Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Theoretical study of vibrations and Raman spectra in pristine and P-doped Si nanocrystals[1] K. H. KHOO, University of Texas at Austin, A. T. ZAYAK, Lawrence Berkeley National Laboratory, H. KWAK, Washington State University, JAMES R. CHELIKOWSKY, University of Texas at Austin — Phonon confinement in Si nanostructures has been widely studied and size-dependent redshifts as well as asymmetric broadening of Raman peaks have been commonly observed. However, a fully *ab initio* study of the Raman spectra in Si nanostructures has yet to be performed. Here, we investigate the vibrational modes and non-resonant Raman spectra of Si nanoclusters using density functional theory. Vibrational modes were calculated using the force constant method and non-resonant Raman spectra were evaluated within the Placzek approximation. We have reproduced the experimental Raman peak shifts and demonstrated that Raman spectra in Si nanocrystals are highly sensitive to the introduction of dopants.

[1]This work was supported in part by the Department of Energy under DE-FG02-06ER15760 and portions of this work were performed at the Molecular Foundry, LBNL.

K. H. Khoo
University of Texas at Austin

Date submitted: 18 Nov 2009 Electronic form version 1.4