Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Storing hydrogen in graphene layers with tunable interlayer spacing[1] YANG LEI, Queen Mary, University of London, WENGUANG ZHU, Harvard University, YAN SONG, Queen Mary, University of London, ENGE WANG, Institute of Physics, CAS, ZHENYU ZHANG, University of Tennessee & ORNL, ZHENGXIAO GUO, Queen Mary, University of London — Carbon nanostructures are being studied for hydrogen storage. However the nature of H-C interactions in such structures is unclear. We use first-principles simulation to model H adsorption between graphene layers. The adsorption of H_2 between layers is evaluated, particularly with respect to inter-layer variation thus simulating the effect of stressing the graphite for H storage. We note that H_2 dissociates when the inter-graphene distance is reduced (the graphite is compressed). When the ratio of H:C=1:1, the graphene changes from a planar to a diamond-like structure. The H-C interaction changes from weak physisorption to strong chemisorption. When the pressure is reduced, H atoms can recombine to form H_2 by overcoming a small energy barrier. Based on this work, we propose a new scheme for H storage in C nanostructures: by way of altering the inter-graphene distance, the C structure can effectively "inhale," store and release hydrogen in a controlled manner.

[1]Supported by USNSF, UCDOE, & EPSRC/UK-SHEC.

Yang Lei
Queen Mary, University of London

Date submitted: 21 Dec 2005 Electronic form version 1.4