



Erasmus + Staff Mobility For Teaching

AVVISO DI SEMINARIO

Il giorno **26 Giugno 2019** alle ore **15.00** nell'aula **COB2**

il **Prof. Gokhan Kacar** (Associate Professor, Department of Genetics and Bioengineering in Trakya University - Edirne) terrà un seminario dal titolo:

Coarse-grained modeling and simulations of hydrophilic polymers for self-healing and drug delivery applications

Ospite: Dr Annalisa Guaragna

Short abstract

In this seminar, I will mainly focus on our efforts in performing coarse-grained simulations to investigate the structure and properties of two sets of materials, namely hydrophilic self-replenishing coatings and drug delivery micelles. These materials are simulated by employing our recently proposed extension of dissipative particle dynamics method to variable bead volumes [1] and hydrogen bond interactions [2, 3]. The experimental swelling behavior and structure are predicted for the hydrophilic polymer [4]. Moreover, the formation of micelles is modelled and drug encapsulation efficiencies are computed. Overall, the coarse-grained DPD simulations predict the structural and drug encapsulation properties of a polymeric system consistent with the experiments, whereby bringing new insights to its molecular understanding in terms of micelle shrinkage upon inclusion of the drug. The results confirm the promising role of the simulation procedure reported in this work to study the drug encapsulation, molecular structure and interactions of polymeric micelles used as drug delivery materials [5].

References

- [1] G. Kacar, E.A.J.F. Peters, G. de With, *EPL*, 2013, 102, 40009.
- [2] G. Kacar, G. de With, *PCCP*, 2016, 18, 9554.
- [3] G. Kacar, *PCCP*, 2018, 20, 12303.
- [4] G. Kacar, P. Albers, C. Esteves, G. de With, *JCTR*, 2018, 15, 691.
- [5] G. Kacar, submitted.