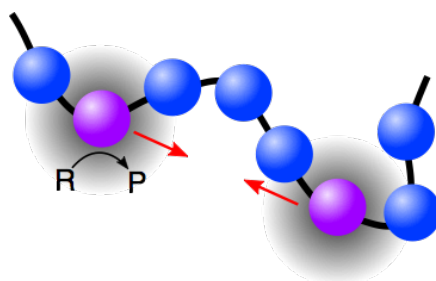


PhD offer – Sorbonne Université – PHENIX lab (UMR 8234)

## Modeling the dynamics of an active polymer

Active matter is made of agents that consume energy from their environment to self-propel. For example, active colloids, which are partially coated by a catalyst, generate gradients of solute concentrations in their environment and respond to these gradients to achieve directional motion. At the molecular scale, active processes may affect the self-assembly of macromolecules, like chromosomes, in complex structures. These nonequilibrium processes usually compete with passive ones, for example due to intermolecular forces. These complex systems can be studied with simple models that reveal the underlying nonequilibrium mechanisms, like chemical reactions. In the recent literature, numerous studies rely on effective descriptions of active processes, for instance by modeling the effect of chemical activity by a propulsion force that acts on the constituents of the system. However, molecular or microscopic descriptions of active particles are still elusive, and remain among the current challenges in the field of active matter.

We will study an active polymer made of monomers that can be active – in the sense that they locally catalyze chemical reactions and generate gradients of substrate concentrations, and respond to these gradients –, or passive, as shown in the figure below. In particular, we will study the structures formed by the chain as a function of different parameters, like the geometrical repartition of the active monomers, their activity, their mobility, and the interactions with the environment. This study will essentially rely on Brownian dynamics simulations, and may be completed by analytical approaches. The effect of hydrodynamic interactions will be studied using a MultiParticle Collision Dynamics (MPCD) algorithm, which accounts for the velocity field in the solvent.



**Candidate's profile** – Masters degree in physics, physical chemistry or theoretical chemistry. Interest for the modeling of physico-chemical systems, and strong interest for computational approaches and numerical simulations. Fluent in English and/or French.

**Salary** – 1768€/month (gross). Funded by ED388 (Ecole doctorale de Chimie Physique et de Chimie Analytique de Paris Centre) for 3 years starting in October 2019. The candidate may teach at the undergraduate level of Sorbonne Université (additional pay).

**Location** – PHENIX lab is located on Pierre et Marie Curie campus (place Jussieu, Paris 5<sup>ème</sup>), in the centre of Paris. Sorbonne Université is part of a vibrant academic community, with numerous higher education and research institutions in its neighborhood.

### Contact

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