ELECTRONIC SUPPLEMENTARY INFORMATION

Doping engineering of thermoelectric transport in BNC heteronanotubes

Leonardo Medrano Sandonas,[*a,b,c] **G. Cuba-Supanta,**[d] **Rafael Gutierrez,**[a] **Carlos V. Landauro,**[d,e] **Justo Rojas-Tapia,**[d] **and Gianaurelio Cuniberti**[a,c,f]

[a] *Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany. Fax: +49 (0)351 4633 1422; Tel: +49 (0)351 4633 1419; E-mail: leonardo.medrano@nano.tu-dresden.de (L.M.S.).*
[b] *Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany*
[c] *Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany*
[d] *Faculty of Physical Sciences, National University of San Marcos, Lima 01, Peru*
[e] *Centro de Investigaciones Tecnológicas, Biomédicas y Medioambientales (CIBTM), Bella Vista, Callao, Peru.*
[f] *Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany*

1 Electron transport properties

We have computed the projected electronic density of states (EDOS) of (6,6)-BNC heteronanotubes as implemented in DFTB+ code.

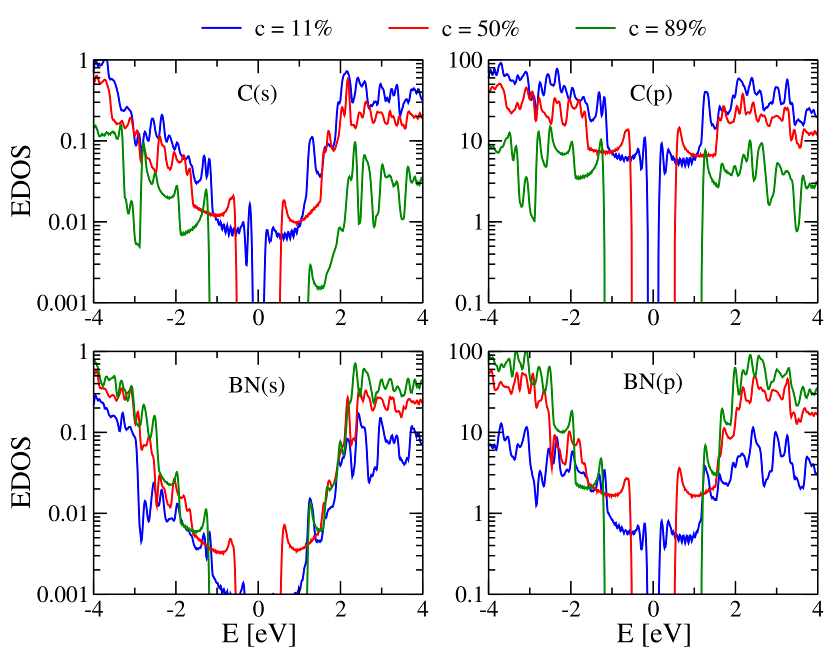


Figure S 1 Orbital-resolved of projected electronic density of states of helical (6,6)-BNC heteronanotubes. We show the contributions of C and BN domains.

