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**Can diamond nanowires grow inside carbon nanotubes?**[1] ZHEN ZHU, DAVID TOMÁNEK, Michigan State University, YANQUAN FENG, Beijing Institute of Technology — 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 "capillary" forces, and orients them in a suitable way favoring fusion and constraining the resulting structure. Based on total energy calculations, we find that fusion of $C_{10}H_{16}$ adamantane molecules requires additional energy, whereas fusion of $C_{14}H_{18}(COOH)_2$ diamantane di-acid molecules in hydrogen atmosphere occurs as an exothermic reaction. Our canonical molecular dynamics calculations at elevated temperatures indicate likely intermediate products occurring during this reaction.

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