Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Quantum Boundary Effect in Nanomaterials: Undo the Quantum Size Effect by Surface Passivation of Silicon Nanofilms YIYANG SUN, XIN LIU, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — It is well known that when the size of a semiconductor is reduced, its band gap will increase due to the increased kinetic energy of the electrons and holes. However, first-principles calculations reveal that there should also be a quantum boundary effect (QBE), which can drastically change the band gap to the extent that the quantum size effect (QSE) is completely erased. It is found that, for Si(001) nanofilms, surface passivations could show such a strong QBE. While the films are passivated by hydrogen, they show a clear QSE with significant increase in band gap. When some of the hydrogen atoms are replaced by =NH ligands, however, the band gap recovers to that of bulk silicon even for film size as small as two nanometers. The concept of zero confinement state for semiconductors will be introduced. It elucidates why it is possible to remove the seemingly universal QSE. The finding here could be highly desirable for certain applications of nanostructured semiconductors where gap increasing due to QSE is detrimental.

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Date submitted: 28 Nov 2010 Electronic form version 1.4