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Phonon stiffening in semiconducting single-walled carbon nanotubes under n-type doping ELENA R. MARGINE, PAUL LAMMERT, VINCENT H. CRESPI, The Pennsylvania State University — The doping dependence of the high-frequency Raman-active modes in single-walled semiconducting carbon nanotubes is studied by density functional theory. We find that the A_{1g} longitudinal mode in $(3 * n + 1, 0)$ zigzag tubes shows a small anomalous upshift, followed by a large downshift under electron doping. This doping-induced stiffening of the A_{1g} mode is related to the large anharmonicity of the mode. Connections are made to recent experiments in the group of P. C. Eklund.

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