

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Preservation of the optical properties of small Si quantum dots in the face of oxidation¹ HUASHAN LI, ZHIGANG WU, MARK LUSK, Department of Physics, Colorado School of Mines — Rapid oxidation occurs when small, unpassivated Si quantum dots are subjected to ambient conditions, and it may at first seem that complete oxidation of 1-3 nm QDs is inevitable, since their initial oxidation rate is expected to be greater than that for bulk Si for a more open surface structure, and the oxide layers on bulk Si tend to be thicker than the dot radii. We use computations based on density functional theory show that sufficiently small, appropriately terminated dots might actually be able to resist oxidation better than their larger brethren. This is because, on well-passivated bulk surfaces, oxygen attacks silicon through vulnerable sites and defects, and defects are much less likely to be present as dot size decreases. Although the more open surface structure of these small dots does leave certain keys sites more vulnerable to oxidation than their bulk counterparts, the oxygen atoms absorbed there are essentially immobile due to large hopping barriers. Furthermore, computations employing the many-body Green function perturbation theory show that the oxidation of these QDs has a relatively small impact on optical character. Therefore, the best defense against oxidation is to eliminate defects; a strategy that becomes increasingly reasonable as dot size decreases.

¹Renewable Energy Materials Research Science and Engineering Center (NSF Grant No. DMR-0820518) at the Colorado School of Mines and the National Renewable Energy Laboratory

Huashan Li
Department of Physics, Colorado School of Mines

Date submitted: 11 Nov 2011

Electronic form version 1.4