Spin-selective transport through helical molecular systems

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Abstract

The majority of existing spintronic devices are based on inorganic materials, although some work has been performed on organic molecules [1–3]. As a rule, the spin sensitivity of molecular based spintronics is rather related to the magnetic properties of the electrodes or of the used molecules, so that the recent experimental demonstration [4, 5] of spin selective effects in monolayers of double-stranded DNA oligomers have drawn a great deal of interest.
On the theoretical side two main lines can be identified: i) Studies based on scattering theory at the level of the Born approximation, including spin-orbit interactions derived from a helically shaped potential [6, 7] and ii) Approaches based on quantum transport [8, 9], which probe the electrical response of DNA self-assembled monolayers in a two terminal setup. Common to both approaches is the assumption that a molecular electrostatic field with helical symmetry can induce in the rest frame of a moving charge an effective, momentum-dependent magnetic field. This field can then couple to the electrons spin leading to a spin-orbit coupling (SOC) which encodes the helical symmetry of the molecular structure.

In the present study, we generalize some of these previous works [8, 9] in important aspects. We consider two concentrical helices, as shown in Figure 1. In addition, we will include two energy levels per site in the tight-binding version of the continuum model, corresponding to the edge orbitals of a molecular monomer building up the helical system. We stress that the two levels do not need to lie on different helices, so that the model only considers transport along a single helical path but with more than one level per site in the tight-binding description. The model can thus be applied to single-helix systems and easily extended to double-helix structures. Our results suggest that two elements are key ingredients to obtain net spin polarization in this class of models: first, including more than one energy level per site (more than one transport pathway), and second, introducing asymmetries in the effective electronic-coupling elements between the different channels, see Figure 2. The model presented is quite general and is expected to be of interest for the treatment of spin-dependent effects in molecular scale systems with helical symmetry.

References

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Figures

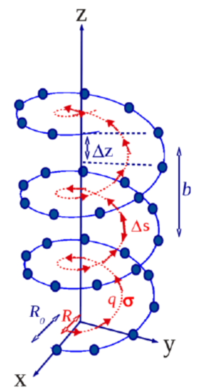

Figure 1. Schematic representation of the system. Along the external helix with radius R_0 point charges are arranged and build the source of the electrostatic field felt by a charge moving along the internal helical path of radius R. The internal helical path is parametrized with the arc length s.

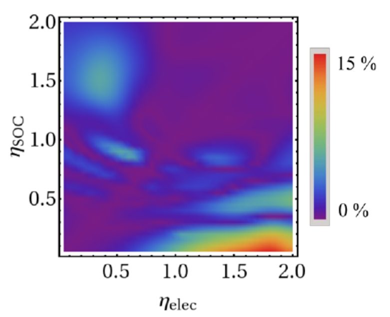

Figure 2. Density plot showing the absolute value of the average spin polarization $\langle P(E)\rangle_E$ as a function of the asymmetry ratios $\eta_{SOC} = \alpha_H/\alpha_L$ and $\eta_{elec} = V_H/V_L$. Parameters are $\alpha_L = 2$ meV nm, $V_L = 30$ meV, $V_{HL} = 50$ meV, $\varepsilon_r = 0.25$, and $L = 2$ helical turns.