The Formation of Novel Crystal Structures in Carbon Nanotubes.

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Atomistic computer simulation models are used to understand the filling of carbon nanotubes by ionic materials. The validity of the models are assessed by reference to high resolution transmission electron microscopy (HRTEM) experiments. The liquids are found to fill narrow width nanotubes to form low dimensional crystallites which display specific distortions in comparison with the idealized bulk fragments. The atomistic origin of the observed distortions are discussed for liquid KI. Molecular dynamics simulation models are then developed to study directly the filling and lead to an understanding of the filling mechanisms. The dependence of the filling structure on the pore radius and morphology of the carbon nanotube is discussed and an effective phase diagram as a function of pore size is produced. Crystal structures incorporating specific twist motifs, which are unique to these low-dimensional confining environments, are predicted. The physical origins of the observed filling mechanisms are discussed. A model wurtzite-forming bulk crystal system is shown to fill the tubes to form alternative structures which represent a potentially new class of tubular structures for these systems. Materials which vary in stoichiometry are inserted and found to lead to crystallite structures with no clear bulk analogues.