Modulating the Conducting Orbitals of Single Molecules Through Chemical Design

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Molecular electronics has primarily been driven by the potential for molecules to be used as miniscule circuit components. A challenge in the field is to design molecules that can perform specific functions in a molecular circuit, which requires the establishment of structure-property relationships. Chemists have the unique ability to modify molecular backbones. Therefore, it is important to exploit chemical modifications to modulate transport in junctions through the intrinsic character of the molecules rather than by external factors.

In this talk, I discuss work on 3 classes of materials – thiophene dioxides, benzotriazinyl-based Blatter radicals, and mixed-valence bis(triarylamines). With these three systems, I show how conducting orbitals can be predictably tuned to control the nature of charge carriers, investigate the interface between metals and the half-filled orbitals of organic radicals, and demonstrate that molecules with conducting orbitals close to the fermi energy of gold can display very efficient length-dependent electronic transport respectively.