Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Optical Properties of Hydrogenated Silicon Nanoclusters: First principles study[1] SEUNG MI LEE, Korea Research Institute of Standards and Science (KRISS), HANCHUL KIM, KYUNG JOONG KIM, DAE WON MOON — Silicon nanoclusters have significant interest due to their potential application to optoelectronic devices in visible range. Using first principles approach, we investigate the electronic and optical properties of hydrogenated silicon nanoclusters. The highest occupied molecular orbital (HOMO) – lowest unoccupied molecular orbital (LUMO) gap dependence on the cluster size show the same trend by using any exchange-correlation functionals. However, a reasonable agreement to experimental absorption spectra peak values cannot be achieved from conventional LDA or GGA functional-based calculations. Using B3LYP hybrid functional within time-dependent density functional theory, we obtain excitonic energies in quantitatively good agreement to experimental data. The passivant effect on HOMO-LUMO gap and excitonic energies will be also presented.

[1]Computing facility support by KISTI under the 7th strategic supercomputing applications support program

Seung Mi Lee
Korea Research Institute of Standards and Science (KRISS)

Date submitted: 30 Nov 2005 Electronic form version 1.4