Supplementary Materials

Density Functional Theory Calculations for
the Quantum Capacitance Performance of Graphene-Based Electrode Material

G.M. Yang[a,b], H. Z. Zhang[a], X.F. Fan[a,*], W.T. Zheng[a,*]

[a] College of Materials Science and Engineering, Key Laboratory of Automobile Materials of MOE and State Key Laboratory of Superhard Materials, College of Physics，Jilin University, Changchun 130012, People's Republic of China

[b]College of Physics, Changchun Normal University, Changchun 130032, People's Republic of China

*To whom correspondence should be addressed: E-mail: xffan@jlu.edu.cn (X.F. Fan); WTZheng@jlu.edu.cn (W. T. Zheng)

The electronic properties of defective graphene can be demonstrated obviously by the band structures near Fermi level. In Figure S1-S5, the band structures of graphene with different types of defects are shown.

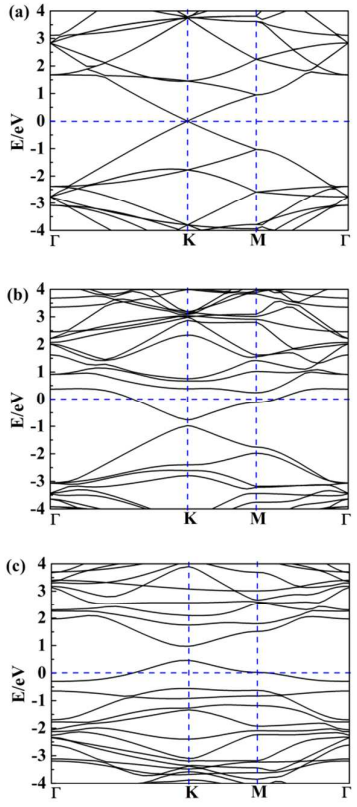

Figure S1. Band structures (corresponding to Figure 2) of (a) pristine graphene, (b) quanternary N-doped and (c) pyridine N-doped graphene. Note the results are obtained with the supercell 4×4.

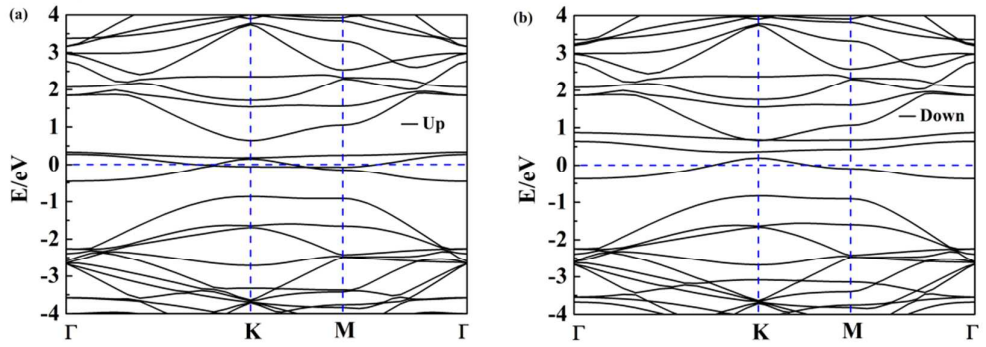

Figure S2. The spin-up (a) and spin-down (b) band structures of single-vacancy graphene (corresponding to Figure 4) with defect concentration of 3.1%, P(4×4).

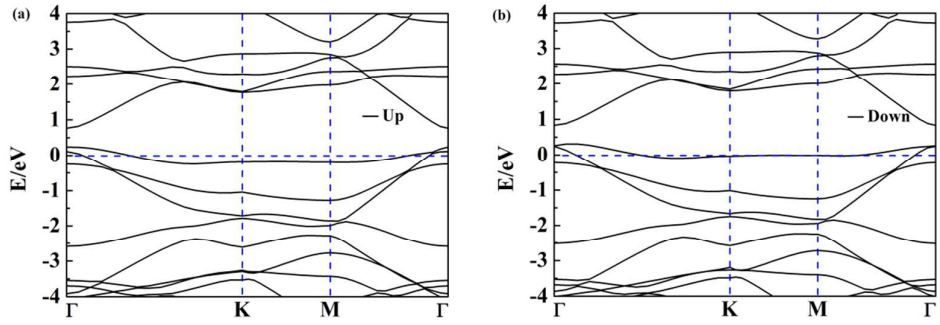

Figure S3. The spin-up (a) and spin-down (b) band structures of pyridine-N doped graphene (corresponding to figure 5) with N-doping concentration of 5.6%, P(3×3).

