Atom-scale computer-aided design of organic-inorganic interfaces

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In this talk I will discuss the difficulties in controlling nanoscale physics and describe how atomic scale computer simulations can aid experiments in the design of functional organic-inorganic interfaces. I will present recent results on experimental/simulation co-design of ferrocene-alkanethiolate self-assembled monolayer (SAM) films on silver; these films exhibit an atom-level sensitivity in their electrical properties.[1] I will also describe combined experiments and simulations of controlled motion of dendrimer molecules on carbohydrate-functionalised SAMs[2] and present the synthesis and interlinking of dendrimer-wrapped gold nanoparticles.[3]

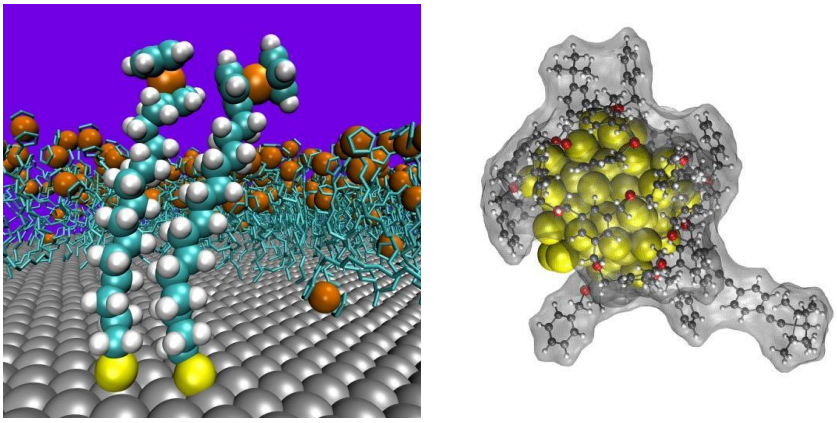

Figure 1. (left) Ferrocene-alkanethiolate molecules with an odd number of alkyl carbon atoms stand tall on silver and form close-packed SAMs that block leakage currents in molecular diodes. [1] (right) Gold clusters stabilised by thioether dendrimer molecules provide building blocks for future molecular electronic devices. [3]

[1] N. Nerngchamnong, Y. Li, D. Qi, L. Jian, D. Thompson and C.A. Nijhuis, *Nature Nanotechnology*, 2013, 8, 113

[2] A. Perl, A. Gomez-Casado, D. Thompson, H. Dam, P. Jonkheijm, D. Reinhoudt and J. Huskens, *Nature Chemistry*, 2011, 3, 317

[3] D. Thompson, J.P. Hermes, A.J. Quinn, M. Mayor, *ACS Nano*, 2012, 6, 3007