Electronic Transport and Thermopower Properties of α-phographene

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The study on new materials made from carbon allotropes has gained prominence due to the diverse applicability that these materials have given to electronics [1, 2]. Among these allotropes, two-dimensional materials play a leading role in the future of electronics due to versatility and wide application [1]. Recently, a class of metallic and semi-metallic materials, called Phographenes, was proposed as a promising for bi-dimensional nanoelectronics. They consist of structures with carbon rings formed by 5-6-8 atoms. In this work, we report the electronic and thermal transport properties of metallic α-phographene [1] obtained by first-principle methods. We used the Density Functional Theory (DFT) combined with Non-Equilibrium Green's Function (NEGF) as implemented in the computational package SIESTA [3] to obtain the results of electronic transport and the GOLLUM [4] package was used to obtain thermal properties. The results for electronic transport in a voltage range from -0.5 V to 0.5 V shown the metallic feature of the α-phographene with a maximum current value of around 4.00μA. Negative Differential Resistance (NDR) was observed at 0.25V, 0.56V, and 0.82V. The density of states confirms the metallic behavior of the device. The maximum value for the dimensionless Figure of Merit (ZT) is aligned with the Fermi level at 0.15 in 0.0 V and is followed by a small contribution of ≈ 0.02 in 0.05V. It indicates the maximum efficiency for heat transfer and the current generation. The shifted to the left demonstrates that the thermal conductance σ becomes lower while increasing the Seebeck coefficient. It implies an increase in the thermoelectric voltage of the device. Finding good values for ZT is a challenge, since conventional devices with good applicability have these coefficients above 3 [4], comparatively, the performance of the α-phographene structure is higher than the devices consisting of graphene nanoribons [4].

References

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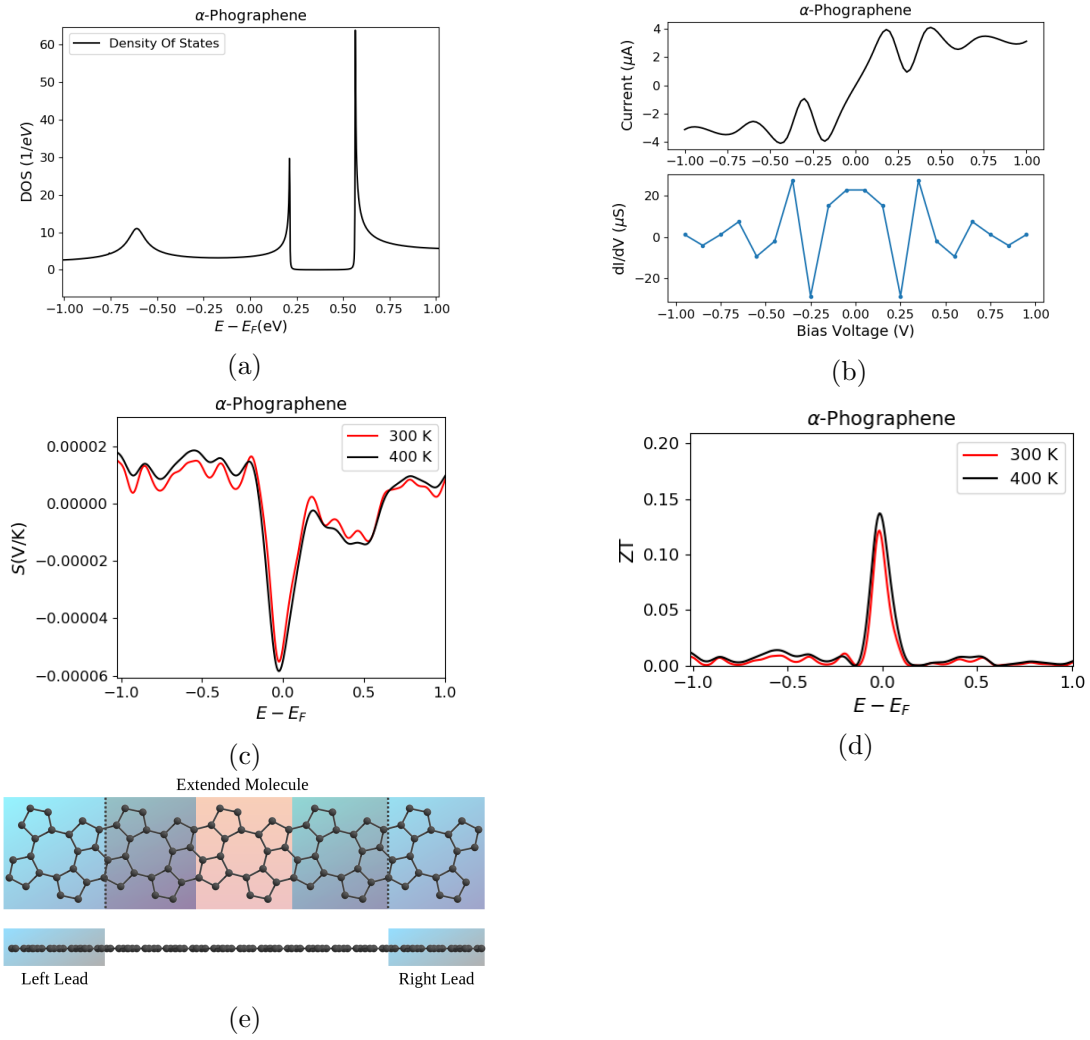

Figura 1: Results to α-phographene, in (a) the density of states (DOS), (b) Current-Voltage and differential conductance-voltage, (c) Seebeck coefficient, (d) ZT coefficient and (e) Geometry of electronic device.