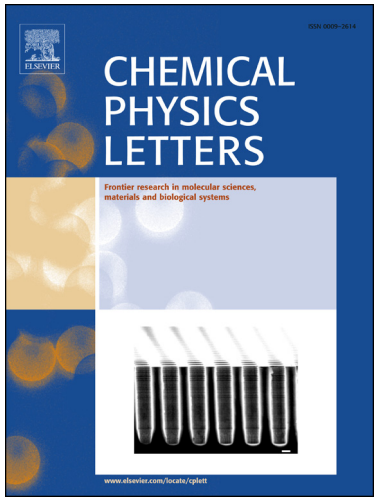

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The structural and Electronic properties of (10,0) zigzag Single-Wall Carbon Nanotubes Modified by Thiophene groups

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Abstract

In this work, modifications of (10, 0) functionalized zigzag Single-Wall Carbon Nanotubes in different sites by thiophene groups were studied using density functional theory. Geometric structures and electronic properties were investigated. After modification a significant change was observed in band structure and density of states and metallic properties were obtained. The best result for application in organic photovoltaic cells was achieved when two organic groups were placed on opposite sides of the wall of the SWCNT symmetrically.

Keywords: Single Wall Carbon Nanotubes; Density functional theory; Band structure; Density of state; Thiophene group; Organic photovoltaic cell

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