Electronic Structure Pseudopotential Calculations of Large (~1000 Atoms) Si Quantum Dots

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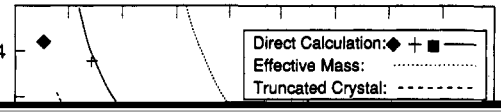
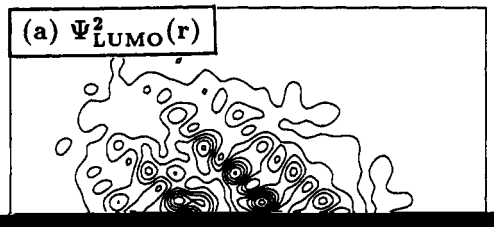
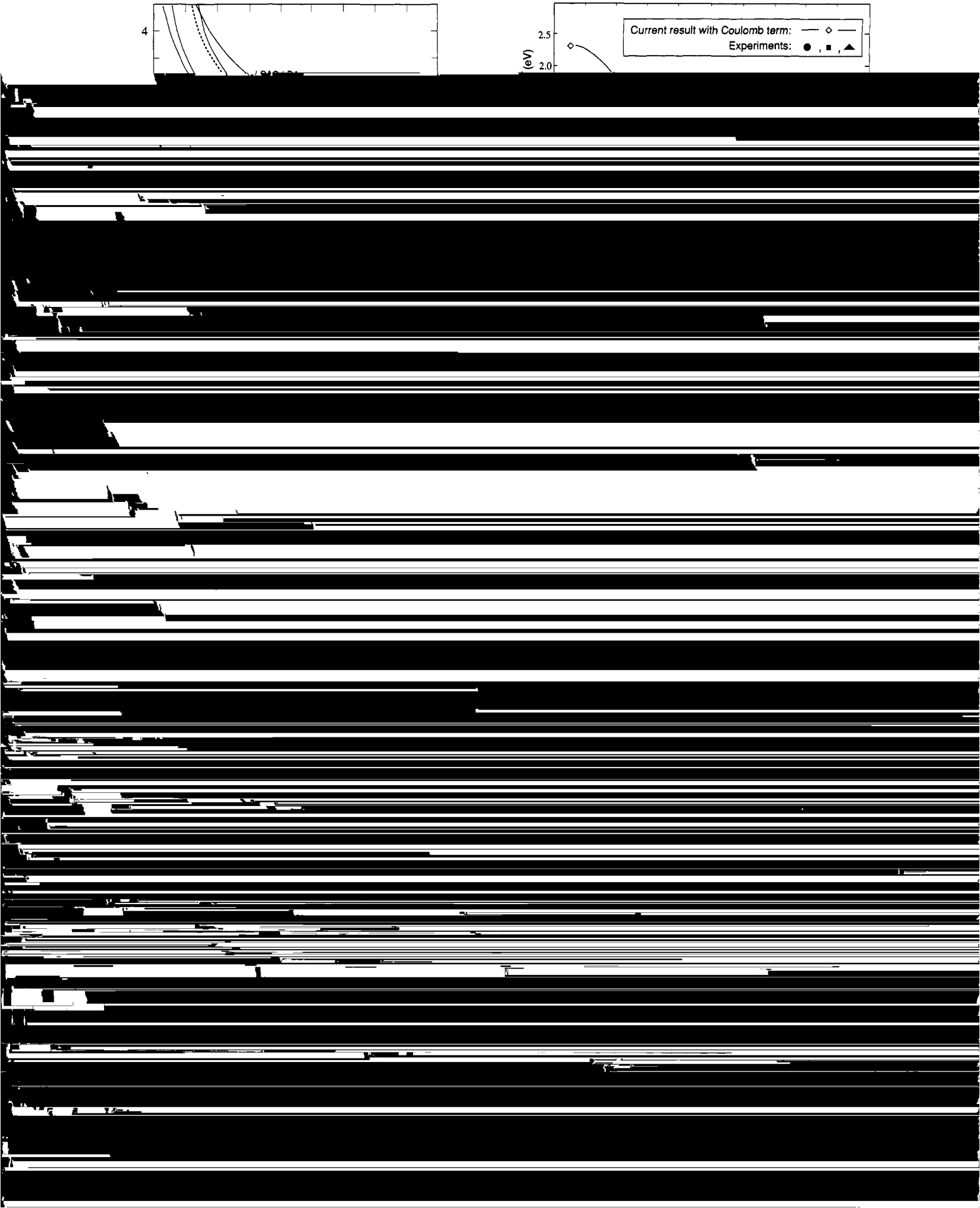
shape of the quantum dot does not change. The precise relaxation of the quantum dot surface atoms is taken from data on these three primary surfaces of H-covered Si films. The reconstructed surface geometries we used are (1×1):H for the (111)-oriented





different treatments of the surface H potentials: In ref 38, the energy levels of the SiH_4 molecule are fitted to give the matrix elements of the TB Hamiltonian. We have tested this procedure using EPM and find a similar surfacelike LUMO state. However, we feel that a SiH_4 molecule is not an adequate model for H-covered Si surfaces. On the (001) film surface, there are two H atoms from neighboring H:Si:H groups which can be quite


4
2.5
2.0
(eV)
Current result with Coulomb term:
Experiments:

[redacted]