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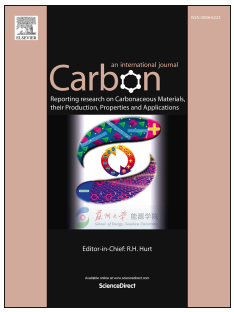

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Effects of pressure on the structural and electronic properties of linear carbon chains encapsulated in double wall carbon nanotubes

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Abstract

High-pressure resonance Raman experiments were performed on linear carbon chains Cn confined in double-wall carbon nanotubes (Cn@DWCNT). Our results indicate that the frequency of the chain mode undergoes a non-linear decreasing as pressure increases, in agreement with previous studies of the behavior of carbon chains into multi-wall carbon nanotubes. After the pressure cycle, the Cn modes present an irreversible frequency downshift together with an irreversible upshift (downshift) of the RBM modes (G^+ band) of the inner tube. These spectral changes are interpreted as evidence of cross-linking between the carbon chain and the wall of the inner tube. Density functional theory (DFT) calculations were performed in order to shed light on the interpretation of the experimental data. The theoretical calculations show a pressure-induced charge transfer from the nanotube to the carbon chain, thus resulting in an increasing of the C≡C bond length, and consequently, a softening frequency of the Cn Raman mode. Furthermore, an irreversible cross-linking between the tube and Cn is

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