Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Atomistic material design by optimization[1] KWISEON KIM, PETER A. GRAF, WESLEY B. JONES, National Renewable Energy Laboratory, Golden, CO 80401 — We cast the problem of discovering atomic configurations with desired properties as a constrained global optimization problem. Here the free variables are the location and identity of every atom in a material and the objective function is built from the desired electronic properties. For example, we can minimize the bandgap or we can optimize for a target of combined bandgap and effective mass. We present two evolutionary optimization methods (a genetic algorithm [1] and a scatter search algorithm [2]), and two applications (semiconductor alloys and quantum dots). We describe the application specific mutation and crossover operation necessary, as well as the constraints and how they are maintained during the search of the space of atomic configurations. We highlight past successes, current challenges, and future prospects for this novel method. [1] D. Levine, PGAPack: Parallel Genetic Algorithm Library (1998). [2] M. Laguna and R. Marti, Scatter Search, Methodology and Implementation in C, Kluwer, Boston (2003).

[1]Supported by DOE-SC-ASCR-MICS.

Kwiseon Kim
National Renewable Energy Laboratory, Golden, CO 80401

Date submitted: 01 Dec 2004 Electronic form version 1.4