

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

First principles comparison of alkyl terminated Silicon dots with Silicon-Carbide dots.¹ FERNANDO A. REBOREDO, GIULIA GALLI, Lawrence Livermore National Lab — Using ab-initio methods, we have studied different quantum dots that could be synthesized using the three elements: Si, C and H. In particular, we have compared hydrogen and alkyl passivated Silicon dots with Silicon-Carbide dots. We find that in Si clusters with reconstructed (100) facets a complete alkyl passivation is possible, but steric repulsions prevents full passivation of Si dots with unreconstructed surfaces. In addition, our calculations show that the stability of alkyl passivated Si clusters depends on the length of the carbon chains. Alkyl passivation weakly affects optical gaps of Si quantum dots, while it substantially affects ionization potentials and electron affinities. We also investigate theoretically the possibility to fabricate silicon-carbide quantum dots passivated with H. We find that the optical properties of this type of dots would be weakly dependent on size but strongly influenced by the structure of the surface, which in turn depends on the growth conditions. We discuss the conditions where quantum confinement could be observed in SiC quantum dots. Our results suggest that depending on the experimental conditions either alkyl terminated Si dots or SiC dots could be form being optical gaps strongly dependent on the core and surface structure.

¹work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

Fernando A. Reboredo
Lawrence Livermore National Lab

Date submitted: 06 Dec 2004

Electronic form version 1.4