A Monte Carlo study of C_{70} molecular motion in C_{70}@SWCNT peapods

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Since their discovery more than a decade ago, fullerene nanopeapods — single-walled carbon nanotubes (SWCNTs) filled with fullerenes — have been the subject of extensive experimental and theoretical research, and have paved the way for a new direction in the field of one-dimensionally confined systems. C_{60}@SWCNT peapods were discovered first [1], but various other fullerenes have been inserted in nanotubes as well, e.g. C_{70} [2]. We present Monte Carlo simulations of chains of C_{70} molecules in a SWCNT. For various tube radii R (6.5 Å $\leq R \leq$ 7.5 Å), we analyze rotational and translational motion of the C_{70} molecules as a function of temperature. We not only reproduce the experimentally well-established lying and standing molecular orientations for small and large tube radii [2], respectively, but we also observe a variety of molecular motions, including orientational flipping of lying molecules and the migration of molecules resulting in a continual rearrangement of the C_{70} molecules in clusters of varying lengths. An analysis of the pair correlation functions reveals a transition from a linear harmonic chain to a hard-sphere liquid with increasing temperature, making C_{70}-peapods tunable physical realizations of two well-known one-dimensional model systems [3]. Our results are in agreement with recent X-ray diffraction experiments [4] and are relevant for possible applications using the dependence of a nanopeapod's electronic properties on the molecules' orientations [5].

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