

Cubane oligomers: A density functional theory study

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Abstract

The cubane molecule, and a few representative oligomers built with cubane units, are examined in order to investigate the feasibility and likelihood of creating covalently bonded arrays with cubane units as building blocks. In this way, oligomers with a variety of structures were obtained, including rods and surface-like networks. B3LYP/6-311G** calculations indicate that, in the bulk limit, the cubane structures do not accept electrons. The electron transfer within the cubane network may occur only through doping or substitution with donor/acceptor groups.