Description for the general public

The word 'durotaxis' stems from the Latin term 'duro', which means 'persistent', and the Greek 'taxis', which means 'arrangement'. It denotes the motion of cells and simple organisms provoked as a response to changes of substrate stiffness. Typically, cells (e.g. human fibroblasts and smooth muscle cells) move towards areas of higher stiffness on a substrate, a motion that becomes less pronounced when cells grow. This behaviour of living matter has inspired engineers to study cases of liquid droplets that use similar mechanisms to move on substrates without the need of external power sources (e.g. chemical reactions or electricity). This is important in the context of nanotechnology as the use of external power sources can damage the substrate having a negative impact on the reproducibility and the long-term efficiency of a process, which translates directly into a cost of maintaining such devices. It was only four years ago that the first experiments were carried out, where durotaxis of liquid drops on substrates of varying stiffness was observed. The difference between drops and cells, which was perceived at that time, was that that fluids preferred softer areas of the substrate, whereas cells the harder ones. However, many issues related to the durotaxis mechanism are still unknown. The aim of this project is to indicate the factors determining spontaneous motion of drops (also those imitating cells made of the so-called active matter), on various substrates using the most modern methods of multi-scale computer modelling. The choice of methodology is dictated by the fact that subtle physicochemical differences of the droplets and the substrate can influence the mechanism and performance of durotaxis. Hence, understanding such phenomena requires a much higher (nanoscale) resolution than what experimental methods used in microfluidics (microscale) can provide. The proposed computer simulations will perform a reliable analysis of parameters affecting the self-sustained motion of nano-objects on substrates with different physicochemical properties, which also includes different substrate patterning that could initiate such motion. These highly precise in silico studies will not only complement observations coming from experimental research, but they will also lead to the knowledge (still insufficient) of durotaxis mechanisms and the suggestion of new guidelines for materials engineering, in this way allowing to increase the efficiency of devices based on this phenomenon and their further miniaturization. The results from this research can contribute to the development of microfluidics and the production of intelligent coatings (self-cleaning and self-healing), as well as other applications requiring flow control, for example, in regenerative medicine. Durotaxis of liquids can also form the basis for obtaining more energy-efficient cooling systems.