Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Computer simulations of the folding mechanism of the GCN4 Leucine zipper YANXIN LIU[1], PREM CHAPAGAIN, JOSE PARRA, BERNARD GERSTMAN, Department of Physics, Florida International University, University Park, Miami, FL 33199 — A modified three dimensional lattice model incorporating a Monte Carlo Metropolis Algorithm is used to investigate the dimerization of the GCN4 Leucine zipper. The model is validated with heat capacity calculations that are seen to match well with experiment measurements. The free energy landscape is investigated as a function of temperature. Evidence of multiple meta-stable states is found during the simulation. The possible folding and dimerization mechanism of the Leucine zipper will be discussed.

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Date submitted: 23 Nov 2007 Electronic form version 1.4