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## Postdoc opening at University of Rouen Normandy

A 12-months postdoctoral position, project "MOUSTIC", funded by the « Région Normandie » and the European Union. Europe invests in Normandy with the European Regional Development Fund (ERDF).

### Atomistic modeling of dynamics of self-assembly in chiral systems

#### Contexte :

A self-organisation is an universal phenomenon in nature and, in particular, is highly important in materials systems. Last decades, computational modelling provided an important tool for understanding pattern formation dynamics and self-organisation in many systems<sup>1</sup>. In the last 25 years, significant progress has been made by using Molecular Dynamic (MD) and Monte Carlo (MC) modeling for study of evolution of multi-atomic system. These methods supplement each other. However, a sheer number of variable in MD modeling limits the size of studied systems to  $N \sim 10^5$  and time of its evolution to  $t \sim 10^{-8}$ sec. The MC alternative complements the MD since it can be applicable to the diffusional time scale. The MC approximates the mechanics of atomic motion by a stochastic dynamics of the Markov chain evolution. A stochastic sampling in the MC dynamics requires a generation of a Markov chain that takes a significant time because it requires a search and update of databases, time scale separation and one process-at-a time execution.

Therefore, there are still significant difficulties of atomic scale prototyping of a slow diffusional self-organization of atoms in complex structures. Recently in University of Rouen en collaboration with the researchers from Berkeley University a new simulation method has been proposed to model a self-assembly kinetics at diffusion time scale and nanometric length scale<sup>1,2</sup>. This new method called « quasiparticle approach » based on the atomic density function theory<sup>3,4</sup> and open the way to model a large variety of complex system. For the first time, the modelling of self-assembly of initially random system to helix and double helix structure was performed. However, several question remain open how to model the dynamics of chiral systems.

The chirality is present in many biomolecules and polymers. In nanomaterials the objects with chirality attract special interest due to their singular properties, which depend from their orientations. One of the well know example is the carbon nanotubes.



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Projet bénéficiaire  
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### Goal :

The goal of this study is a further development of the quasiparticle approach to model a self-assembly dynamics of nanoparticles with chiral structure. The special interest will be done for the objects with the helix structure. The strategy is to include a dipolar interaction in the interaction potential between the nanoparticles and introduce the additional degree of freedom to be able of modelling the folding and tangled of helixes.

### Références :

1. H. Zapolsky, G. Demange, R. Andank-Kozubski « From the Atomistic to the Mesoscopic Scale Modeling of Phase Transition in Solids », *Diffusion Foundations*, 2296-3642, Vol. 12, pp 111-126, 2017.
2. O. Kapikranian, H. Zapolsky, R. Patte, C. Pareige, B. Radiguet, and P. Pareige « Point defect absorption by grain boundaries in alpha iron by atomic density function modelling » *Phys. Rev.B* 92, 224106 ,2015.
3. H. Zapolsky "Kinetics of pattern formation: mesoscopic and atomistic modelling" *ORDER, DISORDER AND CRITICALITY, Advanced Problems of Phase Transition Theory, Volume IV*, .pp 153-193, Ed. Y. Holovach, World Scientific Publishing Co. 2015.
4. M. Lavrsky, H. Zapolsky, A.G. Khachatryan « Quasiparticle approach to diffusional atomic scale self-assembly of complex structures: from disorder to complex crystals and double-helix polymers » *Nature parther journal Computational Materials*, january 2016.

### Profil of candidate:

The candidate should have a PhD in computational physics, a solid background in solid state physics, ideally, in free energy methods. The candidate will also play a central role in interacting with the experimental partners, to suggest the most relevant experiments, and interpret experimental data and observations.

Interested candidates can apply electronically (CV including full publication list and references) by sending an email to: [helena.zapolsky@univ-rouen.fr](mailto:helena.zapolsky@univ-rouen.fr)

The selection process will continue until a suitable candidate is found

### Contacts :

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