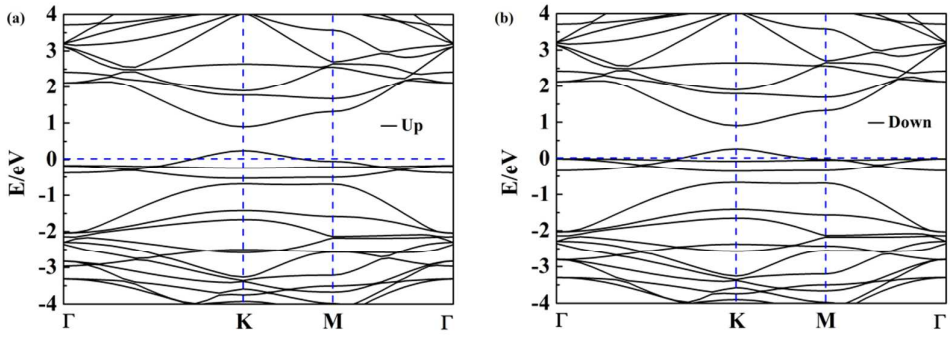

Figure S4. The spin-up (a) and spin-down (b) band structures of N-doped graphene by single vacancy with three N (corresponding to Figure 6) for N-doping concentration of 9.4%, P(4×4).

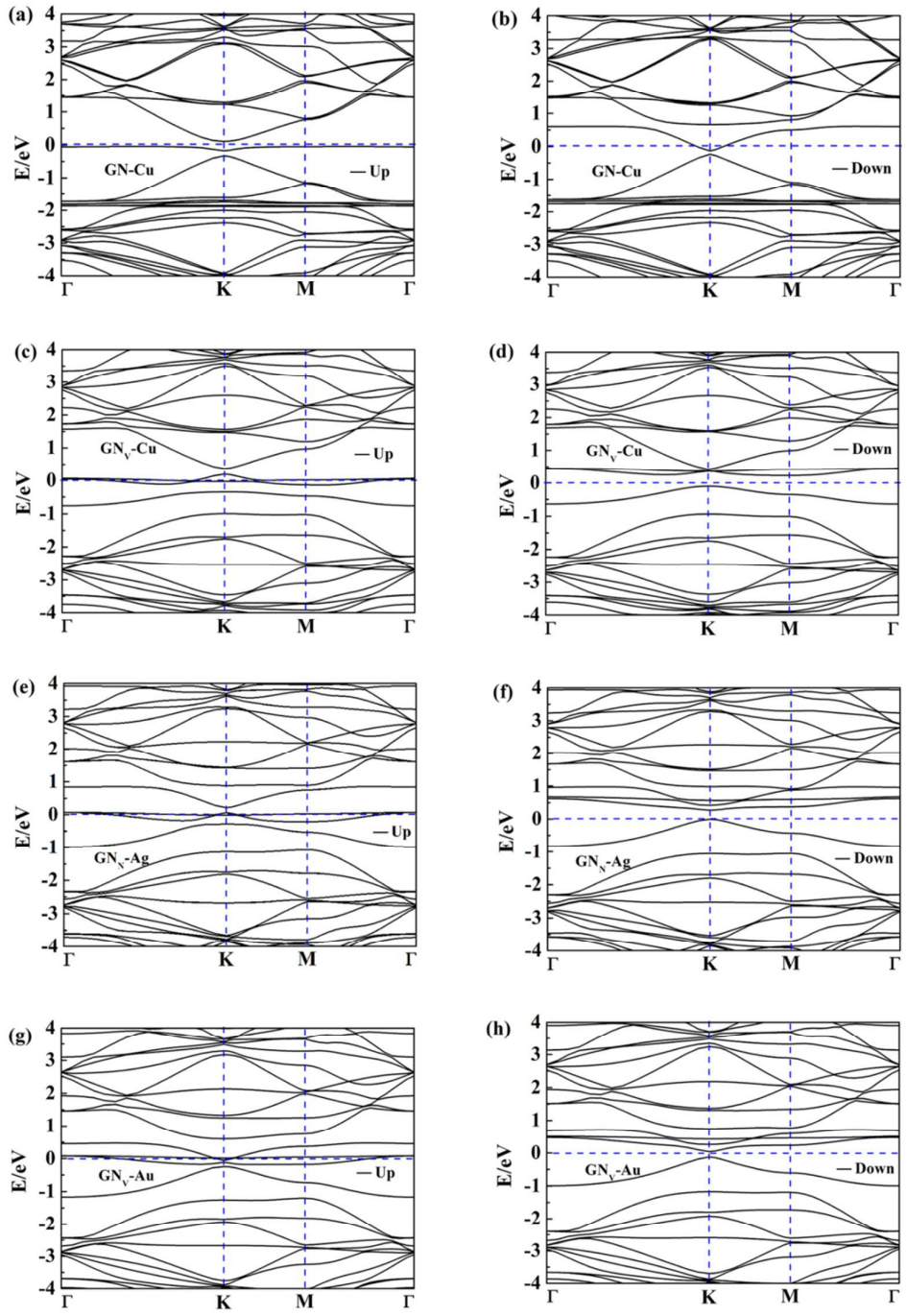

Figure S5. The spin-up and spin-down band structures of pristine graphene with adsorbed Cu atom (a, b), single-vacancy graphene with adsorbed Cu (c, d), Ag (e, f) and Au (g, h) atoms (corresponding to Figure 7). Note the results are obtained with the supercell 4×4.