ELECTRONIC SUPPLEMENTARY INFORMATION

Doping engineering of thermoelectric transport in BNC heteronanotubes

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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

\[ M = \int |\tau_d(E > E_F) - \tau_d(E < E_F)|dE, \]

with \( \tau_d \) 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.
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

\[
\eta(\omega) = \frac{i(G' - G'')\omega}{\pi L}.
\]

(1)

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

\[
R_{DOS} = \frac{\eta_X(\omega)}{\eta_{Total}(\omega)}
\]

(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 $\mu$ 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.