

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Quantum Confinement in PbS nanowire SUBHASISH MANDAL, RANJIT PATI, Michigan Technological University, Houghton, MI 49931 — One dimensional nanowires have become leading candidates in building nano sensor, nano transistor, optoelectronic devices and logic circuit. In last several years, PbS nanowire has drawn considerable interest for their potential applications in optical switch and solar cell. Controlled synthesis of PbS nanowire with diameter ranging from 1.2 nm to 20 nm have been reported with the photo luminescence study revealing wide band gap behavior for the nanowire. This offers exciting opportunities to study theoretically quantum confinement effect in PbS Nanowire. Here we report first principles density functional calculations of the electronic properties of PbS nanowire as a function of diameter. Our calculation shows, by varying the diameter of the nanowire from ~ 1.17 nm to ~ 3.64 nm, the energy band gap is found to change from 1.55 eV to 0.93 eV, substantially higher than the band gap observed for the PbS bulk - confirming the role of quantum confinement.

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Date submitted: 07 Dec 2008

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