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Thermal expansion in carbon nanotubes NICOLA BONINI, NICOLA MARZARI, Department of Materials Science and Engineering, MIT, Cambridge, MA, USA — We present a density-functional study of the thermal expansion properties of carbon nanotubes. The thermal expansion coefficients are calculated from the minimization of the vibrational free energy in the quasi-harmonic approximation. We show that carbon nanotubes contract at low and room temperature and expand at higher temperatures, and that the expansion coefficients strongly depend on the diameter, while chirality has a small effect. The role of different phonon modes in the thermal contraction is discussed togheter with the relation with the thermal expansion properties of graphene.

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