size to mixed bilayers can encourage phase separation by reducing the excess membrane surface area and curvature arising from the size mismatch of the two amphiphiles.

Second, we provide a concrete theoretical demonstration of the basic principle that amphiphile architecture can directly control vesicle radius[2] if the membrane symmetry is broken by the use of copolymers with multiple hydrophilic and hydrophobic sections. We then present a comprehensive investigation of tetrablock (ABCA) copolymers and show how these should be designed to form strongly monodisperse vesicles of a specified size while suppressing the formation of other structures (see Figure 1).

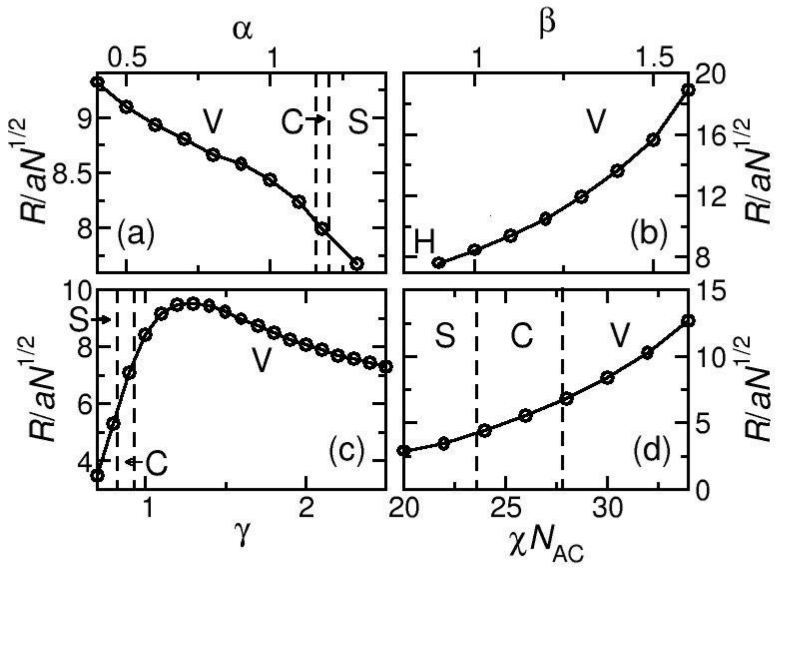

Figure 1: ABCA vesicle radius as a function of block sizes and interaction strength. Increasing the C-block length γ is a highly promising route to the formation of small, monodisperse vesicles unmixed with micelles. The shape transitions between spherical micelles (S), cylindrical micelles (C) and vesicles (V) are also shown.

[1] M. J. Greenall and C. M. Marques, *Soft Matter* **8**, 3308-3314 (2012).
[2] M. J. Greenall and C. M. Marques, *Phys. Rev. Lett.*, accepted (2013).