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Switching Behavior of Carbon Chains Bridging Graphene Nanoribbons: Effects of Uniaxial Strain BRAHIM AKDIM, RUTH PACHTER, Air Force Research Lab — Recently, several experiments [1,2] demonstrated the stability of chain-like carbon nanowires bridged between graphene nanoribbons, paving the way for potential applications in nano-devices. On the basis of density functional tight-binding calculations, we demonstrated switching for chains terminated with a five-membered ring under an applied strain, serving as a model for morphological changes in realistic materials. Electron transport calculations showed an increase of up to 100% in the output current, achieved at a reverse bias-voltage of 2V and an applied strain of just 1.5%. Structural analysis suggested that the switching is driven by conformational changes, in our case triggered by the formation and annihilation of a five-membered ring at the interface of the chain-graphene edge. In addition, we showed that a five-membered ring can easily be formed at the interface under a source-drain bias or through a gate voltage. This mechanism can serve as an explanation of experimentally observed conductance for the materials.

[1] Jin, C.; Lan, H.; Peng, L; Suenaga, K.; Iijima S. *Phys. Rev. Lett.* **2009**, 102, 205501.
[2] Chuvilin, A.; Meyer, J. C.; Algara-Siller, G.; Kaiser, U. *New J. Phys.* **2009**, 11, 083019

Brahim Akdim
Air Force Research Lab

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