Modelling and Design of Nanostructured Interfaces

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Abstract

In this talk I will discuss the difficulties in describing nanoscale physics and describe how computer simulations can aid experiments in the realization of nanostructured materials. I will present recent results on molecular modeling and design of nanostructured interfaces for technology applications. I will focus on self-assembled monolayer films on noble metals [1], metal oxide [2] and graphene [3]. I will also describe recent combined experiments and simulations of dendrimer-wrapped gold nanoparticles [4]. These (ultra)thin films and single-molecule nanostructures are used in molecular devices and also have potential applications in health and energy (Figure 1).

References

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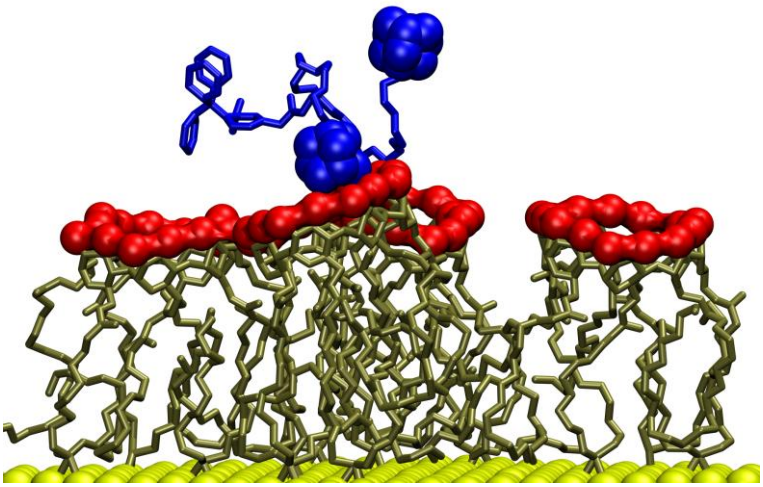

Figure 1 – Molecular simulations and fluorescence microscopy experiments can be combined to determine the structure, dynamics and energetics of the interface between a two-legged dendrimer molecule and a receptor-functionalised self-assembled monolayer on gold [1b].