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Thermal conduction mechanisms in isotope-disordered boron nitride and carbon nanotubes IVANA SAVIC, NATALIO MINGO, LITEN, CEA-Grenoble, France, DEREK STEWART, Cornell Nanoscale Facility, Cornell University, USA — We present first principles studies which determine dominant effects limiting the heat conduction in isotope-disordered boron nitride and carbon nanotubes [1]. Using an ab initio atomistic Green's function approach, we demonstrate that localization cannot be observed in the thermal conductivity measurements [1], and that diffusive scattering is the dominant mechanism which reduces the thermal conductivity [2]. We also give concrete predictions of the magnitude of the isotope effect on the thermal conductivities of carbon and boron nitride single-walled nanotubes [2]. We furthermore show that intershell scattering is not the main limiting mechanism for the heat flow through multi-walled boron nitride nanotubes [1], and that heat conduction restricted to a few shells leads to the low thermal conductivities experimentally measured [1]. We consequently successfully compare the results of our calculations [3] with the experimental measurements [1]. [1] C. W. Chang, A. M. Fennimore, A. Afanasiev, D. Okawa, T. Ikuno, H. Garcia, D. Li, A. Majumdar, A. Zettl, Phys. Rev. Lett. 2006, 97, 085901. [2] I. Savic, N. Mingo, D. A. Stewart, Phys. Rev. Lett. 2008, 101, 165502. [3] I. Savic, D. A. Stewart, N. Mingo, to be published.

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