Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Optimal Silicon for Photovoltaic Applications GEORGY SAMSONIDZE, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — A small overlap of the silicon optical absorption spectrum with the solar emission spectrum limits the efficiency of silicon-based solar cells. We conduct a theoretical search for substitutionally doped silicon with the aim to maximize the spectral overlap. Different dopant species at various concentrations compatible with the existing silicon technology are examined in the virtual crystal approximation using the empirical pseudopotential method. The optimal doping configurations found are further investigated with a first-principles many-electron Green's function approach. The optical absorption spectrum of the doped silicon is calculated by solving the Bethe-Salpeter equation which includes excitonic effects. This work was supported by National Science Foundation Grant No. DMR07-05941, and by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NSF through TeraGrid resources at Indiana University and TACC.

Georgy Samsonidze
Dept of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

Date submitted: 02 Dec 2008 Electronic form version 1.4