

COLLABORATIVE IBEC INTERNATIONAL PhD PROGRAMME

Position

- 1. Project Title: Deformation-driven Motility in Synthetic Cells by Active Motors
- 2. Research project/ Research Group description

Indisputably, the most fascinating and efficient microrobots capable of moving and performing various tasks are natural cells. By engineering simple cell-mimicking systems often referred to as synthetic cells, we can learn about their natural counterparts and derive design principles of soft-matter microrobots capable of performing cell-like and beyond-nature activities. In this project, we aim at engineering motile synthetic cells which will move by reshaping their cell membrane facilitated by adhered self-propelled particles (SPPs) or anchored enzymes. Such type of motion is ubiquitous in cells which exploit appendages or generated protrusions to propel through the surrounding medium. Our goal is to couple force generation at the points of particle attachment, self-organized clustering of these particles, and membrane morphing to generate a feedback loop that will control the motion of this active system. The SPPs decorating vesicle membrane will harvest chemical energy and transform it into forces at the points of contact with the membrane. If these forces are large enough the vesicle will deform during its motion. Thus, the deformation and propulsion become coupled, similar to the motion of SPPs at the membrane, potentially resulting in their emergent collective behavior that can amplify propulsion.

This is a joint project between the IBEC groups "Bioinspired Interactive Materials and Protocellular System", the "Smart-Nano-Bio-Devices" and the TU/e ICMS "Bio-Organic Chemistry" led by Prof Rodriguez-Emmenegger, Prof. Sanchez and Prof van Hest. The Rodriguez-Emmenegger's lab designs materials to interact with living ones, exploiting concepts of polymer science, molecular self-assembly, hierarchy, and biology. Prof. Sanchez's group focuses on the development of self-propelled nanoparticles (so called nanomotors or nanobots) for nanomedicine and fundamental studies of artificial active matter. Prof. van Hest works at the cutting edge of polymer chemistry and biomedicine, pioneering the use of polymersomes and coacervates to build synthetic cells.



3. Job position description

This project will encompass three phases: (1) the synthesis of building blocks (vesicle forming amphiphiles, SPP, linkers for the enzymes, etc) and self-assembly, (2) the design and study of different motion patterns, and (3) the evaluation of emergent behavior such as collective motion or swarming. Each of these phases will demand to go beyond the state-of-the-art. New macromolecules will have to be synthesized to assemble vesicles that are ultra-flexible yet mechanically resistant to withstand the loads during motion and deformation. In particular we will focus on ionically linked comb polymers that assemble into vesicles, which are named combisomes. The backbones arrange in a nematic like fashion at the interface generating anisotropic diffusion coefficients along and across the director vector. This unique feature gives a preferential motion direction and clustering to the SPP or enzyme motors. In the second phase we will study whether the SPP/micromotors preferentially arrange on the membrane and couple force-generation with deformation and motion. The membrane anisotropy may work as "rails" for the SPP. This will provide a means to address the question of whether this organization could generate an active-nematic like system. We will also include simulations of membrane properties (MD) and of the overall vesicle (DPD). Finally, we will study the type of motion and if we can program it to imitate cellular motion such as crawling, pseudopode generation etc. The three mentors are specialists in each of the features of the project, including synthesis of polymers and assembly (Rodriguez / van Hest), SPP and motors (Sanchez), collective motion (Sanchez /van Hest), advanced microscopy (van Hest), etc.

We are looking for an early-career scientist who is willing to immerse into this highly interdisciplinary work to work in the interface of chemistry, physics, nanotechnology and biology to engineer systems that are inspired by nature but that may serve to fulfill non natural tasks.

Group Leaders at IBEC

- 1. Title: PhD, ICREA Research Professor
- 2. Full name: César Rodriguez-Emmenegger
- 3. Email: crodriguez@ibecbarelona.eu
- 4. Research Group: Bioinspired Interactive Materials and Protocellular Systems
- 1. Title: PhD, ICREA Research Professor
- 2. Full name: Samuel Sánchez Ordóñez
- 3. Email: <u>ssanchez@ibecbarcelona.eu</u>
- 4. Research Group: Smart Nano-Bio-Devices

Collaborator at ICMS

- 1. Title: Professor Dr.
- 2. Full name: Jan van Hest
- 3. Email: J.C.M.v.Hest@tue.nl
- 4. Institute: ICMS
- 5. Research group: Bio-Organic Chemistry