Raman spectroscopy of defects C_{60} peapod: theoretical study

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Single walled carbon nanotubes (SWCNT) can encapsulate small and large molecules, including fullerenes [1-4]. C_{60} peapods consist of SWCNT in which C_{60} fullerene molecules are inserted. This hybrid system between C_{60} fullerene and SWCNT have generated a lot of interest for future electronic applications. Carbon peapods have been proposed as possible candidates for novel nanometer scale devices and many efforts led to the synthesis of high-quality 1D fullerene crystals inside SWCNTs [1, 4]. Due to their original one-dimensional nanosized structure and their tunable electronic properties, peapods have several potential applications as high temperature superconductors [5], memory elements [6] and nanometer-sized containers for chemical reactions [3].

In contrast to theoretical considerations, the experimental verifications of the CNTs strength or Young's modulus demonstrate evidently discrepancies that may reach even up to 30% [7]. Structural defects in nanotubes have been identified by STM and HRTEM imaging [8, 9]. Possible single or multiple defects in CNTs provide an explanation for the extant theoretical experimental differences.

The purpose of the current study is to investigate the effect of C_{60} fullerene confined inside defective carbon nanotubes on vibrational properties of peapod, in this aim we use a spectral moment method together with a bond polarizability model. Essentially, the vibrational properties are closely coupled with the atomic structure of the system. The evolution of the Raman spectrum as a function of the spatial arrangement of defects in carbon nanotubes is discussed. The changes of the Raman spectrum as a function of the filling factor is identified.

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