Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Optical absorption of nanoporous silicon: quasiparticle band gaps and absorption spectra[1] GUANGSHA SHI, EMMANOUIL KIOUPAKIS, University of Michigan, Department of Materials Science and Engineering — Silicon is an earth-abundant material of great importance in semiconductors electronics, but its photovoltaic applications are limited by the low absorption coefficient in the visible due to its indirect band gap. One strategy to improve the absorbance is to perforate silicon with nanoscale pores, which introduce carrier scattering that enables optical transitions across the indirect gap. We used density functional and many-body perturbation theory in the GW approximation to investigate the electronic and optical properties of porous silicon for various pore sizes, spacings, and orientations. Our calculations include up to 400 atoms in the unit cell. We will discuss the connection of the band-gap value and absorption coefficient to the underlying nanopore geometry. The absorption coefficient in the visible range is found to be optimal for appropriately chosen nanopore size, spacing, and orientation. Our work allows us to predict porous-silicon structures that may have optimal performance in photovoltaic applications.

[1]This research was supported as part of CSTEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. Computational resources were provided by the DOE NERSC facility.

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Date submitted: 14 Nov 2012 Electronic form version 1.4