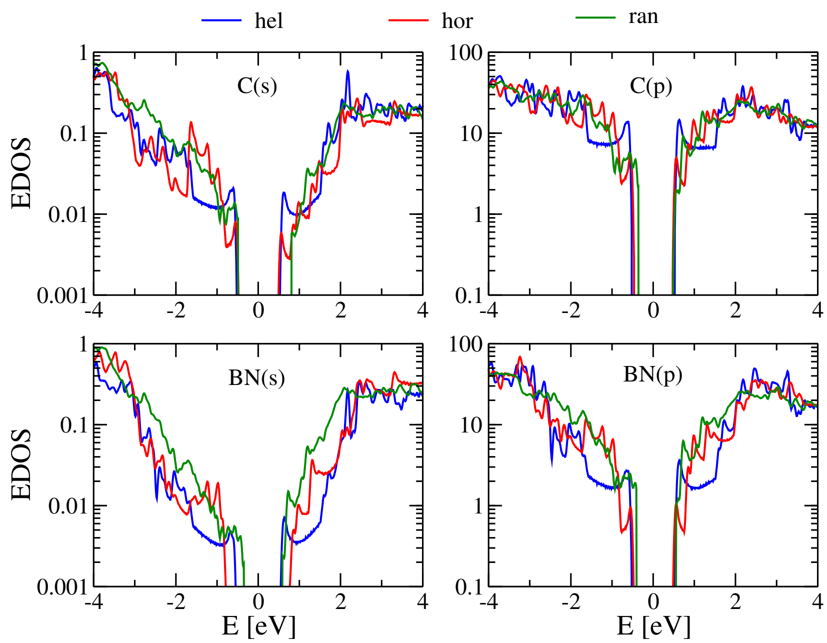


Figure S 2 Orbital-resolved projected electronic density of states of helical, horizontal, and random (6,6)-BNC heteronanotubes with a BN concentration of 50%. We show the contributions of C and BN domains.

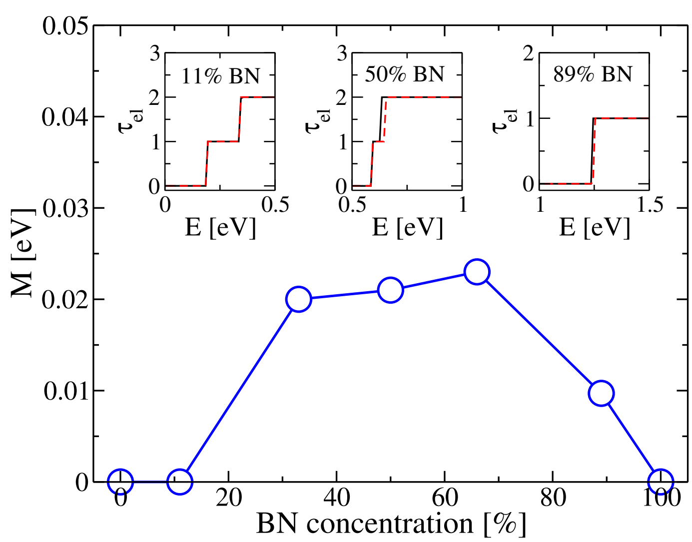
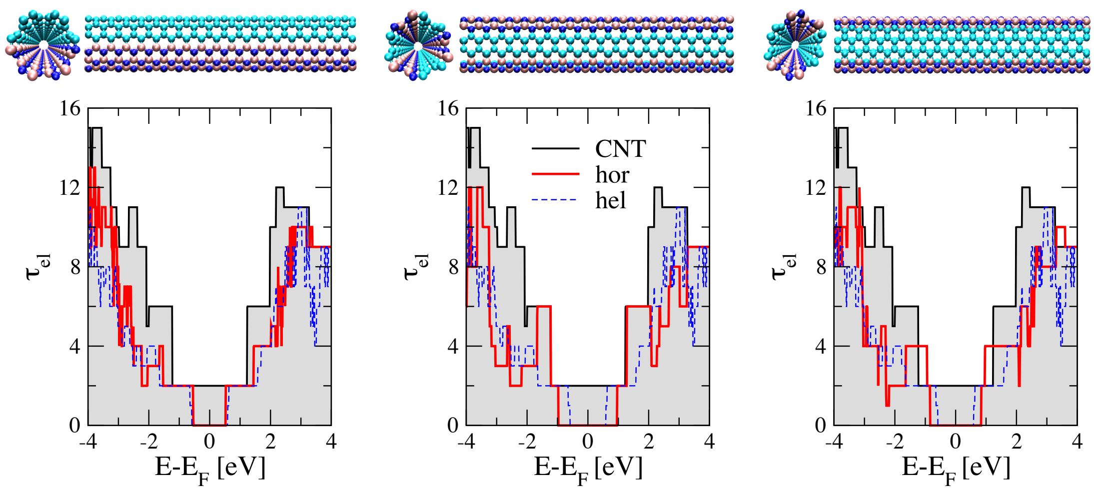


Figure S 3 Variation of the M parameter with the BN concentration in helical (6,6)-BNC heteronanotubes. M is defined as $M = \int |\tau_{el}(E > E_F) - \tau_{el}(E < E_F)| dE$, with τ_{el} as the electron transmission function. Insets: comparison of the transmission probability for the conduction (black solid lines) and valence (red dashed lines) bands of helical (6,6)-BNC heteronanotubes at different doping concentrations.



