AB INITIO TRANSPORT PROPORTIES OF CARBON-BASED NANOSTRUCTURES

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Carbon-based compounds are one most ubiquitous classes of systems in life- and material-science. In particular, hybrid systems composed by carbon-based nanostructures (such as organic molecules, nanotubes, graphene sheets, etc) and transition metal elements are attracting a growing interest in view of their potential for nanoscale applications, single-molecule devices and spintronics. Using first-principles calculations in the framework of density functional theory, we investigate the electronic and transport properties of a few representative systems, i.e. metal-phthalocyanines and graphene stripes, both in a single-molecule configuration and in a model device geometry. We will focus in particular on the magnetic properties induced by the interaction with transition ions (e.g. Mn, Co, Cu). Our results[1,2] show that organometallic devices can act selectively as molecular conductors, as spin valves, and spin filters, confirming the great potential of these systems for molecular nanoelectronics applications.

[1] A. Calzolari *et al*., Nanotechnology **18,** 424013 (2007)

[2] C. Cocchi *et al*., preprint (2008).