Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Crystal structure prediction: a novel approach based on minima hopping MAXIMILIAN AMSLER, STEFAN GOEDECKER, University of Basel — With increasing computational resources the prediction of crystal structures from first principle calculations has become feasible, but still remains a demanding task. A reliable method to perform an efficient, systematic search for the ground state structure based solely on the system's composition is essential. Motivated by the promising results of the minima hopping method obtained on isolated systems, we have generalized the algorithm for crystal structure prediction. Optimized moves in the configurational space spanned by both atomic coordinates and simulation cell variables are performed to escape from local enthalpy minima, and revisiting known minima is avoided, thus allowing a fast exploration of the enthalpy surface. The predictive power of the novel method has been shown in several applications, of which the following will be presented. Superconducting phases in hydrogen rich materials were investigated, leading to the discovery of novel ground state structures. For the longstanding question of the crystal structure of cold compressed graphite a new candidate phase could be identified to perfectly match experimental results. And at last, new low energy structures for materials with possible applications in hydrogen storage are presented.

Maximilian Amsler
University of Basel

Date submitted: 11 Nov 2011 Electronic form version 1.4