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Aggregation of nanoparticles on mixed polymer bilayers

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Polymer vesicles, fluid-filled polymer sacs, have attracted great interest for a range of applications, such as drug delivery vehicles or miniature chemical reactors. Due to their similarity to biological cells they are often considered as minimal synthetic models of cells. However, compared to synthetic systems biological cells possess significantly more complexity and it is natural to ask how much of this can be incorporated into synthetic systems. One aspect of this complexity is the multicomponent nature of the cell membrane, being composed of a myriad of different types of molecules. Mimicking this patchy nature in synthetic systems requires control over the phase separation in them, which may be controlled in a number of ways including the addition of nanoparticles.

Using molecular simulation we have studied the aggregation of nanoparticles on bilayers [1] and the effect these have on phase separation in tyo-component systems. For a uniform bilayer the aggregation of nanoparticles depends strongly on the location of the particles in the bilayer; particles residing on the bilayer exterior cluster strongly under the influence of bilayer-mediated interactions, whereas the inter- action between the particles in the bilayer interior is significantly weaker leading to more loosely bound, dynamic aggregates. The aggregation of nanoparticles on two-component bilayers composed of immiscible components changes due to competition between nanoparticle clustering and their adsorption on the boundary between the bilayer components. This reduces the size of the nanoparticle clusters formed on the bilayer exterior, with the clusters adhering onto the boundary between the bilayer components. Due to their weaker attraction nanoparticles in the interior of a mixed bilayer no longer aggregate and instead form strings along the boundary between the two bilayer components. Nanoparticles with an affinity to one bilayer component nucleate small domains of their favoured component around themselves. For asymmetric mixtures this leads to a notable change in the aggregation behaviour of the nanoparticles.

[1] D L Cheung, *J. Chem. Phys.*, 141, 194908 (2014)