

Abstract Submitted
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Formation **of**
Atomic Carbon Chains from Graphene Nanoribbons¹ RENATO PONTES,
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dade de São Paulo — The formation of one-dimensional carbon chains from graphene
nanoribbons is investigated using spin-polarized ab initio dynamics. We show un-
der what conditions it is possible to obtain a linear atomic chain via pulling of the
graphene nanoribbons. The presence of dimers composed of two-coordinated carbon
atoms at the edge of the ribbons is necessary for the formation of the linear chains,
otherwise there is simply the full rupture of the structure. For a situation where a
linear carbon chain is formed, when a force of 8 nN is reached there is a rupture
of the chain. The presence of Stone-Wales defects close to these dimers may lead to
the formation of longer chains. The local atomic configuration of the suspended
atoms indicates the formation of single and triple bonds, which is a characteristic of
polyynes.

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