

Nanostructured Systems of Diphenylalanine Peptides and Graphene Sheets: an Atomistic Simulation Study

M. Arnittali^{1,2,3,*}, A.N. Rissanou^{1,2,3}, V. Harmandaris^{1,2,3}

¹*Computation-Based Science & Technology Center, The Cyprus Institute, Nicosia Cyprus;*

²*Institute of Applied and Computational Mathematics (IACM), Foundation for Research and Technology Hellas (FORTH), IACM/FORTH, GR-71110 Heraklion, Crete;*

³*Department of Mathematics and Applied Mathematics, University of Crete, GR-71409 Heraklion, Crete, Greece.*

In the current work, the self-assembly of diphenylalanine peptides (FF) on a graphene layer, in aqueous solution, is investigated, through all-atom Molecular Dynamics simulations [1]. The effect of graphene surface on the self-assembly propensity of peptides, as well as on the formed structure, as it has been observed in a corresponding solution of FF in water [2], is examined. Two interfacial systems are studied, with different concentration of dipeptides at room temperature. Atomistic details about the conformational preferences, the orientation of peptides with respect to the surface and the hydrogen bond network are given. Length and time scales of the formed structures are quantified providing important insight into the adsorption mechanism of FF onto the graphene surface. A hierarchical formation of FF structures is observed involving two sequential processes: first, a stabilized interfacial layer of dipeptides onto the graphene surface is formulated, followed by the development of a structure of self-aggregated dipeptides on top of this layer. The whole procedure is completed in almost 200ns, whereas self-assembly in the system without graphene is accomplished much faster; in less than 50ns cylindrical structures, signal of the macroscopic fibrillar ones, are formed. Strong $\pi - \pi^*$ interactions between FF and the graphene led to a parallel to the graphene layer orientation of the phenyl rings. Reduction in the number of hydrogen bonds between FF peptides is observed because of the graphene layer, since it disturbs their self-assembly propensity.

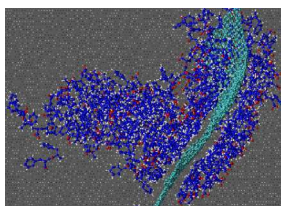


Figure 1: Graphical representation of a model system.

References

- [1] Rissanou, Keliri, Arnittali and Harmandaris, *Physical Chemistry Chemical Physics*, **22**, 27645-27657 (2020).
- [2] Rissanou, Georgilis, Mitraki, and Harmandaris, *The Journal of Physical Chemistry B*, **117**, 3962-3975 (2013).