Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Exploring copper chelation in Alzheimer's disease protein FRISCO ROSE, MIROSLAV HODAK, JERRY BERNHOLC, CHiPS/NCSU — Alzheimer's disease (AD) is a neurodegenerative disorder affecting millions of aging people in the U.S. alone. Clinical studies have indicated that metal chelation is a promising new approach in alleviating the symptoms of AD. Our study explores the as yet undetermined mechanism of copper chelation in amyloid-β, a protein implicated in AD. The structure of amyloid-β is derived from experimental results and incorporates a planar copper-ion-binding structure in a semi-solvated state. We investigate the chelation process using the nudged elastic band method implemented in our *ab initio* real-space multigrid code. We find that an optimal sequence of unbonding and rebonding events as well as proton transfers are required for a viable chelation process. These findings provide fundamental insight into the process of chelation that may lead to more effective AD therapies.

Frisco Rose
CHiPS/NCSU

Date submitted: 11 Nov 2011 Electronic form version 1.4