

THERMAL TRANSFER BETWEEN ULTRA-THIN SHEETS

Agustín M. Mancardo Viotti^{a,b}, Edgar A. Bea^{b,c}, Florencia M. Carusela^{a,b} and Alejandro G. Monastra^{a,b}

^a*Laboratorio de Modelado y Simulación Computacional LMSC ,Instituto de Ciencias, Universidad Nacional de Gral. Sarmiento, Los Polvorines, Buenos Aires, Argentina,
<https://sites.google.com/view/lmsc-ungs>*

^b*Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina*

^c*Comisión Nacional de Energía Atómica*

Keywords: Thermal Conductivity, Thermal Transport, Vibrational Modes, Thin Sheets, DFTB.

Abstract. Thermal conductivity in semiconductors is fundamentally determined by phononic transport. In isolated thin sheets, with a high surface-to-volume ratio, surface effects and their electronic configuration play a relevant role in phononic behavior and, consequently, in thermal properties.

In the case of a system of two facing and separated thin sheets by a distance of a few nanometers, electronic interaction between both surfaces can produce a coupling of vibrational modes, activating a thermal transport process by conduction between both membranes. In this work, the behavior of phononic bands is analyzed as a function of separation distance, in order to determine the vibrational modes involved in this thermal transport across the gap. Atomistic simulations based on the Density Functional Based Tight Binding (DFTB) approximation are employed.