

Abstract Submitted  
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**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 ( $\sim 2$  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.

[1]O. Sugino, Y. Miyamoto, PRB**59**, 2579, (1999);B**66**, 089901(E) (2002)

[2]Y. Miyamoto, H. Zhang, PRB**77**, 165123 (2008)

Yoshiyuki Miyamoto  
Nanosystem Res. Ins., AIST

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