

Abstract Submitted  
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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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