**SELF-ASSEMBLY OF DIPHENYLALANINE PEPTIDES ON GRAPHENE THROUGH DETAILED ATOMISTIC SIMULATIONS**

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**ABSTRACT**

In the field of bio-inspired materials, the non-covalent self-assembly of relatively simple peptidebased molecules has gained increasing attention for the formation of nanostructured, biologically functional materials, including nanofibers and hydrogels, all with nanoscale order. Moreover polypeptide self-assembly is often associated with human medical disorders. Understanding the physicochemical determinants that underlie peptide self-assembly is a fundamental step, in view of the rational design, or redesign of already existed nano building blocks for biotechnological and biomedical applications. Herein, 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 fibrilliar ones, are formed. Strong π – π\* interactions between FF and the graphene lead 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.

**KEYWORDS:** Diphenylanine peptides, Graphene, Self-Assembly, Molecular Dynamics

**REFERENCES**

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