The great versatility of colloidal particles has made them one of the preferred building blocks for assembling and studying complex structures at the microscopic level. In recent years the remarkable ability to synthesize colloids with precise control over their shapes and interactions has endowed them with directionality and shape anisotropy. These advancements enable precise control over their assembly rules, resulting in the creation of novel crystal structures and complex molecules. However, the interplay between shape and interaction that leads to crystal structures is not always trivial, and the parameter space to be explored becomes significantly larger to be approached with experiments.

Therefore, my research aims to develop and simulate models for these new complex systems and to have an in-depth understanding of their self-assembly using molecular dynamics simulations. Different interactions can be implemented using either: a) DNA-mediated interactions, where DNA complementary strands are added to the surface of colloidal particles, thus creating directional interactions, b) depletion interactions, where the addition of smaller particles, known as depletants, to the system induces an effective attractive interaction between colloids, among others.

By using anisotropic colloids with the addition of the aforementioned interactions, we can control the overall local and global structure of the system. For example, by increasing the concentration of depletants on a system of tetrahedral particles with directional interactions[1], we can go from a cubic diamond crystal, to a percolating network with diamond inner structure, to a completely disordered gel (see Figure 1). Thus, by accurately characterizing the space parameters in which the different structures are found, they could serve as guides for experimental exploration.