Tubular fullerenes inside carbon nanotubes: optimal molecular orientation versus tube radius

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Fullerene nanopeapods — carbon nanotubes (CNTs) filled with fullerene molecules — are one of the best-known exponents of materials exhibiting one-dimensional (1D) molecular confinement. The first reported instance of nanopeapods was the observation of C_{60} molecules encapsulated in single-walled CNTs (SWCNTs) [1]. The cylindrical hollow space offered by SWCNTs (the diameter of which can be as small as 4.3 Å [2]) has proven to be a unique environment for studying both experimentally and theoretically the physics and chemistry of 1D arrangements of atoms and molecules [3]. In this work, we focus on the encapsulation of molecules of the family of tubular fullerenes C_{90}, …, C_{200} and investigate their positions and orientations in the CNT [4]. We find that increasing the tube radius leads to the following succession of energetically stable regimes: (1) lying molecules positioned on the tube's long axis; (2) tilted molecules on the tube's long axis; and (3) lying molecules shifted away from the tube's long axis. As opposed to C_{70} and C_{80} molecules encapsulated in a SWCNT [5], standing orientations do not develop. Our results are relevant for the possible application of molecular-orientation-dependent electronic properties of fullerene nanopeapods [6], and also for the interpretation of future experiments on double-walled carbon nanotube formation by annealing fullerene peapod systems.

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