Aggregation of Flavin Mononucleotide Surfactants on Graphene: A Molecular Dynamics Study

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Abstract: Graphene, a single layer of graphite with one atom thickness, has attracted extensive attention due to its extraordinary properties. Especially, owning to the excellent electrical conductivity, ultrahigh ratio of surface area to volume, as well as the extreme sensitivity of its surface atoms to any adsorbed molecules or reaction events, graphene possesses a great potential serving as sensing element, e.g. in biosensors for medical applications. To this day, numerous bottom-up and top-down approaches have been developed to generate pristine graphene. A direct liquid-phase exfoliation of graphite assisted with surfactants is gifted with several significant advantages, including both employing cheap and readily available graphite as well as potential ability of large mass processing [1]. Flavin mononucleotide (FMN), a derivative of vitamin B_2 and biologically benign amphiphilic molecule, has been reported experimentally to act as an efficient surfactant for the exfoliation of graphite to disperse highly stable graphene suspensions with low amount of FMN relative to graphene, recently [2-4]. Unfortunately, it is still not clear how FMN molecules self-assemble on graphene flakes. In this study, we will report results of the aggregate morphology of FMN on graphene flakes as well as the potential of mean force (PMF) between graphene flakes in the presence of aqueous FMN solution, from all-atom molecular dynamics simulations.

References

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[2] Tummala, Naga Rajesh, et al. ACS nano 4.12 (2010): 7193
[3] Ju, Sang Yong, et al. Nature nanotechnology 3.6 (2008): 356
[4] Ayán-Varela, M., et al. ACS applied materials & interfaces 7.19 (2015): 10293

Figures

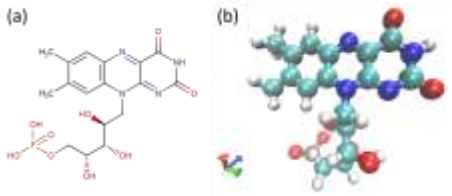

Figure 1: (a) Chemical structure of FMN (b) Ball-and-stick model representation of FMN (blue, red, cyan, white and tan spheres represent nitrogen, oxygen, carbon, hydrogen and phosphorus atoms, correspondingly).

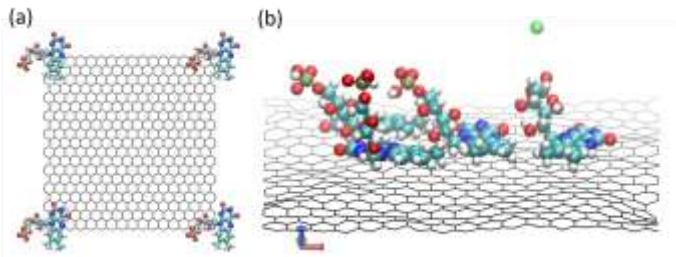

Figure 2: (a) Snapshot of initial configuration of 4 FMN molecules and graphene sheet (b) Snapshot of configuration after 70 ns MD simulation