

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A Density Functional Theory Study of Chain-like Structures Derived from Graphite Nanoflakes BRAHIM AKDIM, RUTH PACHTER, Air Force Research Lab, Ohio — Recently, chain-like structures of about 2 nm in lengths were fabricated from graphite nanoflakes by controlled electron beam irradiation in a 3 stage process [C. Jin, et al. PRL, 102, 205501 (2009)], opening up possibilities for designing all-carbon nano-electronic devices, with sp -hybridized carbon atomic chains as the conducting channel, bridged by the sp^2 -hybridized graphene leads. Although formation, migration and breakage in the material has been addressed theoretically by Jin et al., effects of chain length and chain orientation have not been explored thus far. In this work, we report on the electronic and mechanical properties of chain-like structures bridged between the two-dimensional sheets, to further understanding of the material's behavior.

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Date submitted: 25 Nov 2009

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