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Electronic transport applied to C-57 and hydrogenated C-57

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Abstract:
The evolution of nanoscience and nanotechnology has been one of the most fascinating and dynamic fields of research in recent decades, from its initial concept to the most advanced technologies recently developed. From Greek atomism to the more advanced studies of nanoscience and nanotechnology, where materials are manipulated, observed, and worked with at the manometric scale. In this work, the electronic and transport properties of carbon C-57 and hydrogenated C-57 were investigated by Density Functional Theory combined with the Non-Equilibrium Green's Function (DFT/NEGF) implemented in the TRANSIESTA for application on electronic devices. The molecular systems are composed of a unit cell of C-57 and C-57 with addition of hydrogen atoms at its edges. With the results, it was revealed that the C-57 system in the range of 0.34 V to 0.50 V shows a decrease in current as the voltage increases, indicating points of current suppression influenced by the drop in conductance, due to having few possible accessible states for conduction, as revealed by the Density of States (DOS). This is coupled with an increase in potential barriers and the unavailability of new electronic states for charge transport, resulting in lower conductive performance of the system, as verified by the transmittance of transport. In contrast, for the hydrogenated C-57 system, between the ranges of 0.42 to 0.50 V, there is an increase in current as the voltage rises, revealing points of current elevation, which are consequently influenced by the growth of conductance, due to a slight increase in the density of states available for electrons near the Fermi level. It is possible that there are more accessible states for conduction, as revealed by the DOS, along with a decrease in potential barriers and the availability of new electronic states for charge transport in the hydrogenated system. Based on the results, that the C-57 structure of has characteristics of a conductor; however, the hydrogenated C-57 structure has characteristics of a semiconductor. In this way, influencing the systems for a wide range of applications in molecular electronics and in the field of nanoscience and nanotechnology.

References:

FERREIRA, D. F., *Análise De Transporte Eletrônico Em Junções De Carbyne Com Eletrodos De Nanotubos De Carbono Via Dft/Negf, Trabalho de Conclusão de Curso, 2016.*
FEYNMAN, R. P. *Space-time approach to quantum electrodynamics. Physical Review*, v. 76, n. 6, p. 769-789, 1949.

FEYNMAN, R. P. *There's plenty of room at the bottom. Engineering and Science*, v. 23, n. 5, p. 22-36, 1960.
GUPTA, A. *Carbon nanotubes: Synthesis, characterization, properties, and applications*. Elsevier, 2018.
HAY, P. J.; WADT, W. R. *Ab Initio Effective Core Potentials for Molecular Calculations. Potentials for the Transition Metal Atoms Sc to Hg*. Journal of Chemical Physics, vol. 82, no. 1, pp. 299-310, 1985.
LUZ, S. C., *Investigação do transporte eletrônico em Nanofitas de X-grafeno, Autoria Própria. 2023.*
SOLER, J. M. et al. *The SIESTA Method for Ab Initio Order-N Materials Simulation*. Journal of Physics Condensed Matter, vol. 14, no. 11, pp. 2745-2779, 2002.
SZABO, A.; OSTLUND, N. S. *Modem Quantum Chemistry: Introduction to Advanced Electronic Structure Theory,* Dover Publications, 1996.
ZETTILI, N. *Quantum Mechanics: Concepts and Aplications,* 2nd ed., Wiley, 2001.
ZHAO, et al. *C-57 carbon: A two-dimensional metallic carbono allotrope wih pentagonal na heptagonal rings*,Vol. 100 p. 115 – 119, Elsevier, 2019.