Molecular modelling of bio-adhesive self-assembled monolayers on graphene

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Abstract In this talk I will present recent results on molecular modeling and design of nanostructured films on graphene that can aid the realization of synthetic scaffolds for binding proteins and the electro-stimulated growth of tissue on graphene. Atom-scale molecular dynamics computer simulations were used to probe the structure, dynamics and energetics of alkylamine self-assembled monolayer (SAM) films on graphene, and to model the formation of bilayers and protein complexes on the films (Figure 1). The simulations quantify the changes in film physisorption strength on graphene and alkyl chain packing efficiency as the film surface is made progressively more polar by changing the terminal groups from methyl –CH3 to amine –NH2 to hydroxyl –OH groups. The mode of molecule packing dictates the orientation and spacing between terminal groups at the surface of the SAM, which determines the way in which successive layers build up on the surface, whether via formation of bilayers of the molecule or the immobilization of other (macro)molecules, e.g., proteins, on the SAM-graphene scaffold. We find that monolayers and bilayers of molecules form ordered, stable assemblies on graphene and that molecular films on graphene can serve as protein adsorption platforms, with a hydrophobin protein showing strong and selective adsorption to the scaffold by binding via its hydrophobic and hydrophilic regions to methyl and amine/hydroxyl terminated films. Design rules obtained from modeling the atom-scale structure of the films and interfaces[1] can provide inputs to experiments for rational design of assemblies in which the electronic, physicochemical and mechanical properties of the substrate, film and protein layer can be tuned to provide the desired functionality. As a first step towards this goal, we compare our findings with the latest experimental data from our own labs and others, and provide some perspectives on possible routes to development and exploitation of graphene-based scaffolds, with molecular topology and SAM structure tailored for emerging applications of the layered composite in tissue engineering applications, e.g., electrically stimulated nerve fiber growth via the targeted binding of specific cell surface peptide sequences on the functionalized graphene scaffold.

References

[1] Long, B.; Manning, M.; Burke, M.; Szafranek, B.N.; Visimberga, G.; Thompson, D.; Greer, J.C.; Povey, I.M.; MacHale, J.; Lejosne, G.; Neumaier, D.; Quinn, A.J. Advanced Functional Materials, 22 (2012) Non-Covalent Functionalization of Graphene Using Self-Assembly of Alkane-Amines, 717–725.

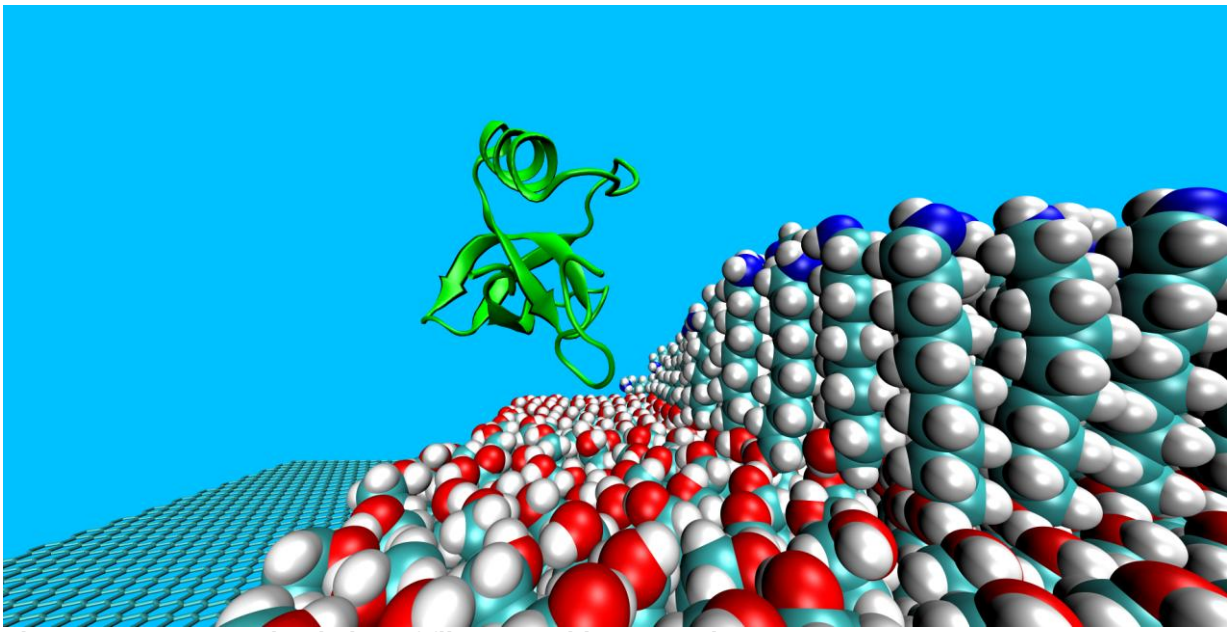

Figure 1. Computer simulation of film assembly on graphene.