# On the Nature of Microscopic Heat Carriers in Nano-Porous Silicon

**Aleandro Antidormi[1],** Xavier Cartoixá[2], Luciano Colombo[1]

[1] *Dipartimento di Fisica, Università di Cagliari, Cittadella Universitaria, I-09042 Monserrato (Ca), Italy,*
[2] *Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona, Spain*

aleandro.antidormi@dsf.unica.it

Porous Silicon (PS), thanks to its small thermal conductivity, is a promising candidate for future thermoelectric applications. Although the effect of morphological properties on thermal conductivity (e.g., porosity, pores' size, ...) has been largely investigated from both a theoretical and experimental perspective, a deep understanding of the microscopic vibrational mechanisms at the core of thermal transport in porous materials is presently necessary in order to properly manage the atomistic features for engineering applications.
In this study we perform an atomistic analysis of the vibrational properties of nano-porous silicon samples for different porosity levels through the calculation and diagonalization of the dynamical matrix. Following recent studies on amorphous materials [1,2], we propose a classification of the vibrational modes into extended and localized modes and calculate participation ratios, stretching factors and phase quotients.
We hence identify the *mobility edge* and argue that a definiton of the *Ioffe-Regel limit* (separating propagons from diffusons in amorphous materials) cannot usefully be applied to PS: for the values of porosity considered no frequency-resolved distinction between the two can be made. We then analyse the low-frequency behaviour of the vibrational density and discuss the modification in the frequency and amplitude of the boson peak.

Finally, we apply a modal analysis [3] to calculate the modal contributions to thermal conductivity and show how porosity induces 1) generally smaller thermal conductivity per mode on one side and 2) strong negative correlations among modes on the other. Hence, we show that these issues concur in the exponentially decreasing thermal conductivity of PS as a function of porosity.

## References

[1] Allen, P. B., et al. ,*Philosophical Magazine B* 79.11-12 (1999): 1715-1731.
[2] Beltukov, Y. M., et al. *Physical Review E* 93.2 (2016): 023006.
[3] Lv, W., and Asegun H.. *New Journal of Physics* 18.1 (2016): 013028.

## Figures

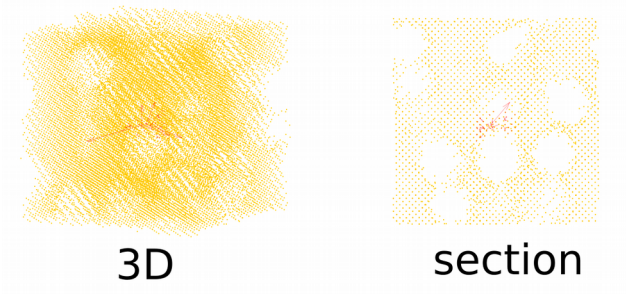


**Figure 1:** Atomic displacements (red arrows) in a localised mode in 30% porosity sample.

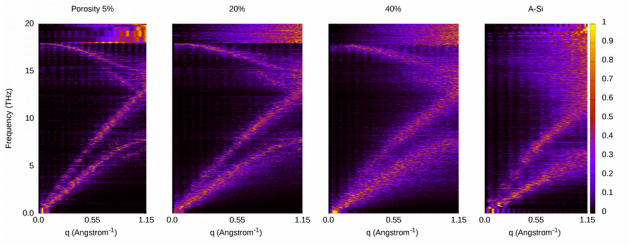


**Figure 2:** Dispersion curves of PS for increasing porosity whence the mobility edge and Ioffe-Regel limit are identified.