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Doping a graphene sheet with impurities[1] CHIH-KAI YANG, Chang Gung University — It has been predicted theoretically and achieved experimentally that a graphene sheet can bond strongly with hydrogen atoms. The resulted hydrocarbon or graphane is a semiconductor with a large band gap around 3.5 eV. In the paper I discuss the density functional calculation that shows how the pristine graphene is attached to lithium, creating instead a metal. In the case of graphane, the calculation also predicts that defects and doping with transition-metal impurities can greatly enhance the conduction and generate high magnetic moments. These properties offer promising application of doped graphane as a nanoelectronic device.

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