POSTDOCTORAL POSITION - LILLE UNIVERSITY
COMPUTATIONAL STUDIES OF AMORPHOUS PHARMACEUTICALS

The team "Matériaux Moléculaires Thérapeutiques (MMT)" (Unité Matériaux Et Transformations (UMET) laboratory - http://umet.univ-lille1.fr) is one of the few French research groups developing an original research activity at the interface between materials science and pharmacy. Researches mostly focus on the physical states of solid materials composed of small organic molecules and/or polymers of pharmaceutical and agrochemical interest. These materials are investigated under different stresses (temperature, pressure, grinding, freeze-drying) aiming to obtain a fundamental understanding of physical mechanisms of the induced transformations. The main goal is to analyse the situations of metastabilities, the glassy states and the phase transformations and out-of-equilibrium evolutions induced by these stresses.

The recruited postdoctoral fellow will basically lead a research programme on the amorphous state of drugs by molecular modelling. Molecular dynamics (MD) simulations particularly offer the possibility to calculate many relevant properties of drug molecules and excipients without the need of long and costly experiments. MD studies have been shown to be of central interest for prediction of valuable physical properties like density, mobility, melting temperature, or for the calculation of solubility parameters.

The amorphous state is omnipresent within the pharmaceuticals. Whether amorphous state is introduced intentionally or unintentionally, it will commonly present stability problems because greater molecular mobility in the amorphous state relative to the crystalline state often lowers the activation barriers for processes such as crystallization or chemical degradations. It is thus of profound importance for the pharmaceutical industry to understand how molecular mobility in the amorphous state changes with temperature. During this postdoctoral position, the main work will be thus to develop theoretical and computational methods to characterize molecular mobility and to predict properties (glass transition, fragility) of small molecules and/or polymers based on MD computations. It would be necessary to validate the approach on a large number of compounds of pharmaceutical/agrochemical interest including mixtures.

The successful candidate will be employed from December 2016/January 2017 for a period of 1 year at the University of Lille1 (Villeneuve d'Ascq, France) with a gross salary of around 45000 €/year.

Candidates profile:
Candidates should have a PHD degree in physics, materials science or chemistry.

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