First principles study of graphene edge properties on Cu(111): Implications for easy delamination

Kester Wong[1,2], 박노정[2,1], Christopher W. Bielawski[1,2], Rodney S. Ruoff[1,2], 곽상규[2,1,†]
[1]기초과학연구원; [2]울산과학기술대학교
(skkwak@unist.ac.kr[†])

CVD-grown graphene exfoliates relatively easily by the oxidation of the copper substrate, yet the inherent oxidation of the graphene-coated copper is conceptually fascinating and poorly understood. Here, we report the study of O_2 and H_2O adsorptions at the graphene/Cu(111) interface using *ab initio* calculations. We demonstrate that intercalation can occur at the interface, via oxidation (dissociative adsorption of oxygen) near the monolayer edge sites. Graphene/Cu(111) interface has a strong oxide formation tendency; lower activation barrier for O_2 and H_2O dissociation into surface oxygen and hydroxyls, respectively. Graphene adsorption energy on the oxidized surface was reduced by a factor of two (per C-atom). As rapid oxidation proceeds, molecular (H_2O or O_2) intercalation may also occur. We propose that O_2 dissociation at the graphene edges as the first step for Cu(111) oxidation, following by H_2O dissociation as the second step for the graphene delamination. While our results provide information on the decoupling of CVD-grown graphene, other important findings can also be extracted from the interaction between graphene edges and the metal surface.