Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Quantum Confined Silicon Clathrate Quantum Dots[1] MARK LUSK, NICHOLAS BRAWAND, Colorado School of Mines — Silicon (Si) allotropes can be synthesized in such a way that tetrahedrally bonded atoms form cage-like structures with bulk mechanical and opto-electronic properties distinct from those of diamond silicon (dSi). We use DFT, supplemented with many-body Green function analysis, to explore the structural stability of clathrate Si quantum dots (QDs) and to characterize their confinement as a function of crystal symmetry and size. Our results show that that there is a simple relationship between the confinement character of the QDs and the effective mass of the associated bulk crystals. Clathrate QDs and dSiQDs of the same size can exhibit differences of gap energies by as much as 2 eV. This offers the potential of synthesizing Si dots on the order of 1 nm that have optical gaps in the visible range but that do not rely on high-pressure routes such as those explored for the metastable BC8 and R8 phases. These results prompt the question as to how minimal quantum confinement can be in dots composed of Si. More broadly, clathrate QDs can in principle be synthesized for a wide range of semiconductors, and the design space can be further enriched via doping.

[1]NSF Renewable Energy Materials Research Science and Engineering Center (REMRSEC) and the Golden Energy Computing Organization (GECO)

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Date submitted: 09 Nov 2012 Electronic form version 1.4