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Molecular ordering in C_{70}@CNT nanopeapods. B. Verberck[a,b], J. Cambedouzou[b], G. Vliegenthart[c], G. Gompper[d], P. Launois[b]. [a]*Departement Fysica, Universiteit Antwerpen, Belgium.* [b]*Laboratoire de Physique des Solides, Université Paris-Sud, France.* [c]*Institute for Advanced Simulation, Forschungszentrum Jülich, Germany.* [d]*Institut für Festkörperforschung, Forschungszentrum Jülich, Germany.*
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The successful insertion of fullerene molecules in carbon nanotubes (CNTs) has opened a new direction in the field of one-dimensionally confined systems. Because of their ellipsoidal shape, C_{70} molecules encapsulated in a CNT adopt lying, tilted, or standing orientations depending on the tube's radius. In addition to the molecule-tube interaction, intermolecular interactions determine the structural and dynamical properties of chains of C_{70} molecules confined in a CNT. Recently, the effect of heating the C_{70}@CNT system—resulting in the coalescence of the molecules into an internal CNT—has been investigated in detail by means of X-ray diffraction [1]. A change in rotational behavior of the molecules prior to coalescence has been inferred from the X-ray diffractograms.

We present Monte Carlo simulations of C_{70}@CNT systems supporting the experimental results and providing insight into the molecular orientations and rotations for varying temperature. In particular, we observe the transition from lying to standing molecular orientations for increasing tube radius. Also, molecular flipping and a temperature-dependent rotational mobility are found. In addition, we address the question of translational motion of the molecules inside the nanotube and predict temperatures above which migration of molecules between adjacent clusters can take place.

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Probing intermolecular interactions in 2-chloro-4-nitrobenzoic acid and nicotinamide. Catharine Esterhuysen. *Department of Chemistry and Polymer Science, University of Stellenbosch, Private Bag X1, Matieland, Stellenbosch, 7602, South Africa.*
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2-chloro-4-nitrobenzoic acid has been found to crystallise in two different polymorphs [1], as well as in a co-crystal with nicotinamide [2]. The intermolecular interactions involved in the two polymorphs have been analysed using Hirshfeld surfaces [3], however the significance of each of the

interactions with respect to the stabilisation that they provide to the crystal structures of the two polymorphs has not been studied. In this paper the different intermolecular interactions undergone by 2-chloro-4-nitrobenzoic acid and nicotinamide are investigated by comparing the results of density functional theory (DFT) calculations with experimental results interpreted through Hirshfeld fingerprint plots. Specific intermolecular interactions are indicated by structural features such as spikes within the Hirshfeld fingerprint plots. The positions of these spikes within the fingerprint plots can be correlated to the strength of the interactions calculated for pairs of molecules using DFT methods. A comparison of nicotinamide-containing crystal structures from literature [4] shows a clear correlation between interaction strength and spike position.

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