Rational design of supramolecular devices

Damien Thompson

Department of Physics, Bernal Institute, University of Limerick, V94 T9PX, Ireland
damien.thompson@ul.ie

In this talk I will describe how a combination of multi-scale computer models, nanoscale materials characterisation and macroscopic electrical device measurements has bred a new class of high-performing, long-lived molecular devices that are approaching the performance of CMOS electronics but which are based on monolayers of redox-active molecules trapped between conductive electrodes. I will show how judicious choice of molecule length, headgroup, electrode material and electrode quality (Fig. 1) has a large impact on device performance that can be rationalised using molecular models [1] that in turn provide a virtual sandbox for the rational design of junctions with pre-programmed functionalities for a broad range of applications in nanoelectronics as well as plasmonics and nanomedicine.

References

[1] Thompson, D.; Nijhuis, C.A. Even the Odd Numbers Help: Failure Modes of SAM-Based Tunnel Junctions Probed via Odd-Even Effects Revealed in Synchrotrons and Supercomputers. Accounts of Chemical Research, 49 (2016), 2061-2069.

Figures

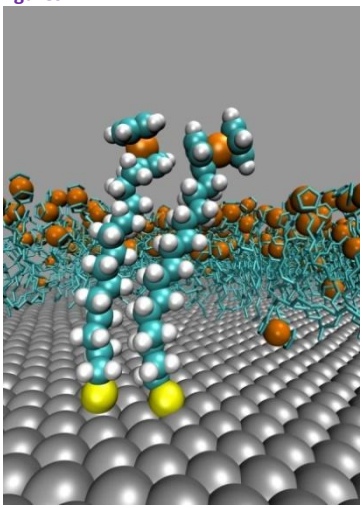

Figure 1: Ferrocene-alkanethiolate self-assembled monolayers (SAMs) on silver electrodes provide robust high-performance molecular rectifiers.