Electronic and transport properties of graphitic nanostructures

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In this poster we discuss the use of first-principles density function theory (DFT) methods using Gaussian basis sets for calculating the electronic band structure of periodic graphitic nanostructures such as carbon nanotubes and graphene nanoribbons. We use the one-electron wavefunctions as inputs to effective principal layer electron transport calculations for systems with localized defects, including periodic, helical nanostructures. We present results for single-wall carbon nanotubes and graphene nanoribbons, as well as for inorganic silicon nanowires. We also 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. This work was supported at OSU by the US DOE and at NRL by the US ONR.