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Effect of intertube bond formation on mechanical and vibrational properties of nanotube ropes ANDRIY H. NEVIDOMSKYY, GÁBOR CSÁNYI, MIKE C. PAYNE, Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — Based on first-principles electronic structure calculations, we predict the formation of chemical bonds between boron nitride (BN) nanotubes, if doped with carbon. Similarly, intertube bonds are predicted to form in ropes of Nitrogen-doped carbon nanotubes. The effect of such bonds on the mechanical properties of carbon and BN nanotube ropes has been analysed, from which we find that the shear modulus of a nanotube rope appears to be greatly enhanced by the presence of intertube bonds. The analysis of phonon vibration spectra of BN nanotube ropes shows the up-shift in the frequency of the radial breathing mode due to the intertube bridging. These findings open prospects both for experimental detection of intertube bonds and possible technological applications.

Andriy Nevidomskyy
Theory of Condensed Matter, Cavendish Laboratory
University of Cambridge, Cambridge CB3 0HE, UK

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