M2 Research internship

Simulations of attractive polymer nanocomposites

Polymer nanocomposites are suspensions of **solid particles** (carbon, silica) dispersed in a **polymer matrix.** Due to their unique properties, they can be found in a variety of applications, ranging from LED devices, to materials for aeronautics and car tires [1]. Despite their wide use, their mechanical properties are still poorly understood. It is well known experimentally that poorly dispersed nanoparticles and **fractal-like aggregates** display the most interesting features in terms of mechanical properties. However, a microscopic understanding of the relation between the material structure and the resulting **rheological properties** is still missing. The goal of the internship is to establish such a link by simulating a new model of fractal-like aggregate nanocomposites, based on a generalized **Langevin equation.**

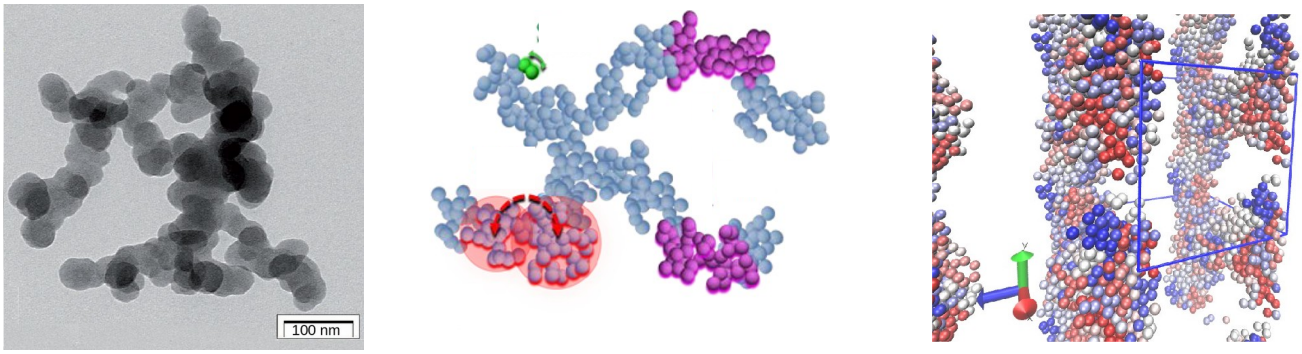

Figure: Individual solid aggregates (left) placed in a polymer matrices form superstructures (middle) which modify the rheology of the material. To understand this phenomena, we use simulations of a model nanocomposite (right).

To this end, the student will benefit from a **molecular dynamics code** developed by a former PhD student [2,3]. Of particular interest will be the properties of attractive nanocomposites, for which preliminary results were already obtained [2], showing enhanced elastic properties. This internship is best suited for students having a taste for numerical simulations and statistical physics. Depending on the student tastes, parallel **analytical work** is also possible. No prior knowledge of rheology or viscoelasticity is required. In the long term, our numerical approach offers many directions to explore.

Opening toward a PhD : yes (funding with «bourse ministère»)

[1] Vilgis, Heinrich, Kluepell. *Reinforcement of Polymer Nano-Composites:Theory, Experiments and Applications,* 2009
[2] Y. Wang, PhD thesis (Université de Lyon, mars 2018)
[3] Y. Wang, G. Maurel, M. Couty, F. Detcheverry and S. Merabia, manuscript in review.

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