Supporting Information

Possible Oxygen Reduction Reactions for Graphene Edges from First Principles

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Figure S1 shows the local density of states (LDOS) for the three kinds of binary-doped GNRs we considered. Compared to LDOS for N_{edge-1}-doped graphene shown in Figure 8 of ref 1, the density of π (i.e., p_z) states is significantly reduced (enhanced) just below (above) the Fermi level at C1 site in all the binary-doped GNRs, which is able to adsorb O_2 molecules with the activation barrier of $\sim$0.3 eV.

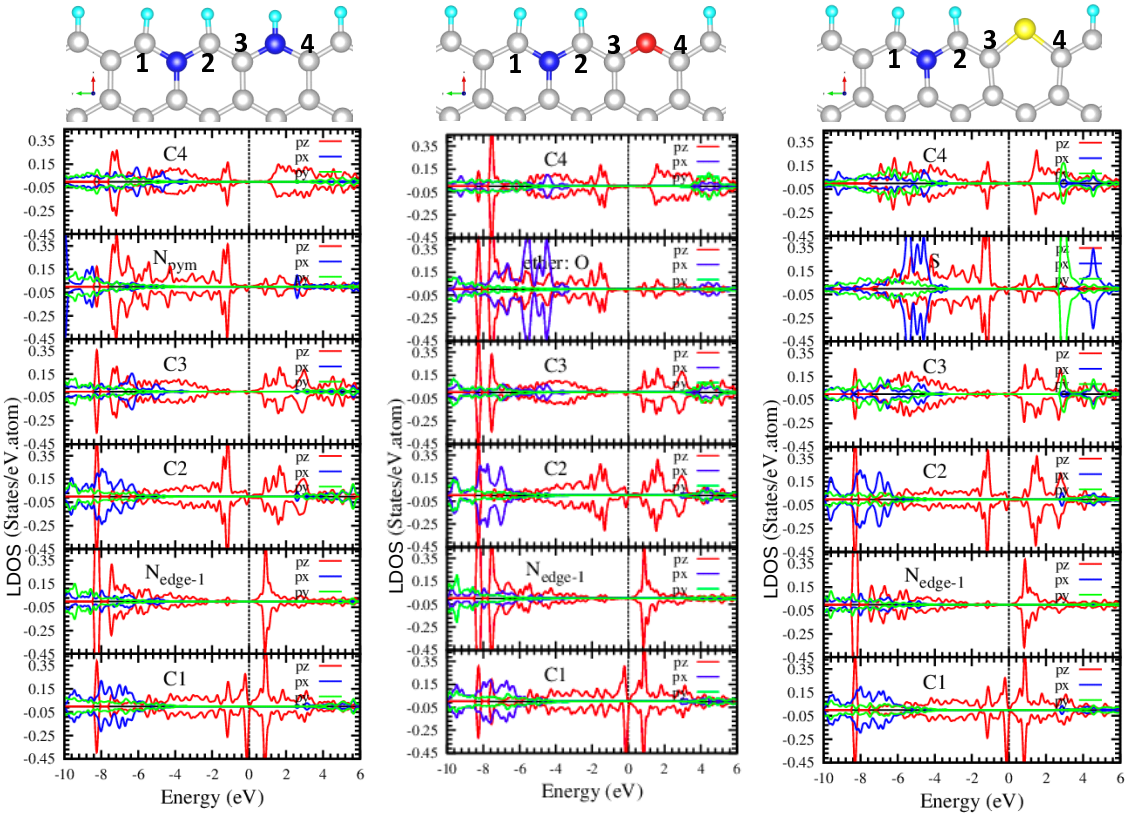

Figure S1: LDOS for p orbitals of dopants and their neighboring C atoms for GNR co-doped with pyridiniumlike N (left), pyranlike O (middle), and thiopyranlike S (right) along with N_{edge-1}. Atom colors are cyan for H, gray for C, red for O, blue for N, and yellow for S.

References

(1) Huang, S.-F.; Terakura, K.; Ozaki, T.; Ikeda, T.; Boero, M.; Oshima, M.; Ozaki, J.; Miyata, S. First-principles calculation of the electronic properties of graphene clusters doped with nitrogen and boron: Analysis of catalytic activity for the oxygen reduction reaction. *Phys. Rev. B* **2009**, *80*, 235410.