## Optimizing the thermoelectric figure of merit of aperiodic solids

## Enrique Maciá

Dpto. Fisica de Materiales, Facultad CC. Fisicas, Universidad Complutense de Madrid, E-28040, Madrid (Spain) emaciaba@fis.ucm.es

During the last few years we have witnessed a growing interest in searching for novel, high performance thermoelectric materials (TEMs) for energy conversion in small scale power generation and refrigeration devices. Some time ago the appealing question regarding the best possible electronic structure of thermoelectric materials (TEMs) was discussed by Mahan and Sofo [1]. It was proposed on sound theoretical basis that the best TEMs are likely to be found among materials exhibiting a sharp singularity in the density of states (DOS) close to the Fermi level, along with a substantial depletion of the DOS at the Fermi level. In this contribution I will describe the thermoelectric properties of two different classes of materials are representatives of quasicrystalline alloys exhibiting semiconductor-like, rather than metallic electronic transport properties, along with extremely low thermal conductivity values. Accordingly, quasicrystals can be regarded as an unexpected instance of the so-called electron crystal-phonon glass approach introduced by Slack [2]. Thus, quasicrystals occupy a very promising position in the quest for novel TEMs, naturally bridging the gap between semiconducting materials and metallic ones [3].

As an alternative to bulk materials the study of the thermoelectric properties of single molecules may underpin novel thermal devices such as molecular-scale Peltier coolers (figure) and provide new insight into mechanisms for molecular-scale transport. In this way, the thermoelectric potential of some conducting polymers, like polythiophene and polyaminosquarine, has been recently reviewed on the basis of their electronic band structures. I will focus on the electronic structure and transport properties on DNA based devices, with an special attention to the possible use of a thermoelectric signature for different codons of biological interest in order to explore new sequencing techniques based on physical processes instead of the usual chemical ones [4-7]. In fact, the thermoelectric properties of molecular systems have received a lot of attention during the last few years and it is expected that this attention to increase fast as the necessary experimental techniques are progressively refined [8-10].

## References

[1] G. D. Mahan and J. O. Sofo, "The best thermoelectric", Proc. Natl. Acad. Sci. USA, 93 (1996) 7436.

[2] G. A. Slack, CRC Handbook of Thermoelectrics, edited by D. M. Rowe (CRC Press, Boca Raton, FL, 1995).

[3] E. Maciá, "Aperiodic Structures in Condensed Matter: Fundamentals and Applications" (CRC Press, Boca Raton, FL, 2009).

[4] E. Maciá, "Codon thermoelectric signature in molecular junctions", Phys. Rev. B 82 (2010) 045431.

[5] E. Maciá "DNA based thermoelectric devices" in Charge Migration in DNA: Physics, Chemistry and Biology Perspectives, Ed. Chakraborty T (Springer, Berlin, 2007).

[6] E. Maciá "DNA-based thermoelectric devices: A theoretical prospective", Phys. Rev. B **75** (2007) 035130

[7] E. Maciá, "The role of aperiodic order in science and technology", Rep. Prog. Phys. 69 (2006) 397.

[8] P. Reddy, S. Y. Jang, R. A. Segalman, and A. Majumdar, "Thermoelectricity in molecular junctions", Science **315** (2007) 1568 .

[9] K. Baheti, J. A. Malen, P. Doak, P. Reddy, S. Y. Jang, T. D. Tilley, A. Majumdar, and R. A. Segalman, "Probing the chemistry of molecular heterojunctions using thermoelectricity", Nano Lett. **8** (2008) 715.

[10] A. Tan, S. Sadat, and P. Reddy, "Measurement of thermopower and current-voltage characteristics of molecular junctions to identify orbital alignement", Appl. Phys. Lett. **96** (2010) 013110.

## Figures



Figure caption

Sketch illustrating the basic features of a nanoscale DNA based Peltier cell. A polyA-polyT (polyG-polyC) oligonucleotide, playing the role of n-type, left (p-type, right) semiconductor legs, are connected to organic wires (light boxes) deposited onto ceramic heat sinks (dark boxes).