Formation of diamond nanowires inside carbon nanotubes: An *ab initio* study

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We investigate the possibility of templated growth of diamond nanowires from functionalized diamondoid molecules enclosed in a carbon nanotube (CNT). Our *ab initio* density functional theory studies identify suitable candidate molecules and conditions, under which such molecules may fuse to narrow diamond nanowires with C_8H_8 or C_7H_8 unit cells inside a CNT. We find that the unique environment inside a narrow carbon nanotube, which can be suitably represented by a cylindrical potential, subjects enclosed molecules to a high pressure, caused by a "capillary" force. The surrounding narrow nanotube orients the enclosed molecules in a suitable way favoring fusion within the constraining volume. Our calculations indicate that $C_{10}H_{16}$ adamantane molecules do not fuse to diamond nanowires in a reaction that requires additional energy, but rather convert to carbon chains [1]. On the other hand, $C_{14}H_{18}(COOH)_2$ diamantane di-acid molecules may fuse in an exothermic reaction to $-C_8H_8-$ diamond nanowires in hydrogen atmosphere [2]. Our canonical molecular dynamics calculations at elevated temperatures indicate likely intermediate products that occur during these reactions and agree with experimental observations [1,2].

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