Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**Conformational space annealing scheme in the inverse design of functional materials**[1] SUNGHYUN KIM, KAIST , IN-HO LEE, Korea Research Institute of Standards and Science, JOOYOUNG LEE, Center for In Silico Protein Science, School of Computational Science, YOUNG JUN OH, KEE JOO CHANG, KAIST — Recently, the so-called inverse method has drawn much attention, in which specific electronic properties are initially assigned and target materials are subsequently searched. In this work, we develop a new scheme for the inverse design of functional materials, in which the conformational space annealing (CSA) algorithm for global optimization is combined with first-principles density functional calculations. To implement the CSA, we need a series of ingredients, (i) an objective function to minimize, (ii) a 'distance' measure between two conformations, (iii) a local enthalpy minimizer of a given conformation, (iv) ways to combine two parent conformations to generate a daughter one, (v) a special conformation update scheme, and (vi) an annealing method in the 'distance' parameter axis. We show the results of applications for searching for Si crystals with direct band gaps and the lowest-enthalpy phase of boron at a finite pressure and discuss the efficiency of the present scheme.

[1]This work is supported by the National Research Foundation of Korea (NRF) under Grant No. NRF-2005-0093845 and by Samsung Science and Technology Foundation under Grant No. SSTFBA1401-08

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Date submitted: 13 Nov 2014 Electronic form version 1.4