(a) (b) (c)

Figure S 4 Electron transmission function for the different atomic configurations of horizontal (6,6)-BNC heteronanotubes with $c = 50\%$. We compare the results with those corresponding to a (6,6)-CNT and full helical (6,6)-BNCNT with the same concentration. The atomic configurations for each case are also shown.

2 Phonon transport properties

The phonon density of states per atomic site has been calculated by using Green's function formalism as

$$\eta(\omega) = \frac{i(G^r - G^a)\omega}{\pi L}. \tag{1}$$

Then, we defined the ratio between the phonon DOS corresponding to C and BN domains with the following expression

$$R_{DOS} = \frac{\eta_X(\omega)}{\eta_{Total}(\omega)} \tag{2}$$

where X can be either C or BN.

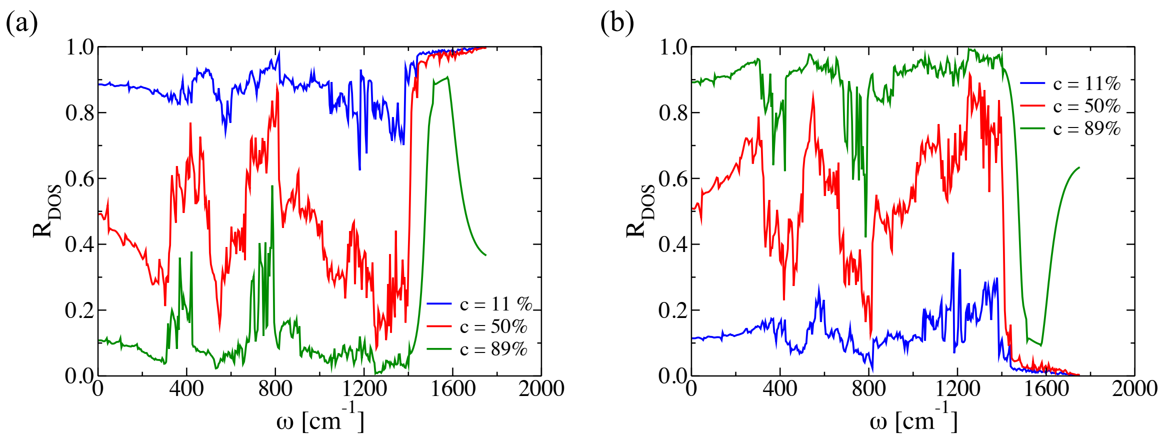


Figure S 5 Variation of R_{DOS} as a function of the vibrational frequency for helical (6,6)-BNC heteronanotubes with different concentrations. We show the values corresponding to (a) carbon and (b) boron-nitride domains.

