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Tuneable Electronic and Magnetic Properties of Hybrid Silicene/Silicane Nanoribbons Induced by Nitrogen Doping

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Abstract

The geometric, electronic and magnetic properties of N-doped zigzag and armchair silicene/silicane nanoribbons (Z- and A-SSNRs) have been studied by using density functional theory calculations, where silicane is the fully hydrogenated silicene. It is confirmed that the substitution of N for Si atom is preferred at the silicene/silicane interface and silicane edge. The large hydrogen diffusion energy barriers indicate high interface stability of the N-doped SSNRs. When the doping concentration is larger than a critical value, the doped Z-SSNR with N at silicene/silicane interface shows ferromagnetic semiconducting character with a magnetic moment of about 1 μB, while the doped Z-SSNR with N at silicane edge shows metallic character and tuneable magnetic moments dependent on the silicane width. For armchair SSNR, the A-SSNR with doping N at silicene/silicane interface is a semiconductor with a local magnetic moment of about 1 μB. However, the A-SSNR with doping N at silicane edge shows nonmagnetic metallic state. In addition, the Z- and A-SSNRs with doping N at silicene/silicane interface exhibit decreased band gaps and oscillatory band gaps, respectively, with increasing silicene width. This work provides fundamental insights for the applications of SSNRs in nanoelectronics

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