

decreases this must imply a greater role of surface

approximation (EMA) of Takaoahara and Takeda [6]

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 $d = 34.1 \text{ \AA}$ ($N_{\text{Si}} = 1035$ atoms). The VBM and CBM states are found to be localized in the interior of the quantum dot, with zero amplitude on

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-



