Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Strain-engineered Surface Transport in Si(001): Complete Isolation of the Surface State via Tensile Strain[1] MIAO ZHOU, ZHENG LIU, ZHENGFEI WANG, University of Utah, ZHAOQIANG BAI, YUANPING FENG, National University of Singapore, MAX G. LAGALLY, University of Wisconsin-Madison, FENG LIU, University of Utah, UNIVERSITY OF UTAH TEAM, NATIONAL UNIVERSITY OF SINGAPORE COLLABORATION, UNIVERSITY OF WISCONSIN-MADISON COLLABORATION — When silicon channel layer grows increasingly thinner in microelectronics, surface conductance becomes increasingly dominant, opening an opportunity to use surface states for novel devices. By combining density functional theory, non-equilibrium Green's function formulism, and effective-Hamiltonian approaches, we demonstrate strain-engineered surface transport in Si(001), with the complete isolation of the Si surface states from the bulk bands. Our results show that sufficient tensile strain can effectively remove the overlap between the surface valence state and the bulk valence band, because of the drastically different deformation potentials. Isolation of the surface valence state is possible with a tensile strain of $\sim$1.5%, a value that is accessible experimentally. Quantum transport simulations of a chemical sensing device based on strained Si(001) surface confirm the isolation of dominating surface conductance, giving rise to an enhanced molecular sensitivity. Our results show the promise for combining surface engineering with strain engineering to further our ability to manipulate surface states for quantum information processing and surface-state based devices.

[1]This research was supported by DOE (Grant No: DEFG02-04ER46148).

Miao Zhou
University of Utah

Date submitted: 13 Nov 2013 Electronic form version 1.4