Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Recombination pathways for atomic hydrogen on the graphite (0001) and single-wall carbon nanotubes ZELJKO SLJIVANCANIN, Institut Romand de Recherche Numerique en Physique des Materiaux (IRRMA), CH-1015 Lausanne, Switzerland, LIV HORNEKAER, EVA RAULS, BJORK HAMMER, Department of Physics and Astronomy, Aarhus University, Ny Munkegade bygn. 520, 8000 Aarhus C, Denmark — Using density functional theory we investigated the lowest energy configurations of two H atoms on a graphite surface, and found two states with an approximately identical binding energy. These states are the dimer A state with two hydrogen atoms adsorbed on two neighbour carbon atoms and the dimer B state with two hydrogen atoms adsorbed on carbon atoms at opposite sides of a carbon hexagon. Hydrogen atoms in the dimer A state will recombine via diffusion into state B and then directly recombine from B. We also studied the corresponding pathways for molecular hydrogen formation from H atoms adsorbed at the single-wall carbon nanotubes and compared results to those obrained for the graphite surface.

Zeljko Sljivancanin
Institut Romand de Recherche Numerique en Physique des Materiaux (IRRMA), CH-1015 Lausanne, Switzerland

Date submitted: 27 Nov 2006 Electronic form version 1.4