Spin selective transport through helical molecular systems

Elena Díaz[1], R. Gutierrez[2], R. Raaman[3] and G. Cuniberti[2]

[1]Departamento de Física de Materiales, Universidad Complutense, E-28040 Madrid, Spain
[2]Institute for Materials Science, Dresden University of Technology, D-01062 Dresden, Germany
[3]Department of Chemical Physics, Weizmann Institute, 76100 Rehovot, Israel

elenadg@fis.ucm.es

Abstract

The concept of spintronic devices operating without a magnetic field has been proposed some time ago for solid state devices in which the spin-orbit coupling (SOC) is large [1, 2]. In recent years, a new type of magnet-less spin selective transmission effect has been reported [3–7]. It was found that electron transmission through self-assembled monolayers (SAM) of chiral molecules is highly spin selective at room temperature. These findings are so far surprising as organic molecules typically have a small SOC that cannot support significant splitting between the spin states. Although it has been suggested both by theory [8, 9] and experiments [10] that there is a cooperative contribution to the value of the SOC, making this quantity larger in molecules or nanotubes than in a single carbon atom, the values calculated or experimentally found are still relatively small [8–11], e.g. few meV for nanotubes [10]. Hence, even including this cooperative contribution, the spin polarization (SP) in electron transmission through SAMs of chiral molecules [6, 7] seems to be too high to be rationalized by such SOC values.

Recently, a theoretical model based on scattering theory has been proposed for explaining the spin selectivity of chiral molecules [12]. Although the results are in qualitative agreement with the experimental observations, they could not explain them using reasonable SOC values.

In this work [13], a minimal model is presented, describing electron transmission through a helical potential, see Fig. 1. Main goal of the model is to highlight the role of some crucial parameters, which will lead to a high SP while still keeping a moderate SOC strength. Although the recent transport experiments on DNA SAMs [7] are our main motivation, the model is generic enough to encompass other molecular systems with chiral symmetry. In short, there are two main key factors in the model allowing for a high SP: i) Lack of inversion symmetry due to the chiral symmetry of the scattering potential, and ii) Narrow electronic band widths in the helical system, i.e. the coupling between the units composing the helical structure is relatively weak. A physically meaningful estimation of the SOC is further obtained by taking into account that first, in the present study the electric field acting on the electron needs to include the effective influence of all the electrons belonging to a molecular unit [7, 14], and second, due to proximity effects, the Coulomb interaction between the transmitted electron and those in the molecular unit scales as 1/R for short distances R.

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Figures

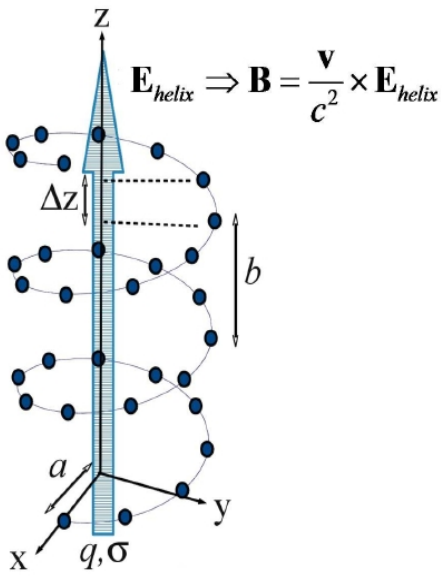

FIG. 1. A charge q in spin state σ is moving along through helical electric field. The parameters a, b and Δz are the radius and the pitch of the helix and the spacing of the z-component of the position vector of the charges distributed along it, respectively. The helical field induces a magnetic field B in the rest frame of the charge and hence influences its spin state.

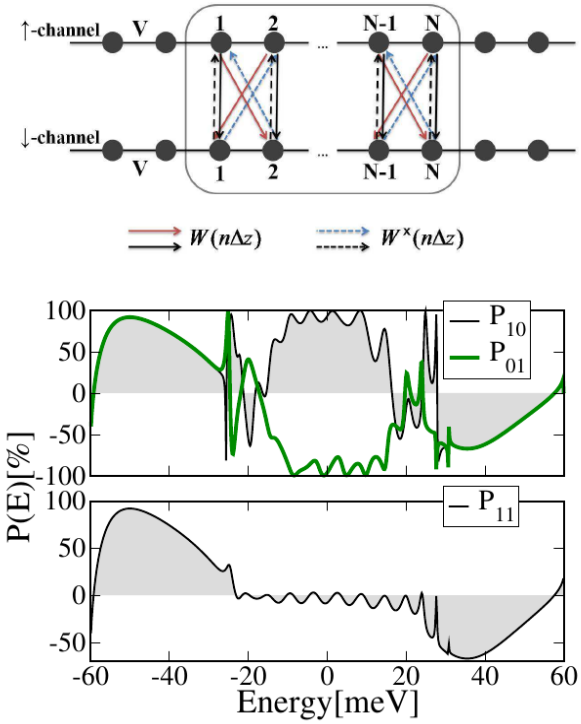

FIG. 2. Top panel: Schematic representation of the tight-binding model. The two channels interact via the SOC (framed region). To the left and right of the spin scattering region, both channels are independent and are modeled by semi-infinite chains. Bottom panel: Energy dependence of the SP P (E) for L0 =3 helical turns, and for injected electrons polarized with their spin pointing up (P10), down (P01), or unpolarized (P11). A spin-filter effect takes place only for energies near the band edges, where all SPs have the same sign.