## Abstract Submitted for the MAR06 Meeting of The American Physical Society

The silicon di-vacancy investigated with density functional theory

RYAN WIXOM, ALAN WRIGHT, Sandia National Laboratories — As part of a larger effort to quantitatively model the behavior of point defects in silicon, we have investigated the silicon di-vacancy using density functional theory with three different exchange-correlation functionals and super-cells containing as many as 1000 atoms. The literature on this defect contains two proposed atomic structures and disagreement on the relative stability of the configurations. Our study indicates that the determination of the ground state configuration is dependant on the particular choice for exchange and correlation. We will report on the atomic and electronic structures of this defect as well as formation.

Ryan Wixom Sandia National Laboratories

Date submitted: 07 Dec 2005 Electronic form version 1.4