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Energy barrier for carbon nanotube collapse RAFAEL DEL GRANDE, RODRIGO CAPAZ, Univ Fed Rio de Janeiro — Small-diameter carbon nanotubes have circular cross section shapes, but the ground state of large-diameter tubes correspond to collapsed structures, stabilized by the van der Waals attraction of opposite sides of the nanotube wall. For those tubes, the circular cross section shape is metastable and it is interesting to investigate the energy barrier for jumping from one configuration to another. This barrier is shaped by the energetic compensation between van der Waals interactions and the elastic energy related to nanotube deformation. Previous theoretical works calculate the energy barrier by considering a transition pathway in which the nanotube collapses uniformly along its length, normally using periodic boundary conditions along the nanotube axis. In reality, this assumption is unphysical since it would lead to an infinite barrier for a nanotube of infinite length. In this work, we calculate the true energy barrier for carbon nanotube collapse by considering a transition pathway that consists of an initial local deformation that subsequently propagates itself along the carbon nanotube axis. This leads to finite and physically meaningful energy barriers in the limit of infinite nanotubes. Surprisingly, we find large energy barriers for the collapse of large-diameter carbon n

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