Self-Assembly of Tetra-Peptides on Surfaces of Two-Dimensional Materials

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As the novel “bottom-up” strategy for fabricating nanomaterials, molecular self-assembly has attracted considerable attention worldwide. On one hand, two-dimensional (2D) materials such as graphite and molybdenum disulfide (MoS_2) have been demonstrated as the platform for this self-assembly due to their unique electrical, optical properties, and atomically flat surfaces, etc [1,2]. On the other hand, amphiphilic peptides with both of the hydrophobic and hydrophilic nature also have already been used as ideal building blocks for forming various sophisticated self-assembling materials with certain applications. Therefore, in order to functionalize the 2D material surface by peptides self-assembly, it is necessary for a deliberate understanding of the interaction between biomolecules and 2D substrate materials [3].

In this work, we aim to combine the experimental and computational approaches to understand the molecular mechanism. For this purpose, we started with a small peptide composed of four amino acids, “FEFE”, where charged and aromatic amino acids may play a role for the self-assembly. Firstly, we focused on the concentration dependence of their self-assembled structural morphology on graphite surface. FEFE solution (F: Phenylalanine; E: Glutamic) were diluted by 10 mM Phosphonate Buffer to be 10 nM, 100 nM, 1 uM, 10 uM, 20 uM and 40 uM, respectively. The solutions were placed on a fresh mechanically exfoliated 2D material substrate, and were incubated in a humid chamber at room temperature for 1 hour. After the incubation, the droplet was removed with a blow of nitrogen gas and dried in a vacuum desiccator.

Finally, we use atomic force microscopy (AFM) to measure out the morphology of the tetra-peptide self-assembled structures. Besides, we performed the molecular dynamics simulation (MD) using GROMACS starting with single FEFE on graphene surface. According to the calculations such as center-of-mass distance between peptide and graphene surface, two benzene rings angle change and binding energy distribution, we can ensure the most stable FEFE structure on graphene surface.

Through the comparison between AFM and MD results, the information about periodicity of FEFE self-assembly structure can be obtained so that it can pay foundation for building the conformation-property relation of amphiphilic peptide self-assembly on 2D material surfaces.

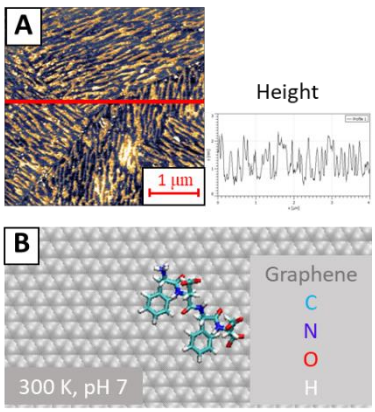

Figure 1: An image of AFM and MD calculation of FEFE peptide on graphene

Reference: [1] Li P, Sakuma K, Tsuchiya S, et al. ACS applied materials & interfaces, 2019.

[2] Chen J, Zhu E, Liu J, et al. Science, 2018, 362(6419): 1135-1139.

[3] Qiu F, Chen Y, Tang C, et al. International journal of nanomedicine, 2018, 13: 5003.