Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

**Lithium Intercalation Induced Decoupling of Epitaxial Graphene on SiC(0001): Electronic Property and Dynamic Process** YUANCHANG LI, GANG ZHOU, Department of Physics, Tsinghua University, Beijing, JIA LI, Institute of Advanced Materials, Graduate School at Shenzhen,Tsinghua University, Shenzhen, JIAN WU, BING-LIN GU, WENHUI DUAN, Department of Physics, Tsinghua University, Beijing, CMT TEAM — This work presents first-principles investigations of the dynamic process of lithium (Li) penetration through the buffer layer on 6H-SiC(0001) surface, as well as the Li-insertion induced change of electronic structure. It is found that the penetration is kinetically forbidden for perfect buffer layer, because of the size confinement of its honeycomb structure. From the analysis of rate coefficient under the experimental conditions, topological defects no smaller than 8-membered ring are predicted to be essential for Li intercalation. Along with the Li insertion, the electronic property of the buffer layer is changed from n-type doping (Li-adsorption) to that of quasi-free-standing graphene (Li-intercalation). It is the electron injection by Li that results in the dissociation of the Si-C bonds and the decoupling of Li-intercalated buffer layer from the substrate. Moreover, we demonstrate the influence of such topological defects on the electronic property of epitaxial graphene, which provides some useful hints for understanding the observed gap and midgap state behavior.

Yuanchang Li
Department of Physics, Tsinghua University, Beijing

Date submitted: 01 Nov 2011 Electronic form version 1.4