Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Atomic structure of the carbon-induced Si(001)-c(4x4) surface
G.W. PENG, Y.Y. SUN, Department of Physics, National Univeristy of Singapore, Singapore 117542, A.C.H. HUAN, Institute of Materials Research and Engineering, 3 Research Link, Singapore 117602, Y.P. FENG, Department of Physics, National Univeristy of Singapore, Singapore 117542 — First-principles methods are employed to identify the reaction pathways for Si dimer rotations on the carbon-induced Si(001)-c(4x4) surface. The nudged elastic band calculations show that the recently proposed rotated dimer model can be obtained from the refined missing dimer model by dimer rotations with small energy barriers. The energy barriers are found to be sensitive to the rotation directions of Si dimers. The energy barrier along the minimum energy path is 0.82 eV. A new low-energy structure with a single rotated dimer is identified along the minimum energy path. This new structure is energetically more favorable than the rotated dimer model, the previously most stable structure, by 0.25 eV per c(4x4) cell.

Guowen Peng
Department of Physics, National University of Singapore, Singapore 117542

Date submitted: 03 Dec 2006 Electronic form version 1.4