Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Combinatorial design of high-temperature ferromagnetic semiconductors from first principles ALBERTO FRANCESCHETTI, SERGEY DUDIY, SERGEY BARABASH, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401, J. XU, M. VAN SCHILFGAARDE, Arizona State University, Tempe, AZ 85287 — The Curie temperature T_C of Mn-doped GaAs depends strongly on the arrangement of the substitutional Mn dopants. For example, the highest T_C reported so far was attained in thin GaMnAs layers embedded in GaAs. However, an exhaustive search of all possible configurations to find those that maximize T_C is difficult, due to the astronomically large number of possibilities. Here we address this problem by parametrizing the Curie temperature of a set of $\sim$ 50 input configurations, calculated from first principles using linear-response theory and Monte Carlo simulations, in terms of configuration variables (cluster expansion). Once established, this expansion allows us to search almost effortlessly the Curie temperature of arbitrary configurations of Mn dopants in GaAs. We find that the highest T_C (>350K) is achieved for $(GaAs)_m/(MnAs)_n$ superlattices in the (201) crystallographic orientation, with (m,n)=(4,1). Our general approach of cluster expanding *electronic or magnetic properties* of complex systems opens the way to first-principles combinatorial design of materials with prescribed transition temperatures. This work was supported by DARPA, under NREL contract No. DEAC36-98-GO10337.

Alberto Franceschetti
NREL

Date submitted: 23 Nov 2005 Electronic form version 1.4