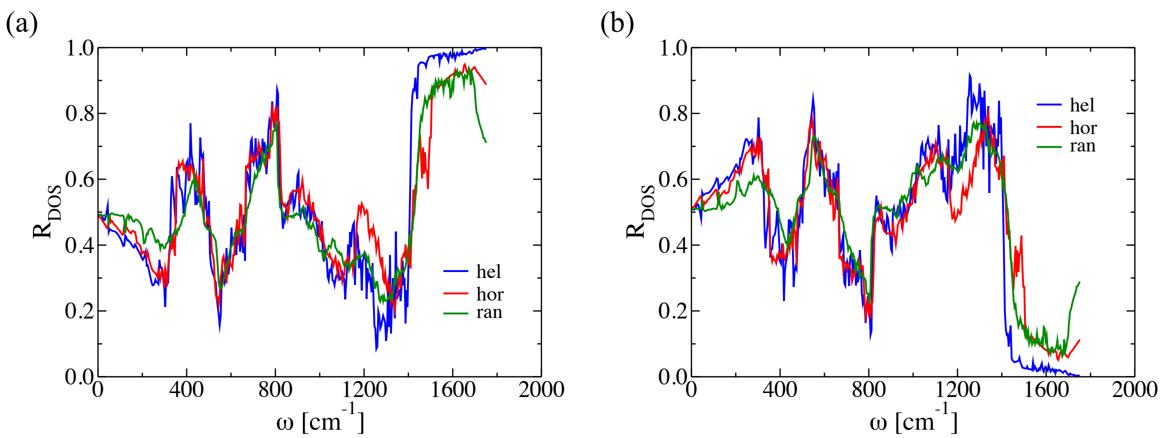


Figure S 6 Variation of R_{DOS} as a function of the vibrational frequency for helical, horizontal, and random (6,6)-BNC heteronanotubes with a BN concentration of 50%. We show the values corresponding to (a) carbon and (b) boron-nitride domains.

