

# Phase behaviour of active particles in block copolymer melts

Javier Díaz Brañas<sup>1</sup> and Ignacio Pagonabarraga<sup>1,2,3</sup>

<sup>1</sup> CECAM, Centre Européen de Calcul Atomique et Moléculaire, École Polytechnique Fédérale de Lausanne, Lausanne, 1015 Switzerland

<sup>2</sup> Departament de Física de la Matèria Condensada, Universitat de Barcelona, Martí i Franquès 1, Barcelona, 08028 Spain

<sup>3</sup> Universitat de Barcelona Institute of Complex Systems (UBICS), Universitat de Barcelona, Barcelona, 08028 Spain

Block copolymer (BCP) materials are perfect matrices to control the position and orientation of nanoparticles (NPs) with anisotropic shapes or chemically inhomogeneous surfaces[1]. This is due to the ordered structures that BCP melts can form in the nanoscale (e.g. lamellar, BCC spheres). On the other hand, active self-propelled particles can self-assemble into a rich phase behaviour in the bulk[2], or in the presence of obstacles and under confinement[3].

In this work, self-propelled particles, modelled as active Brownian particles (ABPs), are guided by the BCP morphology, which in turn is deformable and reacts to the presence of active motile particles. The hybrid BCP/ABP system co-assembled into a rich phase behaviour both for interface-segregated and selective ABPs. In the presence of confinement induced by the BCP (at the interface or within compatible drop-like domains) ABPs can form train-like structures that flow continuously, as shown in figure 1. Lower activity rates and higher concentrations promote aggregation of ABPs, specially when dispersed within immiscible phases. The formation of clusters deform the BCP structure.

For higher activity rates, the ABPs and the BCP dynamics are largely decoupled, which leads to large deformations in the BCP morphology and the emergence of global polar order in the ABPs.

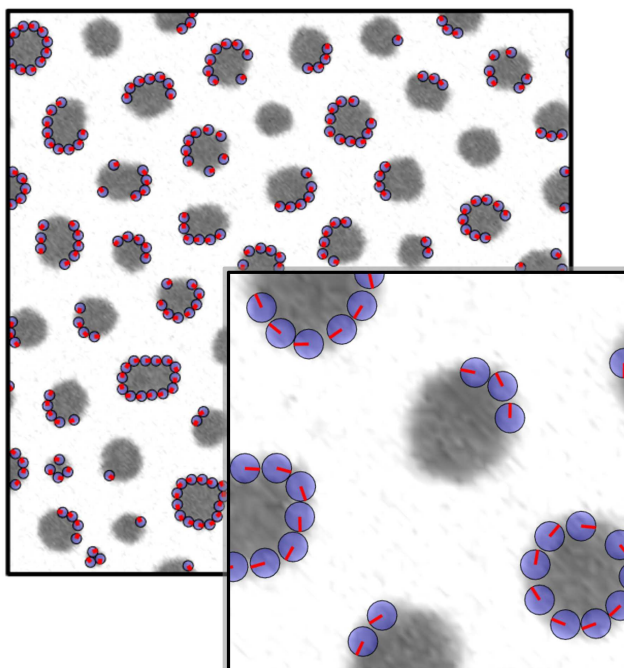


Fig. 1. ABPs (blue) organise in train-like structures with polar order when confined within the interface of circular-forming BCP domains(gray/white). The self-propulsion direction of each particle is indicated in red. This co-assembled configuration occurs for intermediate activity and intermediate ABP concentration.

---

[1] E. Ploshnik, A. Salant, U. Banin, and R. Shenhar. *Phys. Chem. Chem. Phys.*, **12** (2010).

[2] Telezki, V. and Klumpp, S., *Soft Matter*, **16** (2020)

[3] Bechinger, C., Di Leonardo, R., Löwen, H., Reichhardt, C., Volpe, G. and Volpe, G., *Rev. Mod. Phys.*, **88** (2016)