Molecular Penetration through the Basal Plane of Graphene, Density Functional Theory Study

Seung Mi Lee[1,*], Dinh Loc Duong[2], and Young Hee Lee[2]

[1] Korea Research Institute of Standards and Science Daejeon 305-340, Korea
[2] Sungkyunkwan Advanced Institute of Nanotechnology, Sungkyunkwan University, Suwon 440-746, Korea

The atomic and molecular diffusions through the basal plane of graphene have been theoretically investigated using density functional theory. We studied an H atom, an O atom, and an OH molecule for penetrating atom/molecule and the graphene with Stone-Wales (SW) defect for penetration surface. Functionalization of the SW defect widened the heptagonal area and deformed the graphene in basal direction as clearly shown in Figure 1. Penetration energy barriers were lowered by the functionalization of graphene defect. We systematically studied the functionalization effect on the penetration energy barriers according to the surface adatom/admolecules of H, O, and OH. Comparison to the experimental observations will be also presented.[1]

Reference

[1] D.L. Duong, G.H. Han, S.M. Lee, F. Gunes, E.S. Kim, S.T. Kim, H. Kim, Q.H. Ta, K.P. So, S.J. Yoon, S.J. Chae, Y.W. Jo, M.H. Park, S.H. Chae, S.C. Lim, J.Y. Choi, and Y.H. Lee, "Probing graphene grain boundaries with optical microscopy", Nature **490**, 235-239 (2012).

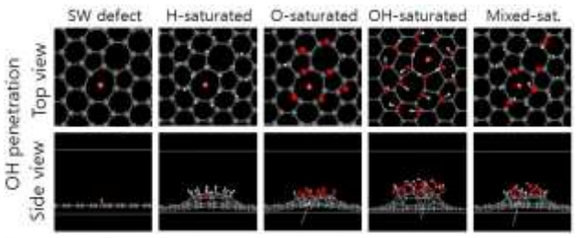

Figure 1. The atomic geometries of transition states for the penetration of OH molecule through the basal plane of graphene Stone-Wales defect by density functional theory calculations. [1]