Abstract Submitted for the MAR05 Meeting of The American Physical Society

Microscopic dielectric function in semiconductor quantum  $dots^1$ XAVIER CARTOIXA, LIN-WANG WANG, Lawrence Berkelev National Laboratory, Berkeley, CA, 94720 — Dielectric function and screening effects within a quantum dot is of paramount importance in describing the optical properties and energy levels in a quantum dot. Previously it was believed that the dielectric function inside a quantum dot decreases compared to the bulk due to the increase of the band gap. Recently[1], using macroscopic electric fields and response analysis, it was suggested that the reduction of dielectric constant in a quantum dot is due to surface bond breaking, not due to the opening of the band gap. We have investigated this issue by studying the microscopic response function using plane wave ab initio calculations. Indeed, we found that the microscopic response function  $f(r_1, r_2)$ is identical to the bulk value when both r1 and r2 are within the quantum dot. We have provided a model which allows one to accurately approximate the quantum dot microscopic dielectric function  $f(r_1, r_2)$  from its bulk values without doing explicit calculations. The model also produces accurately the overall dielectric constant reduction for a quantum dot compared to its bulk value. [1] C. Delerue, M. Lannoo, G. Allan, Phys. Rev. B 68, 115411 (2003).

<sup>1</sup>Supported by U.S. Department of Energy under Contract No. DE-AC03-76SF00098

Lin-Wang Wang Lawrence Berkeley National Laboratory, Berkeley, CA, 94720

Date submitted: 06 Dec 2004

Electronic form version 1.4