

Abstract Submitted  
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**Electronic and mechanical properties of phosphorus and phosphorus-nitrogen doped carbon nanotubes** E. CRUZ-SILVA<sup>1</sup>, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6367, F. LOPEZ-URIAS, E. MUNOZ-SANDOVAL, Advanced Materials Department, IPICyT. Mexico, B.G. SUMPTER, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6367, H. TERRONES, Advanced Materials Department, IPICyT. Mexico, J.-C. CHARLIER, Unité de Physico-Chimie et de Physique des Matériaux (PCPM), European Theoretical Spectroscopy Facility (ETSF), Université Catholique de Louvain, V. MEUNIER, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6367, M. TERRONES, Advanced Materials Department, IPICyT. Mexico — Carbon Nanotubes have high potential for new materials based on their unique electronic and mechanical properties. They have found use in several fields, including composite materials, electronic nano-devices, catalysis, and energy storage, among others. Doping of nanotubes by exohedral or endohedral methods has been found to substantially modify their electronic structure, as well as their chemical reactivity. In this work, we present a density functional theory study of the electronic and mechanical properties of phosphorus and phosphorus-nitrogen substitutionally doped carbon nanotubes. It is found that doping with these atoms create localized states which modifies electron transport properties. The effects on mechanical properties will also be presented. These new doped nanotubes could have new applications in composite materials or in applications such as gas sensing or molecular detection.

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