Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Si diffusion on and between graphene sheets LEDE XIAN, M.Y. CHOU, School of Physics, Georgia Tech — The growth of epitaxial graphene (EG) on the SiC substrate is accompanied by the evaporation of Si atoms during the growth process. The continuing loss of Si atoms takes place even after the surface graphene sheets have been formed. This atomic transport is believed to be a key element in establishing a growth mechanism to model and control the process. Using density functional theory (DFT) calculations, we have studied the diffusion of Si atoms on a single layer of graphene and between graphene sheets. The potential energy surfaces are explored. For single-layer graphene, the diffusion barrier for Si is relatively low. While for multilayers, some buckling of graphene sheets will appear and the stacking pattern also plays a role. The connection with the growth process will be discussed.

Lede Xian
School of Physics, Georgia Tech

Date submitted: 20 Nov 2008 Electronic form version 1.4