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► **To cite this version:**

Virginie Hugouvieux, Monique Axelos M.A.V, Max Kolb. Micelle formation, gelation and adsorption of amphiphilic multiblock copolymers: A Monte Carlo study. International soft matter conference (ISMC), Sep 2013, Rome, Italy. hal-01837769

HAL Id: hal-01837769

<https://hal.science/hal-01837769>

Submitted on 6 Jun 2020

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Micelle formation, gelation and adsorption of amphiphilic multiblock copolymers: A Monte Carlo study.

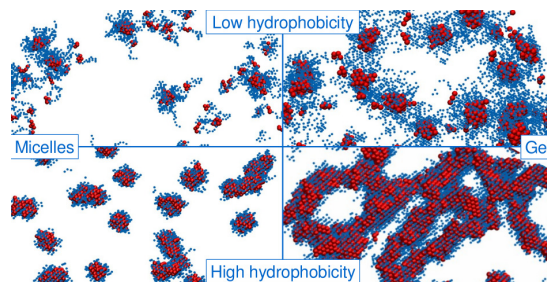
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Amphiphilic multiblock copolymers are versatile macromolecules able to form a large variety of structures, both intra- or intermolecular. Applications range from stabilizing, emulsifying or foaming agents to rheology modifiers and drug vectors. In this study we focus on the structures and properties of copolymers with a large number of hydrophobic and hydrophilic blocks, both in solution or close to a surface. For this purpose, we use a lattice Monte Carlo simulation approach.



Low hydrophobicity leads to spherical micelles and a weak, hydrophilically connected gel (top), high hydrophobicity to tubular micelles and a strong hydrophobically linked gel (bottom).

In solution, multiblock copolymers self-assemble because of the hydrophobic effect, which leads to an effective attraction between the hydrophobic blocks. At low concentration they form intramolecular structures ranging from pearl-necklaces of micelles to lamellar structures depending on the quality of the solvent and the ratio of hydrophobic to hydrophilic monomers⁽¹⁾. At higher concentrations (semi-dilute solutions) intermolecular micelles and percolating networks are observed. The topologies of the networks depend on the hydrophobic content of the copolymers⁽²⁾ (see Figure).

In the presence of a solid hydrophobic surface, the hydrophobic blocks tend to adsorb and form isolated surface micelles with a well-defined size whenever bulk micelles are present. With increasing surface hydrophobicity the surface micelles arrange in a regular manner. Surface percolation is favoured by the multiblock nature of the copolymers. Long multiblock copolymers also lead to the presence of a secondary bulk micellar layer attached to the layer of surface micelles.

- (1) V. Hugouvieux, M.A.V. Axelos & M. Kolb. *Macromolecules*, **42** (2009) 392-400.
- (2) V. Hugouvieux, M.A.V. Axelos & M. Kolb. *Soft Matter*, **7** (2011) 2580-2591.