decreases this must imply a greater role of surface effects on the electronic structure. This is true only if the wavefunction has an amplitude on the surface atoms. We test this next.

Shown in Fig. 2a,b are the wavefunction square of the CBM and VBM of the rectangular quantum box with $d = 34.1$ Å ($N_{Si} = 1035$ atoms). The VBM and CBM states are found to be localized in the interior of the quantum dot, with zero amplitude on

proximation (EMA) of Takagahara and Takeda [6] and the model of Rama Krishna and Friesner (RKF) [7].

2.3.1. Comparison with the effective mass method

As could be seen in Fig. 2, the VBM and CBM states found in our direct calculations are not surface states, hence a comparison with the results of the (surfaceless) EMA is warranted. Our 'exact' calcula-

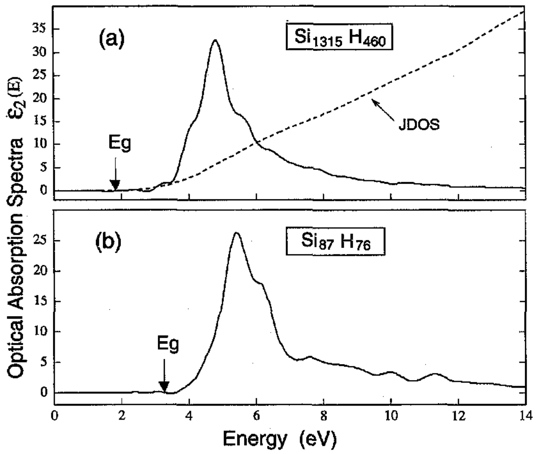

Fig. 7. Calculated optical absorption spectra $\epsilon_2(E)$ of spherical Si

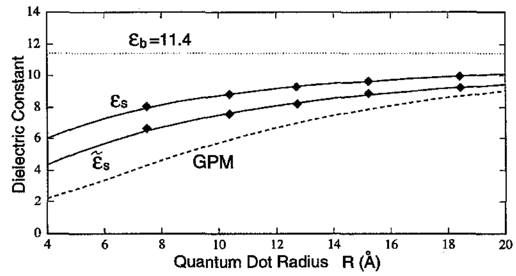

Fig. 9. Dielectric constants as a function of spherical quantum dot radius R. Here ϵ_s is for total polarization and $\tilde{\epsilon}_s$ is for exciton screening. The diamond symbols are the calculated results while the solid lines are the curves fitted to Eq. (5). The dashed curve corresponds to the generalized Penn model (GPM) given by Ref. [17].