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

Lin-Wang Wang and Alex Zunger*

National Renewable Energy Laboratory, Golden, Colorado 80401

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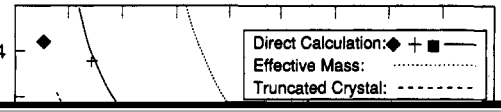
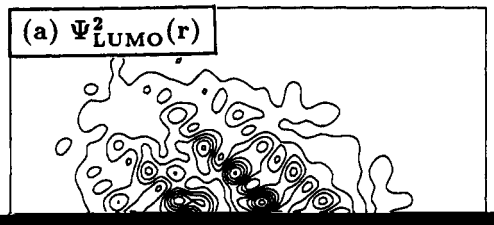
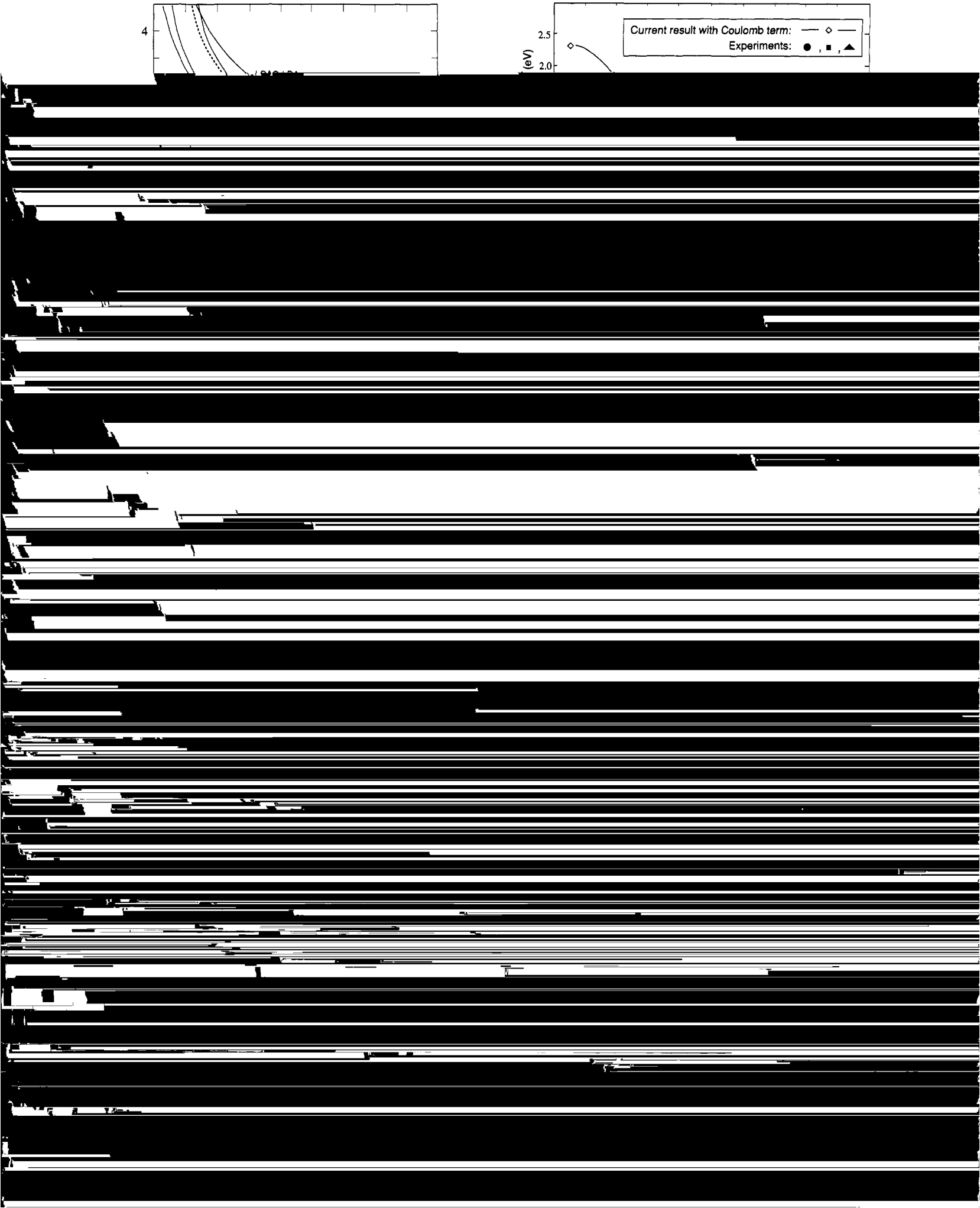
The electronic structure of quantum dots containing $N \geq 1000$ atoms is difficult to calculate by conventional molecular methods since the effort scales as N^3. Our newly developed method allows calculation of eigenstates

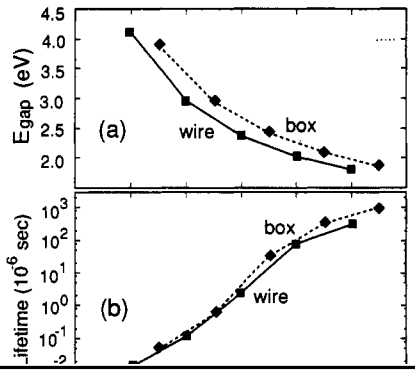
shape of the quantum dot does not change. The precise relaxation of the quantum dot surface atoms is taken from data on these three primary surfaces of H-covered Si films. The reconstructed surface geometries we used are (1×1):H for the (111)-oriented





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:



lifetimes for these two systems are very close, within a factor of 2. The fact that the gap of a dots is larger than that of the wire is consistent with the larger quantum confinement for finite L_z (i.e., box). However, the nearly identical radiative lifetimes of these two systems is surprising given that in the wire $k_z = 0$ for the HOMO and LUMO while in the box $k_z \neq 0$ for both of them. This implies that, in this case, the radiative lifetime is mostly determined by the x, y directions, while the z direction has little effect.

IV. Conclusions

We have used the empirical pseudopotential method to calculate the electronic structure of Si quantum dots of different sizes

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