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Control of Negative Differential Resistance from benzene ring chains attached in carbon nanotubes

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ABSTRACT

Since the design of a single molecule device started by Aviram and Ratner in 1974 [1], encouraged mainly by the dimensional limits of the microtechnology, there is much research for the effective use of these nanodevices [2]. Organic materials have been the focus of many researchers for the generation of systems with more precision of control and with greater energy efficiency [3]. In this respect, the evolution of advanced theoretical studies for the prediction of nanosystem electronic properties has been widely used, due to its prediction being very efficient to direct and predict with great success experimental applications [4]. The present work investigates the study of the electronic properties in different chains of benzene rings with defects attached in carbon nanotubes [5]. Using advanced theoretical methodology based on the Functional Theory of Density and Non-Equilibrium Green Functions in the formalism of Landauer-Buttiken [6-8]. The results showed negative differential resistance (NDR) and resonance with diode characteristic, being the main importance visualized the control of the same in the signature of the electronic current of the system, favoring the indication of use for possible applications in control engineering for components that need tuned bands at low voltages [9,10]. In this sense, the direction of the work entails the possibility of NDR control in nanosystems using carbon-based materials for advancement in nanoelectronic engineering.

REFERENCES

- [1] AVIRAM, M. A.; RATNER, M. A. Molecular Rectifiers. *Journal of physical chemistry*, **114** (48), 20299–20319 (1974).
- [2] HULLA, J. E.; SAHU, S. C.; HAYES, A. W. Nanotechnology: History and future. *Human & experimental toxicology*, **34** (12), 1318-1321 (2015).
- [3] TALAWAR, M. B. et al. Environmentally compatible next generation green energetic materials (GEMs). *Journal of Hazardous Materials*, **161** (2), 589-607 (2009).
- [4] ARTACHO, Emilio et al. The SIESTA method; developments and applicability. *Journal of Physics: Condensed Matter*, **20** (6), 064208 (2008).
- [5] REIS-SILVA, J.C.; FERREIRA, D.F.S.; LEAL, J.F.P; DEL NERO, J.; Enhancing and optimizing electronic transport in biphenyl derivative single-molecule junctions attached to carbon nanotubes electrodes. *Solid State Communications* **252**, 46-50 (2017).
- [6] HOHENBERG, P.; KOHN. Inhomogeneous electron gas. *Physics Review*, **136**, 864-871 (1964).
- [7] DATTA, S. Exclusion principle and Landauer-Büttiker formalism. *Physical Review B*, **45**, 1347-1364 (1992).
- [8] DATTA, S.; TIAN, W.; HONG, S.; REIFENBERGER, R.; HENDERSON, J. I.; KUBIAK, C. P. Current-voltage characteristics of self-assembled monolayers by scanning tunneling microscopy. *Physics Review Letters*, **79**, 2530-2533 (1997).
- [9] LEHMANN, B.; DORER, V.; GWERDER, M.; RENGGLI, F.; TÖDTLI, J. (2011). Thermally activated building systems (TABS): Energy efficiency as a function of control strategy, hydronic circuit topology and (cold) generation system. *Applied Energy*, **88**(1), 180-191.
- [10] KULKARNI, Shriram; MAZUMDER, Pinaki; HADDAD, George I. Digital logic design using negative differential resistance diodes and field-effect transistors. U.S. Patent n. 5,903,170, (1999).