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A twist on graphene nanoribbons[1] JOHN MINTMIRE, JUNWEN LI, Oklahoma State University, DANIEL GUNLYCKE, CARTER WHITE, Naval Research Laboratory — Although two-dimensional graphene might exhibit some microscopic structure, viewed macroscopically it is essentially flat. In contrast, many one-dimensional materials are helical in nature. Because of the strong sp^2 bonds in graphene nanoribbons, these ribbons are generally assumed to be flat like graphene. In this presentation, first-principles calculations on graphene nanoribbons are presented that suggest that narrow ribbons could in fact be helical depending on size and edge species. Twisting nanoribbons is also shown to affect the electronic properties near the Fermi level. If the twist is large enough, our calculations show that it might even be possible to reduce the semiconducting band gap to well below room temperature, effectively making the ribbons metallic.

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