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Light emitting peapods: A first-principles study MATUS MILKO, TAYEBEH MOVLAROOY, CLAUDIA AMBROSCH-DRAXL, Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — Nanohybrids i. e. single wall carbon nanotubes with encapsulated organic molecules have been proposed for opto-electronic devices as they combine the unique mechanical and electronic properties of nanotubes with the desired optical properties of π-conjugated molecules. We investigate structural, cohesive and optical properties of these hybrid systems using density functional theory. Including the contributions for the non-local dispersive interactions, we examine in a systematic manner the effect of tube diameter and chirality on the stability and bonding characteristics of the peapod as well as the position of the molecule inside the tube. We find that these systems are almost exclusively van-der-Waals bound. Based on a series of oligo-thiophenes encapsulated into zig-zag nanotubes, we explore how the presence of the molecules inside the cavity can alter the electronic and optical properties. In particular, we inspect new features in the dielectric and loss functions due to transitions between the states of the molecule and the nanotube.

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