Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Effects of Shape-Dependence and Diameter-Dependence on Photoluminescene properties of Silicon Nanowires and Porous Silicon[1]
DMITRI MIGAS, Department of Physics, University of Louisville, C.S. JAYANTHI, Department of Physics, University of Louisville, S.Y. WU, Department of Physics, University of Louisville — It is well known that photoluminescence (PL) in porous silicon arise from silicon nanostructures. In this work in order to shed light on PL from porous silicon, we have carried out the first-principles electronic structure calculations of silicon nanowires (SiNWs). Specifically, we considered (001)-oriented SiNWs of different diameters and cross-sectional shapes with their dangling bonds passified by hydrogen atoms. Our work demonstrates that the PL originates from the inner core of hydrogenated SINWs, and that enhanced dipole matrix elements are obtained when the surface of the SiNW is characterized by dimers and covered by SiH species. However, we find that a surface covered by SiH_2 species obtained by breaking the dimer bonds helps in stabilizing the direct nature of the gap. This work also presents the interplay between the nature of the energy gap, the diameter, and the shape of the wire on the PL from porous silicon..

[1]This work was supported by the NSF (DMR-0112824), the U.S. DOE (DE-FG02-00ER45832) and the NCSA (DMR-040039).

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Date submitted: 30 Nov 2004 Electronic form version 1.4