

# Thermoelectric coefficients and quantum interference effects in trilayer silicene flakes

Natalia Cortés, L. Rosales, M. Pacheco, P. A. Orellana and Leonor Chico

Departamento de Física, Universidad Técnica Federico Santa María, Casilla 110-V, Valparaíso, Chile.

[natalia.cortesm@usm.cl](mailto:natalia.cortesm@usm.cl)

The thermoelectric efficiency in different materials is measured by the quantity  $ZT$ , known as figure of merit. This quantity in bulk materials have values not higher than the unit, but in nanostructured systems can be improved by different mechanisms, such as quantum size effects and the reduction of the thermal conductance, reaching values greater than 1 [1]. In this work, we propose a two-dimensional analogue of graphene to achieve this goal. We present a theoretical study of the electronic and thermoelectronic properties of a trilayer silicene flake device. This system can be studied with the same  $\pi$ -orbital tight-binding Hamiltonian model in trilayer graphene flakes [2]. The trilayer silicene flake is composed by an infinite central nanoribbon connected with two finite flakes symmetrically placed above and below it, as shown in Fig. 1. We have considered a gate voltage  $\Delta$  applied to the flakes, which controls the symmetries of the electronic potentials into the system. This allows us to explore the appearance of bound states in the continuum (BICs) and Fano antiresonances in the system to produce sharp changes in the electronic transmission. We show that the thermoelectric quantities as electronic conductance, thermal conductance, Seebeck coefficient and figure of merit can be tuned by means of the parameters of the system like the gate voltages, length of the flake and temperature. The optimal figure of merit is achieved at  $\Delta=0.032$  eV,  $T=50$  K and length of the flake  $L=27$  unit cells, as shown in Fig. 2. This theoretical study suggests an efficient way to enhance the thermoelectric efficiency of silicene devices.

## References

[1] R. Venkatasubramanian, E. Siivola, T. Colpitts, and B. O'Quinn, *Nature*, **413** (2001) 597.

[2] Natalia Cortés, L. Chico, M. Pacheco, L. Rosales, and P. A. Orellana, *EPL (Europhysics Letters)* **108** (2014) 46008.

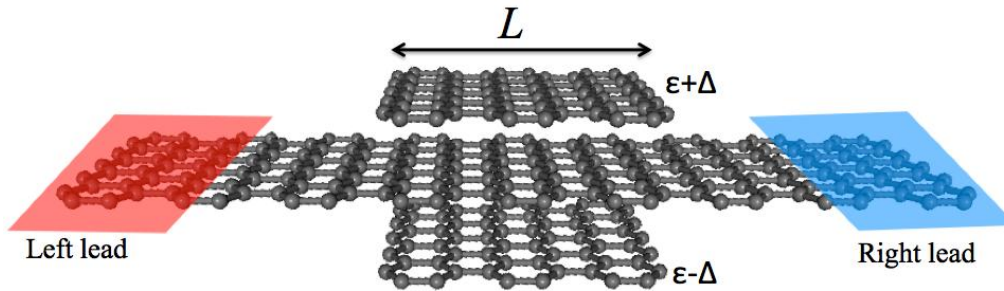


Fig. 1. Trilayer silicene nanostructure with AAA stacking.

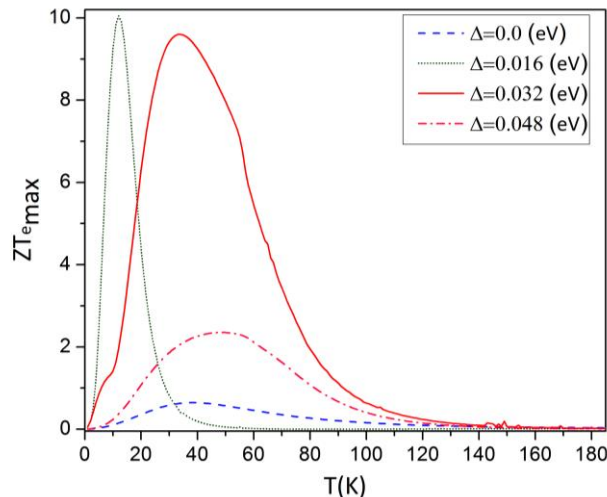


Fig. 2.  $ZT_{\max}$  as a function of the temperature for  $L=27$  flake length.