UNIMORE Dipartimento di Scienze Fisiche, Informatiche e Matematiche

UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

CNRNANO MODENA S3

FIM-S3 SEMINAR

Computer simulation of the diffusion of proteins and nanoparticles in crowded environment

Tuesday May 7th, 2024 – 15.00 (sharp)

S3 Seminar Room, 3rd Floor, Physics building
Link: https://tinyurl.com/FIMS3HLOPEZ

Speaker

Hender LOPEZ – Technological University Dublin, Ireland

Abstract

In this seminar we will present results on the diffusion of proteins and nanoparticles in naturally crowded environments. Firstly, we show our results on short-time diffusion of proteins in lysate, both experimentally and with the aid of computer simulations [1]. We show how using a method based on Stokesian Dynamics in which hydrodynamic interactions are considered explicitly, the short-time properties of the dispersion can be calculated and used to understand the experimental finding. In our approach, the lysate polydisperse system is modeled using hard spheres and we demonstrate an intricate dependency between the diffusion of a tracer on the crowder composition. The simulation results further show that polydispersity slows down larger macromolecules more effectively than smaller ones even at nanosecond timescales. We then extend the simulation methodology to study the long-time diffusion and study the impact of model used to incorporate the the short-time diffusivity on the dynamics of the proteins at long times.

Secondly, we present results on the diffusion of nanoparticles (NPs) in crowded media. When NPs are exposed to biological fluids, they are rapidly covered by a layer of biomolecules, commonly refer to as the protein corona. In particular, the transport properties of the NP-protein complex is central on how fast and efficient NPs interact with cells in a living organism. Here we show how coarse-grained molecular dynamic simulations can be used to study the diffusion of NPs in protein solution [2]. We later discuss how to extend this methodology to more realistic crowded environments by simulating systems for which the proteins corona is already formed and it is constant in time [3]. We finally discuss how to relax this constraint by incorporating NP-protein interactions obtained from a bottom-up approach [4].

[1] Grimaldo M., Lopez H., et al. (2019) J. Phys. Chem. Lett. 10, 1709–1715
[2] G. Brancolini, H. Lopez, S. Corni and V. Tozzini. (2019) International Journal of Molecular Sciences 20, 3866.
[3] Cipriani B and Lopez H. (in preparation)
[4] D. Power, I. Rouse, S. Poggio, E. Brandt, H. Lopez, A. Lyubartsev and V. Lobaskin. (2019) Modelling and Simulation in Materials Science and Engineering 27, 084003.

In collaboration with

Finanziato dall'Unione europea NextGenerationEU

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