Effect of structural disorder and chemical doping on thermal transport in Nanoporous Graphene

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Graphene nanostructures have gained increasing attention due to their great potential for applications in electronics, optoelectronics, spintronics, chemical sensing, thermoelectricity, etc. The synthesis of graphene nanostructures via top-down methods such as exfoliation and chemical reduction present well-known disadvantages such as nonregular edge structures or uncontrollable sizes. In contrast, the bottom-up organic synthesis approach has emerged as a powerful tool to design structurally well-defined nanographenes. Among them, Nanoporous Graphene (NPG) has attracted particular interest in the last years for the possibility to finely tune the structural properties of the material via the controlled manipulation of nanopores in the basal plane. The possibility to control the density and structure of the pores represents indeed a promising strategy to tune also the electrical and thermal transport in the material.
In this work, we focus on the thermal properties of NPG by studying the impact of the structural features of the material and of the chemical doping. In particular, by means of classical molecular dynamics we investigate the vibrational properties at the microscopic level. The effect of structural disorder and chemical doping on the density of states, the participation ratio, and the intrinsic character of the vibrational modes is analyzed. Finally, the contribution of each single mode to the overall thermal conductivity is calculated, highlighting the most effective vibrations responsible for heat transport in NPG.

References

[1] Moreno, César, et al. "Bottom-up synthesis of multifunctional nanoporous graphene." *Science* 360.6385 (2018): 199-203.

Figures

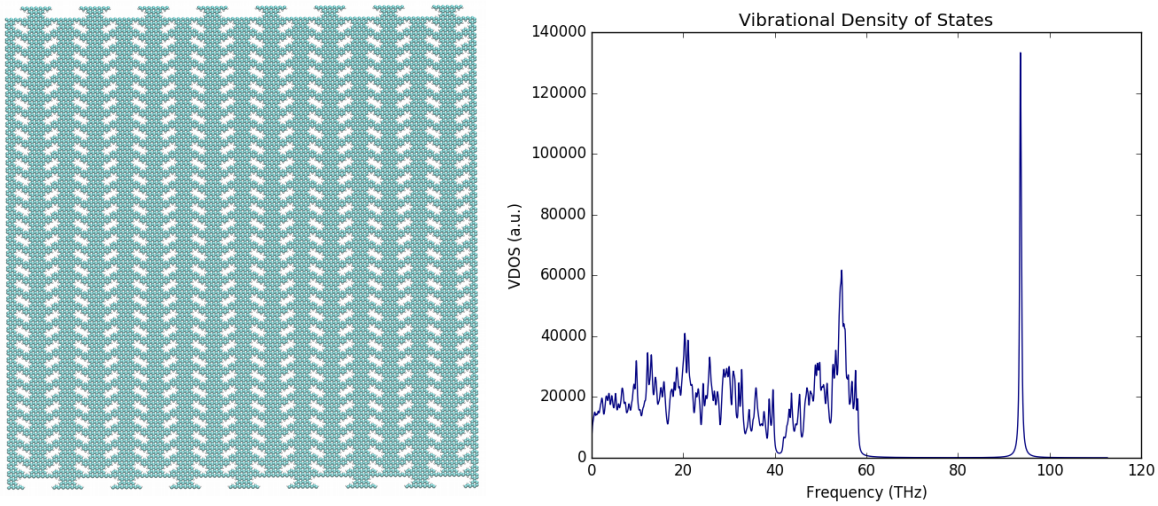

Figure 1. (Left) Nanoporous Graphene sample with 24800 atoms. (Right) Vibrational Density of states of NPG.