3 Thermoelectric transport properties

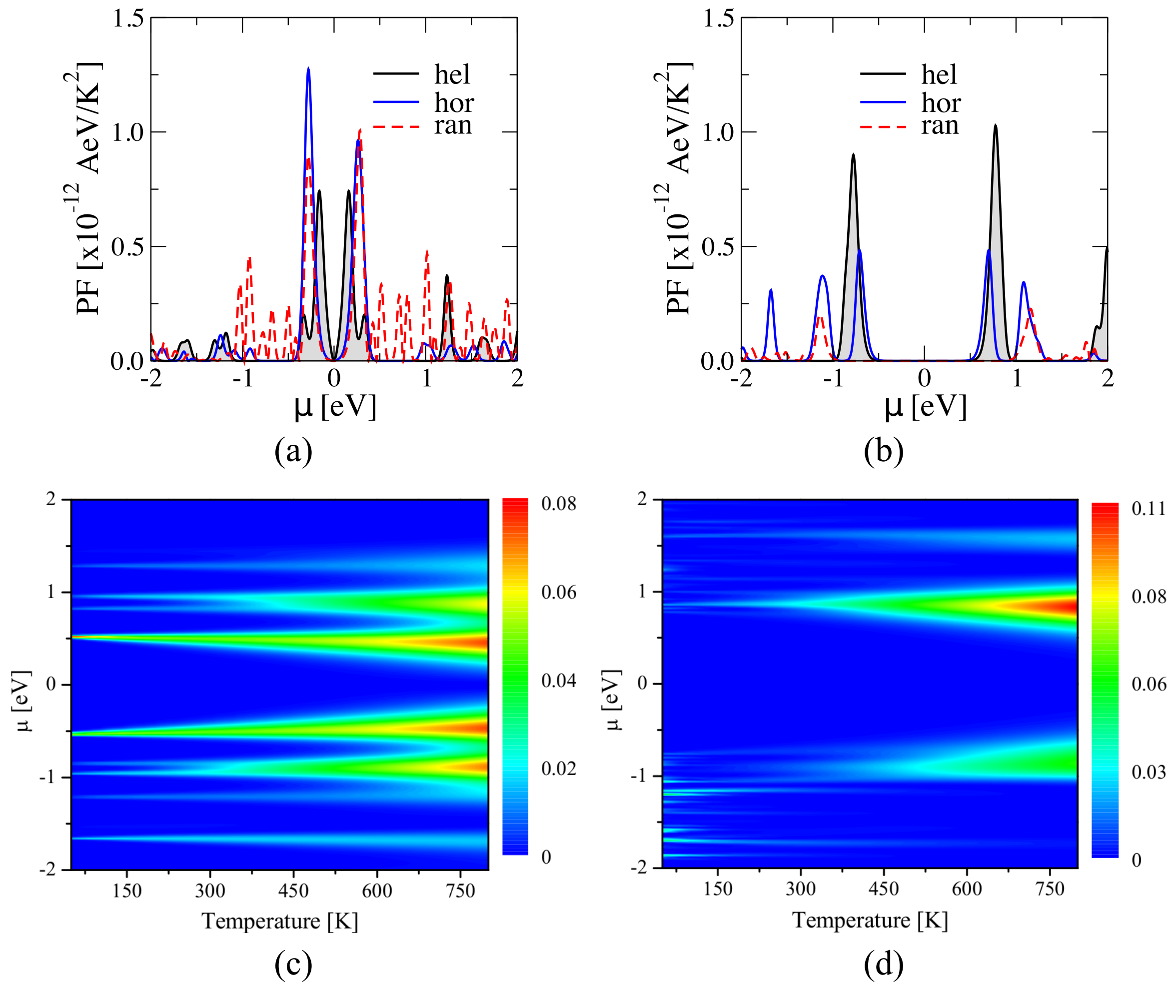


Figure S 7 Variation of the Power Factor (PF) as a function of the chemical potential for helical, horizontal, and random (6,6)-BNC heteronanotubes with a BN concentration of (a) 16% ($c = 11\%$ for helical case) and (b) 66%. Figure of merit ZT as a function of the temperature and chemical potential μ for (6,6)-BNC heteronanotubes with (c) horizontal and (d) random doping distribution at $c = 50$ %.

