Controlling desorption of H, O, atoms and OH group from graphene by pulse laser

YOSHIYUKI MIYAMOTO, Nanosystem Res. Ins., AIST, HONG ZHANG, College of Physical Science and Technology, Sichuan University — Possibilities of reduction of graphene oxide and one-side dehydrogenation of graphane (H-terminated graphene) with using ultra-short pulse (∼2 fs) laser are discussed. We have performed molecular dynamics (MD) simulation of O-, H-, and OH-adsorbed graphene sheets induced by electronic excitation upon irradiation with laser pulse. The time-dependent density functional theory treating real-time propagation of electron wave functions combined with the Ehrenfest approximation for the MD was employed and FPSEID [1] code was used to check the energy conservation rule under dynamical external field [2]. We found asymmetric pulse shape as a function of time causes an efficient desorption of O atoms and OH groups from graphene which can be applicable for reduction of graphene oxide alternative to chemical and thermal treatment. Meanwhile, such asymmetric pulse shape is beneficial for one-side H-desorption from graphane that will trigger further structural changes such as spontaneous shrink/rippling or heterogeneous termination on side-by-side.