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Gapping by Twisting: Analysis of the Band-Gap Variations in Rippled Carbon Nanotubes TRAIAN DUMITRICA, DONG-BO ZHANG, University of Minnesota — Recent experimental and theoretical [1] developments represent an opportunity to further our understanding on the carbon nanotubes electronic response in rippled morphologies. The mechanisms effective in collapsed nanotubes are not sufficient to explain the band-gap changes in rippled states. In this talk we uncover the important role played by the inhomogenous shear strain present in the nanotubes wall, a mechanisms that was not considered before. Relying on objective molecular dynamics combined with density-functional-based tight-binding, and introducing the concept of effective strain, we are able to delineate the physical mechanisms responsible for the band-gap variations and formulate a perturbative model in terms of the shear stress located at the ridges. This approach offers a clear interpretation such that the previous observations can be convincingly explained. We first focus on an isolated wall and later study the consequences of the gradual presence of inner walls, until the idealized behavior is regained. The galore of band-gap variations with the applied strain encuntered in the intermediate behavior has clear experimental implications. It suggests that some caution should be taken when interpreting the conductivity measurements carried out in nanotube-pedal devices. [1] D.B. Zhang, R.D. James, and T. Dumitrica, "Electromechanical Characterization of Carbon Nanotubes in Torsion via Symmetry-Adapted Tight-Binding Objective Molecular Dynamics," Physical Review B 80, 115418 (2009).

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