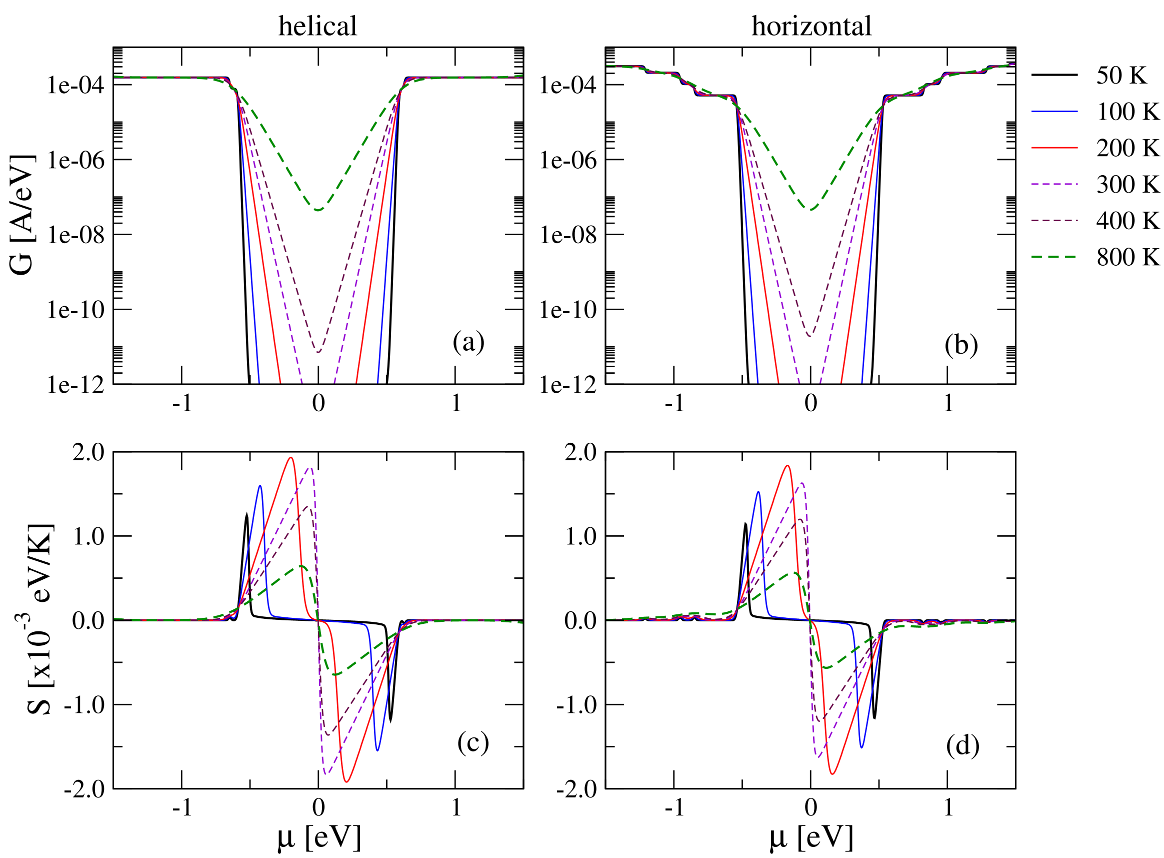


Figure S 8 Temperature dependence of the (a,b) electrical conductance G and the (c,d) Seebeck coefficient S for (6,6)-BNC heteronanotubes at a doping concentration of 50 %. We show the results for helical and horizontal doping distributions.

4 CNT - helical BNCNT - CNT system

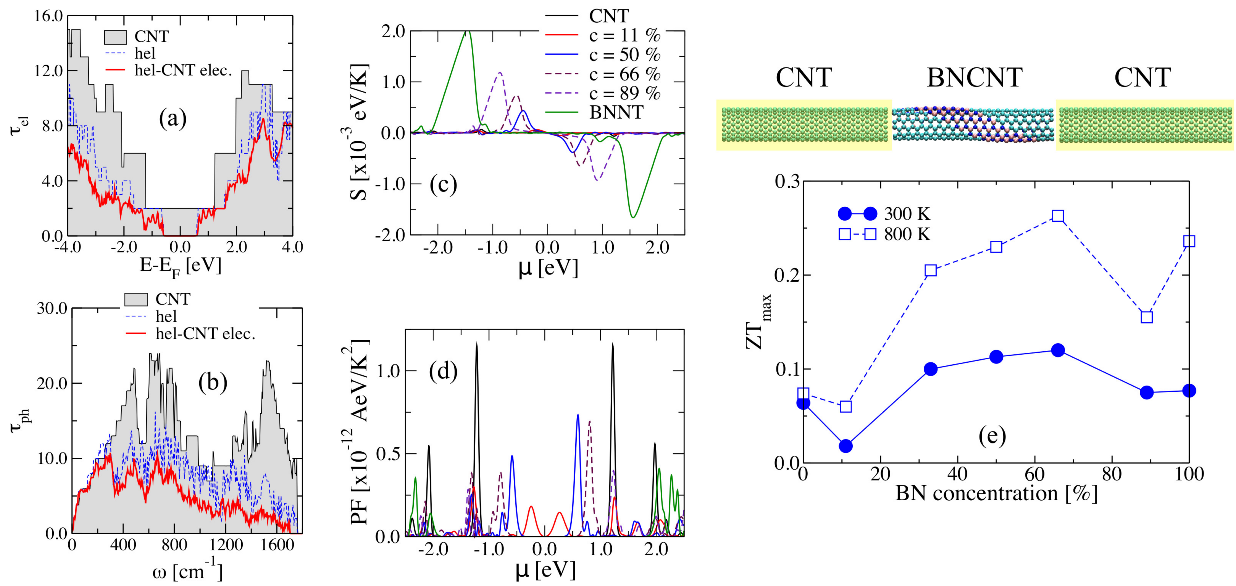


Figure S 9 (a) electron and (b) phonon transmission functions for the two cases of helical (6,6)-BNC heteronanotubes. We compare the results to the corresponding functions for (6,6)-CNT. BN concentration dependence of (c) Seebeck coefficient and (d) Power Factor for helical (6,6)-BNCNTs connected to (6,6)-CNT electrodes. (e) Variation of the Figure of merit as a function of the BN concentration for CNT-helical BNCNT - CNT system at 300 K and 800 K.