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 C₈H₈ or C₇H₈ 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 C₁₀H₁₆ 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, C₁₄H₁₆(COOH)₂ diamantane di-acid molecules may fuse in an exothermic reaction to −C₈H₈-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].

* Supported by the National Science Foundation Cooperative Agreement No. EEC-0832785, titled “NSEC: Center for High-rate Nanomanufacturing”. Email of the corresponding author: zhuzhen@msu.edu