Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Surface passivation optimization using DIRECT[1] KWISEON KIM, PETER A. GRAF, WESLEY B. JONES, National Renewable Energy Laboratory, Golden, CO 80401, LIN-WANG WANG, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720 — The calculation of the electronic structure of a nanostructure must take into account surface effects. In experiments, the dangling bonds at the surface of a semiconductor nanostructure are passivated by other semiconductors or by organic ligands. In either case, photoluminescence measurements reveal that the emission comes from bulk-like, dot-interior states. These observations suggest that an approach to passivating a simulated nanostructure would be to attach pseudo-atoms to each dangling bond. Here we present an automated methodology for generating surface passivating pseudo potentials for bulk empirical pseudo potentials. Our method is based on the global optimization method DIRECT. We apply it to two materials, CdSe and InP. Incorporated into a larger computational nanoscience infrastructure, our work represents a much needed improvement in the usability of the empirical pseudo potential method.

[1]supported by US DOE-SC-ASCR-MICS.

Kwiseon Kim
National Renewable Energy Laboratory, Golden, CO 80401

Date submitted: 29 Nov 2005 Electronic form version 1.4