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Thermal transport in graphitic nanostructures: Analytic force constants and first principles calculations YIFENG CHEN, THUSHARI JAYASEKERA, B. D. KONG, K. W. KIM, M. B. NARDELLI, North Carolina State University — Graphitic nanostructures such as graphene, nanoribbons and carbon nanotubes have shown to be potential candidates for device applications that may revolutionize the future of nanoelectronics. However, very little is known about their thermal properties. In fact, understanding the heat transfer at the nanoscale is essential for optimal thermal management and heat removal in device applications. In this talk, we will discuss an efficient approach to compute the phonon contribution to thermal transport in a broad range of carbon nanostructures using models based on analytic force constants and validate them against state of the art ab initio calculations based on Density Functional Theory. This work was supported, in part, by the NERC/NIST SWAN-NRI and the DARPA/HRL CERA programs.

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