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Conductance Through Single Organometallic Molecules[1]

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We have undertaken ab initio calculations of the conductance and I-V curve of a variety of single molecules bridging two metallic leads. The method adopted is a non-equilibrium Green function (NEGF) approach to transport combined with density functional theory (DFT) calculations for the electronic structure.

A principal motivation comes from experiments in the U. Maryland group [1]: they showed that a molecule containing a ferrocene moiety conducts nearly perfectly, in striking contrast to the severely impaired conduction through all fully conjugated but non-metallic molecules. Our calculations show that, indeed, there is a transmission resonance at the Fermi energy of the leads connected to the iron atom in the molecule. However, the comparison of theory and experiment also points to significant weaknesses caused by approximations in the standard NEGF+DFT approach.

Thus, on a much simpler system – a H atomic chain – we carry out much improved calculations involving exact exchange, hybrid functionals, and the optimized effective potential method. These provide a cautionary illustration of the kind and magnitude of errors in the standard approach.

Finally, emboldened by our success with the ferrocene-containing molecule, we turn to developing a true molecular spintronics based on cobaltocene moieties (spin 1/2). A simple molecule with a single cobaltocene provides a spin filter; we demonstrate a spintronic switch and spin valve using a dicobaltocene molecule [2].

(1.) S.A. Getty, et al. (groups of M.S. Fuhrer, and L.R. Sita), PRB 71, 241401(R) (2005).
(2.) R.Liu, S.-H. Ke, H.U. Baranger, and W. Yang, Nano Lett. 5, 1959 (2005).

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