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**DFT properties of Quasi-One-Dimensional Nanostructured Materials**[1] JOHN MINTMIRE, Oklahoma State University, JUNWEN LI, University of Pennsylvania, DANIEL GUNLYCKE, CARTER WHITE, US Naval Research Laboratory — Over the past several years we have made substantial progress in developing an approach for density-functional electronic structure calculations on quasi-one-dimensional nanostructures with helical symmetry. In this talk we discuss the application of these first-principles methods using Gaussian basis sets for calculating the electronic band structure of periodic graphitic nanostructures such as carbon nanotubes and graphene nanoribbons In particular we discuss how chemical effects at the edges of saturated graphene nanoribbons can cause ribbons to twist and form three-dimensional helical structures. Our calculations show that F-terminated armchair ribbons twist into helices, unlike flat H-terminated strips. Twisting ribbons of either termination couple the conduction and valence bands, resulting in band gap modulation.

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