Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Strong Enhancement of Doping in Graphene via Substrate BING HUANG, SU-HUAI WEI, National Renewable Energy Lab — Controlling the type and density of charge carriers by doping is the key step for developing graphene electronics. Based on first-principles calculations, we demonstrate that doping could be strongly enhanced in epitaxial graphene on silicon carbide (SiC) substrate. Compared to free- standing graphene, the formation energies of dopants decrease dramatically by $2 \sim 8$ eV. The dopants prefer to stay in the interface buffer layer between epitaxial graphene and substrate, which could tune the interface dipoles evidently. The type and density of charge carriers of epitaxial graphene layer can be effectively manipulated by suitable dopants and surface passivation. Contrasting to the direct doping of graphene, the charge carriers in epitaxial graphene layer are weakly scattered by dopants due to the spatial separation between dopants and conducting channel, in the spirit of modulation doping, which takes advantages in maintaining the high carrier mobility of graphene. Beyond controlling the charge carriers via buffer layer doping, we find that the reconstructed vacancy in the interface buffer layer breaks the spin symmetry of epitaxial graphene, which induces a half-metallic state without magnetic impurities doping.

Bing Huang
National Renewable Energy Lab

Date submitted: 16 Nov 2010 Electronic form version 1.4