Mapping electron transport pathways in complex systems

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As system complexity increases, in either biological or synthetic molecules, understanding of structure-function relationships makes it possible to identify the essential functional units controlling physical properties from what may be a vast sea of spectator components. Until recently, the range of theoretical tools that have been implemented for elucidating structure-function relationships in molecular electron transport have been limited and consequently the ability to build chemical intuition for the behaviour of complex systems has been hindered.

Here we present our efforts developing a local description of molecular electron transport[1], which has allowed us to map the interactions in a molecule that mediate the tunnelling current in a range of chemically interesting molecules, for example the system shown in Figure 1. With this description of the local transport we can understand the behaviour of a complex, fluctuating system[2] as a force is applied that induces conformational change. We can isolate the interactions in the molecule responsible for high or low currents and can use this information to refine the system design.

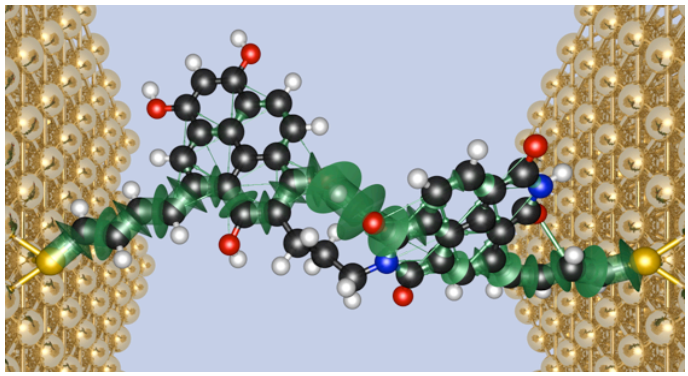

Figure 1 The local transmission through a complex molecule, illustrating the interactions in the molecule that mediate the tunnelling current.

References

[1] G. C. Solomon, C. Herrmann, T. Hansen, V. Mujica and M. A. Ratner, Nature Chem, **2** (2010), 223
[2] I. Franco, C. B. George, G. C. Solomon, G. C. Schatz and M. A. Ratner, J. Am. Chem. Soc. **133** (2011) 2242