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NEW DEFECTS IN GRAPHENE NANORIBBONS

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Graphene, one-atom thick sheet of carbon atoms arranged in hexagonal rings, has become the hottest new material in physics and nanotechnology due to its exotic properties. In particular, graphene can be patterned with various experimental methods to give graphene nanoribbon (GNR). The electronic properties of these new quasi-one dimensional materials depend on the ribbon width and edge geometry zigzag or armchair. Especially, the zigzag GNR (ZGNR) is predicted to exhibit interesting electronic properties very required for future nanoscale devices. It is usually subjected to various types of defect in the atomic structure like adatoms, vacancies, doping and geometric defects. The introduction of Stone-Wales defect, obtained by a 90^0 rotation of a C-C bond, replacing four hexagons into two pentagons and two heptagonal, shows an electronic transition from half-metallicity to semiconductor. Using DFT calculations, we model new defects and we exploit their effects on the electronic properties of GNR to make novel nanoelectronic devices.