

Probing Molecular Chirality via Electronic Transport

F. A. Pinheiro ^{(1)*}, S.J.S. da Silva ⁽²⁾, E.R. Granhen ⁽²⁾, F.M. Souza ⁽³⁾, J. Del Nero ^(1, 2)

(1) Instituto de Física, Universidade Federal do Rio de Janeiro, Rio de Janeiro (RJ), email: fpinheiro@if.ufrj.br

(2) Departamento de Física, Universidade Federal do Pará, Belém (PA)

(3) Instituto de Física, Universidade Federal de Uberlândia, Uberlândia (MG)

* Corresponding author.

Abstract – Molecular devices have attracted attention due to promising application in electronics. Chirality is a very important molecular property that manifests itself in several physical observables such as the well-known natural optical activity. In this work we demonstrate that molecular chirality also manifest itself in the electronic transport properties in a crucial way. In particular, we show, by *ab initio* Hartree-Fock derivative as well nonequilibrium Green function, that the electronic current through molecular devices is proportional to the degree of chirality, which is calculated using group theory.

Recently Nitzan raised up a competitive relationship between ballistic and diffusive heat transport on molecular scale for larger systems taking into account non-linear/linear effects as well as the needs to find out fundamental rules for the nature of these interactions on nanostructured systems [1,2]. Beside that, it has been investigated and proposed systems presenting ballistic molecular rectification for two-terminal nano-device with saturated and conjugated backbone. In particular, for a complex helicoidal molecular structure it was found a nanowire behavior due to the electronic coupling in a conjugated bridge [3,4,5 and references therein]. Also, molecules with p bridges and octupolar termination groups have been synthesized and investigated with particular attention to the two-photon optical properties.

We calculate the chiral index, using group theory [6], for several structures of the whole family of the oligo-(para)phenylene-vinylene attached to orto-propyl and demonstrate that the chiral index is proportional to the modulus of the current for all the considered structures (Fig. 2). This result suggests that electronic transport may be interpreted as a new manifestation of molecular chirality, as well as many other physical observables such as the natural optical activity [6] and light scattering [7]. Also, our findings suggest that we can probe and measure the degree of molecular chirality by means of transport properties.

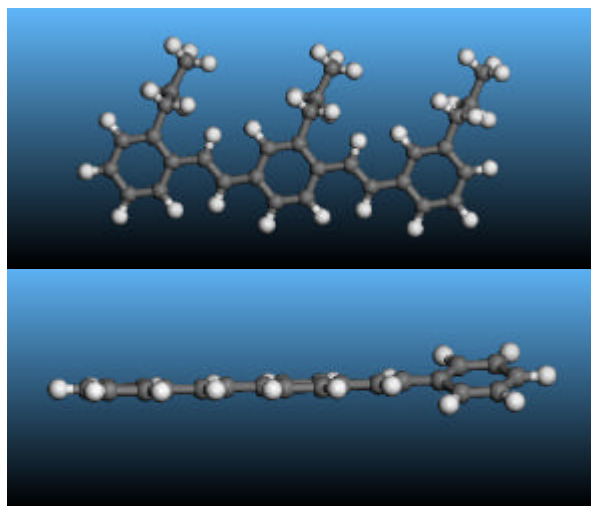


Figure 1 (Top) Pictogram of PPV oligomer. Parallel conformation with (a) front view and lateral view with (bottom) 15° and (c) 30° as dihedral angle (The C₆H₅ radicals were removed from (bottom) for better view) under external electric field, respectively.

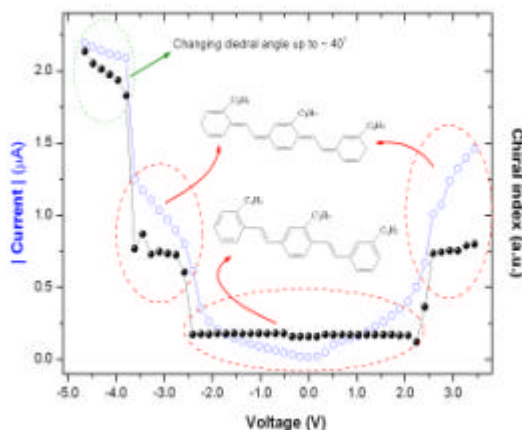


Figure 2: Current (blue) and Chiral index (black) versus bias voltage for PPV derivative showing three different conduction behaviors as: a) aromatic when the device is under low voltages (ohmic characteristic); b) quinoidal, after resonance (+ and – bias V) and c) Changing of dihedral angle.

[1] P. Delaney, and J.C. Greer, Phys. Rev. Lett. 93 (2004) 036805.

[2] A. Nitzan, Science 317 (2007) 759.

[3] M.A. Reis, and J. Del Nero, J. Comp. Theor. Nanoscience. 5 (2008) 567.

[4] D.B. Lima, and J. Del Nero, J. Comp. Theor. Nanoscience. 5 (2008) 1445.

[5] D.B. Lima, M.A. Reis, F.M. Souza and J. Del Nero, J. Comp. Theor. Nanoscience. 5 (2008) 563.

[6] A. B. Harris, R.D. Kamien, and T. C. Lubensky, Rev. Mod. Phys.71 (1999) 1745.

[7] F.A. Pinheiro, and B.A. van Tiggelen, Phys. Rev. E 66 (2002) 016607.