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Ab initio electronic structure and transport studies of N_2^{AA}-doped armchair and zigzag graphene nanoribbons JONATHAN OWENS, Rensselaer Polytechnic Institute, EDUARDO CRUZ-SILVA, University of Massachusetts Amherst, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Recent work by Lu, et al. (Nature Scientific Reports, DOI: 10.1038) on large sheets of nitrogen-doped graphene, determined that a highly predominant amount of nitrogen dopants (80 %) form in pairs on the same sub-lattice. Graphene nanoribbons, which are essentially narrow strips of graphene, have a natural band gap and tunable electronic properties, making them a promising candidate for scalable nanoelectronics. In this work we explore various electronic structural (density of states, local density of states, and STM images) and transport properties of armchair (aGNR) and zigzag (zGNR) graphene nanoribbons under different orientations of the N_2^{AA} dopants with respect to the ribbon growth direction. For all configurations of zGNRs and aGNRs, we see a substantial decrease in conductance due the dopants, as well as spatially localized states opening around the dopant sites. Most notably, however, we observe the emergence of a new stable spin configuration, wherein the spin-up spin-down polarizations of the edges in zGNRs (denoted the antiferromagnetic state) flip near the doping sites, while being in the normal zGNR AFM ground state away from the dopants.

Jonathan Owens
Rensselaer Polytechnic Institute

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