Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Large scale ab initio calculations for shallow acceptor levels in bulk Si[1] LIN-WANG WANG, Lawrence Berkeley National Laboratory — Accurate calculation of shallow donor levels in conventional semiconductors is a long standing challenge due to the large supercell needed for such calculation. We have used the charge patching method and local density approximation (LDA) to study the acceptor levels in bulk Si, including B, Al, Ga, In and Tl acceptors. The atomic positions are relaxed under LDA using 512 atom cells, and 64,000 atom supercells are used to calculate the acceptor energy levels to achieve the converged results. The calculated impurity binding energies reproduce the experimental trend from B to Tl. However, there is still a significant difference between the calculated binding energies and the experimental results, especially for Tl. This raises the question of whether the LDA can be used to calculate the shallow impurity level accurately.

[1]This work is supported by U.S. Department of Energy, BES, under contract No. DE-AC02-05CH11231 and it used the resource of the National Energy Research Scientific Computing Center.

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Date submitted: 04 Dec 2007 Electronic form version 1.4