Short Visit Scientific Report

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Purpose of the visit

The goal of this short visit of three days was to set up the basis to define a long-term collaboration between Pol Vilaseca, post-graduate student from Barcelona University with a master in Computational Physics, and the Centre for BioNano Interactions (CBNI) leaded by Prof. Kenneth A. Dawson at University College of Dublin. During his master, Vilaseca developed a computational approach for studying soft-core interaction potentials under the supervision of Prof. Giancarlo Franzese of Barcelona University, now visiting the CBNI for three months.

Description of the work

Soft-core isotropic potentials can be used to describe complex liquids and protein solutions. These potentials are known to exhibit a rich phenomenology, including polyamorphysm (i.e. more than one fluid or amorphous phase), polymorphysm (i.e. more than one crystal phase), metastable fluid phases, and anomalies in the thermodynamics and the dynamics. Isotropic potentials could be used to describe interactions between nanoparticles and proteins forming the protein corona, and the interactions among the protein coronas. We plan to design experiments suitable to elucidate the main contributions to these interactions and, in such a way, constituting the starting point for analytic theories, in the context of molecular and statistical physics for nano and biosystems. This theoretical work, in turn, will allow performing computer simulations to predict the properties of these complex systems and guide future experiments. The aim is to reach a better understanding of the properties of these fascinating protein coronas.

Future prespectives

After the visit the long term collaboration between Pol Vilaseca and the Center for Bio Nano Interactions has been satisfactorilly accorded to start at the beginings of 2010, possibly finalized to a Ph.D. Vilaseca is now apllying for an exchange grant of three months as a starting point for the long term collaboration.