Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

A simple and efficient approach to calculating the density of states of a fluid CHENGJU WANG, RICHARD M. STRATT, Department of Chemistry, Brown University, Providence, RI 02912 — Knowledge of the density of states (DOS) is not only of fundamental thermodynamic significance but is also critical to designing stochastic methods in molecular simulations. Contrary to conventional methods which include bias from temperature or other order parameters, we showed that sampling the potential energy surface by a random walk in the *energy landscape ensemble* enables us to calculate DOS directly from the potential energy distribution of the configurations within the ensemble. The ensemble itself is defined to include all the configurations with a potential energy less than a given value. Using this approach, we studied the relationship between the configuration entropy and the configurational temperature for the Kob-Andersen model, a typical glassy system. The results were in excellent agreement with the literature reports while showing a significant improvement in computational efficiency.

Chengju Wang
Department of Chemistry, Brown University, Providence, RI 02912

Date submitted: 16 Nov 2006 Electronic form version 1.4