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Spontaneous Boron-doping of Graphene at Room Temperature LIDA PAN, Vanderbilt Univ, YANDE QUE, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, SOKRATES T. PANTELIDES, Vanderbilt Univ — Doping graphene with boron or nitrogen is an effective way to modify its electronic properties. However, the reaction barrier for introducing these impurities is quite high, making the doping process difficult. In this work, we propose a low-energy reaction route derived from first-principles calculations and subsequently validated by experiments. The calculations show that, when graphene is placed on a ruthenium substrate and exposed to atomic boron, boron atoms can incorporate substitutionally into the graphene sheet with an energy barrier about 0.1 eV, displacing carbon atoms below the graphene sheet where they migrates away. This result suggests that spontaneous doping by boron can take place at room temperature. Following the prediction, we grew high-quality graphene on the Ru(0001) surface and then expose it to B2H6 which decomposes into atomic boron. XPS and STM results indicate that boron dopes graphene substantially without disturbing the graphene lattice, confirming the theoretical predictions. Doping by nitrogen and co-doping by B and N will also be discussed.

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