Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Diffusion and Self-alignment of Atomic Oxygens on the Graphene Surfaces: First Principles Calculations TAKAZUMI KAWAI, YOSHIYUKI MIYAMOTO, Nano Electronics Labs., NEC Corp. — Graphene is attracting much attention for the application of nano-devices due to its interesting electronic properties, and its robustness. For the device applications, it is very important to know the behaviors of atmospheric molecules such as adsorption, diffusion, and desorption on the graphene surface since the reaction with such chemicals cause the significant change in the electronic properties at Fermi level and even break the sp^2 network. Here, the oxygen is one of the most important impurities that we want to know and control the behavior. In this paper, we performed density function calculations for the diffusion of atomic oxygens on a graphene sheet in a periodic boundary condition. The results for a single atomic oxygen in our calculations are consistent with the previous works with cluster models. However, the favorable adsorption site for the next oxygen atom and diffusion barriers are completely different from them. The atomic oxygens prefer to align along armchair direction but not zigzag one. We will further discuss the stability and diffusion of the next oxygen atom on the other side of the graphene.

Takazumi Kawai
Nano Electronics Labs., NEC Corp.

Date submitted: 18 Nov 2008 Electronic form version 1.4